

Electronic Supporting Information

for

**Computational Identification of Bi-functional Metal-modified ZSM-5 Catalysts
to Boost Methane-Methanol Coupling**

Mengnan Sun^{1,#}, Xiaowa Nie^{1,#,*}, Xinwei Zhang², Sirui Liu¹, Chunshan Song^{1,3},
Xinwen Guo^{1,*}

¹*State Key Laboratory of Fine Chemicals, Frontier Science Center for Smart Materials, PSU-DUT*

Joint Center for Energy Research, School of Chemical Engineering, Dalian University of

Technology, Dalian 116024, China

²*Dalian Research Institute of Petroleum and Petrochemicals, SINOPEC, Dalian 116041, China*

³*Department of Chemistry, Faculty of Science, The Chinese University of Hong Kong, Shatin, NT,*

Hong Kong, China

***Corresponding Authors**

Dr. Xiaowa Nie

Email: niexiaowa@dlut.edu.cn

Dr. Xinwen Guo

Email: guoxw@dlut.edu.cn

These authors contributed equally to this work

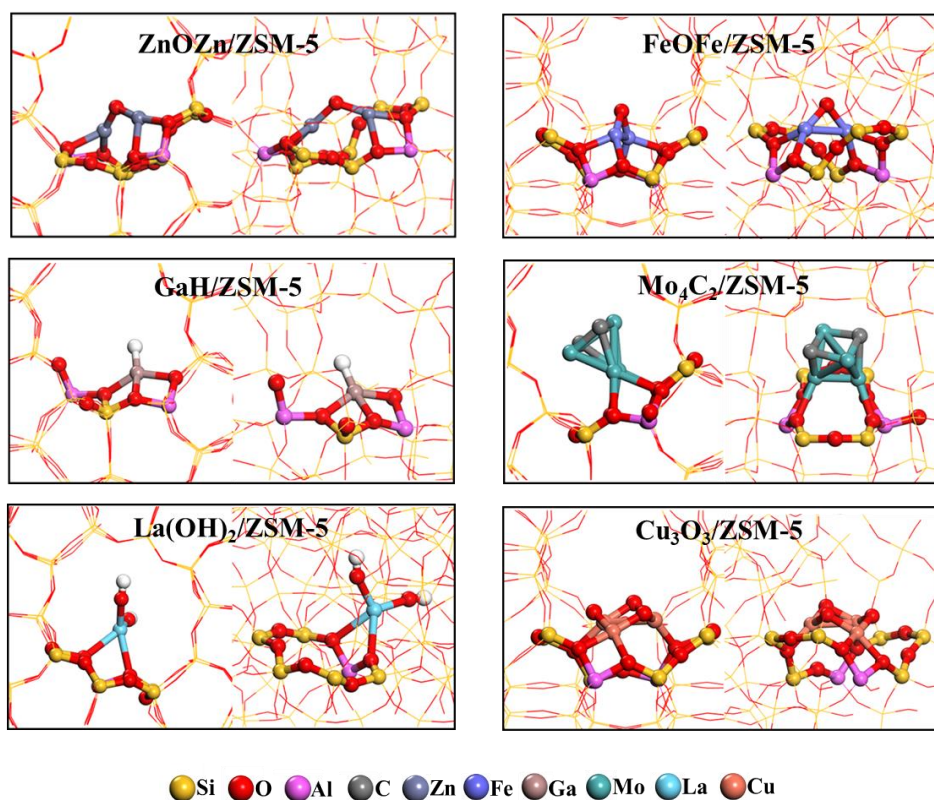


Figure S1. Optimized structures of active site models of M/ZSM-5 (M=Zn, Fe, Ga, Mo, La, Cu)

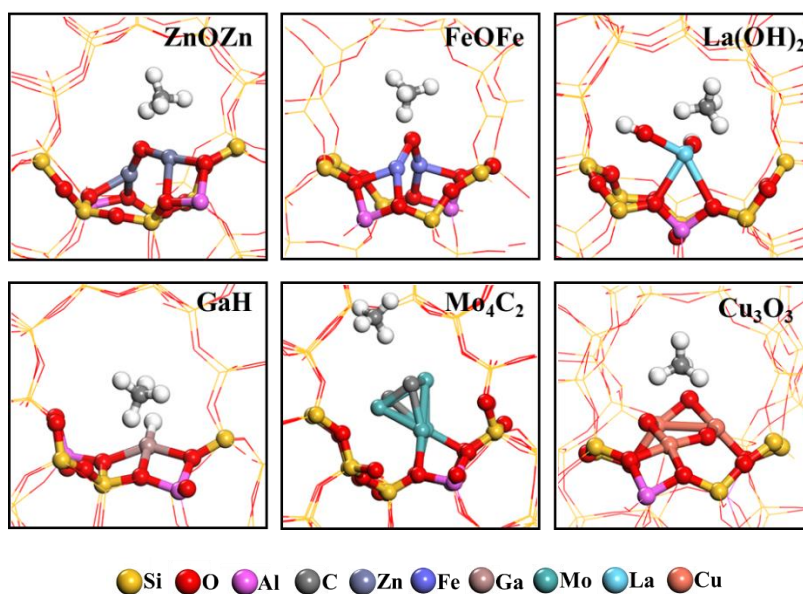


Figure S2. Optimized structures of methane adsorption over M/ZSM-5 (M=Zn, Fe, Ga, Mo, La, Cu).

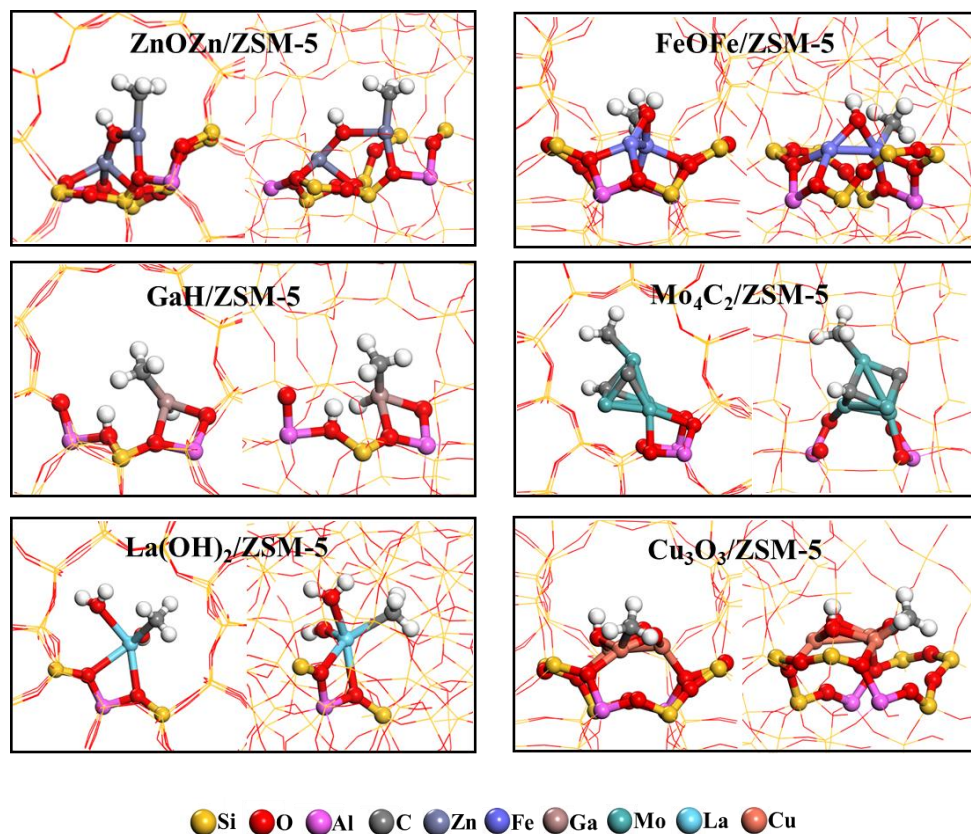


Figure S3. Optimized final state structures of methane activation via C-H bond cleavage over M/ZSM-5 (M=Zn, Fe, Ga, Mo, La, Cu).

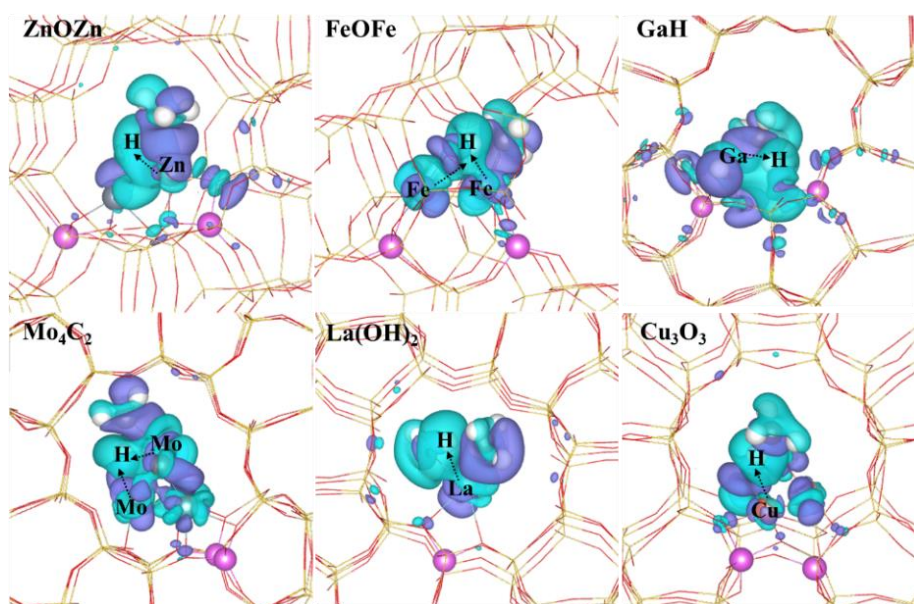


Figure S4. The charge density difference maps of the transition state for methane activation over M/ZSM-5 (M=Zn, Fe, Ga, Mo, La, Cu).

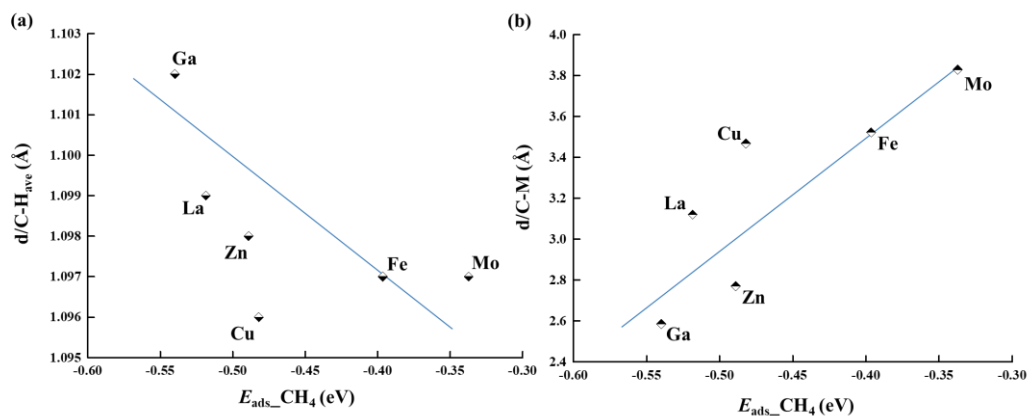


Figure S5. The relationship between methane adsorption energy versus (a) the average C-H bond length of methane and (b) the C-M interatomic distance in adsorbed methane over M/ZSM-5 (M=Zn, Fe, Ga, Mo, La, Cu).

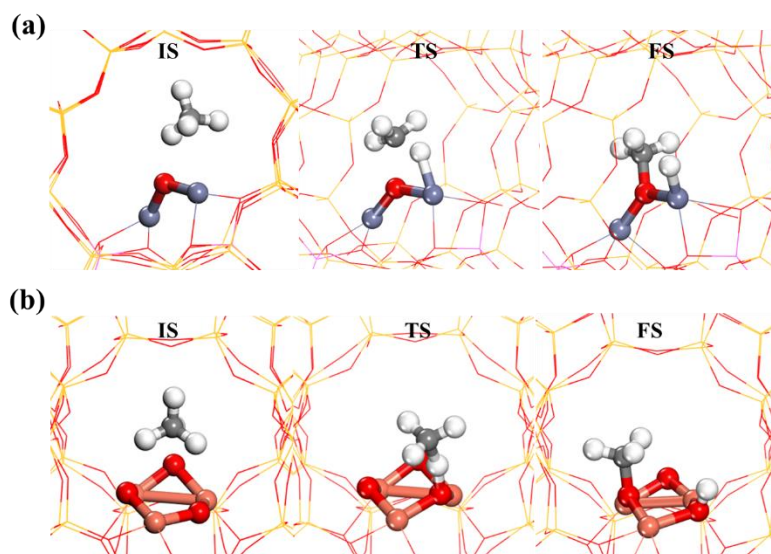


Figure S6. Optimized structures of adsorption state, transition state, and final state for methane C-H bond activation to form $\text{O}_M\text{-CH}_3$ species over Zn/ZSM-5 and Cu/ZSM-5.

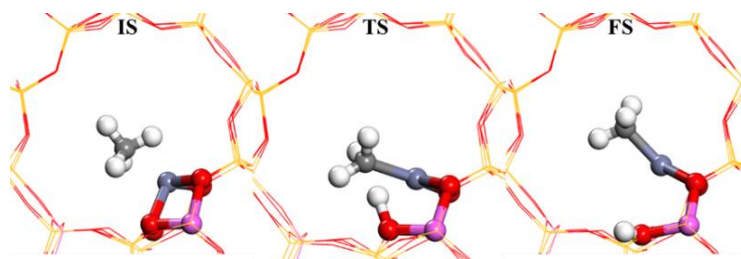


Figure S7. Optimized structures of adsorption state, transition state, and final state for methane C-H bond activation over $\text{Zn}^{2+}/\text{ZSM-5}$ catalyst model.

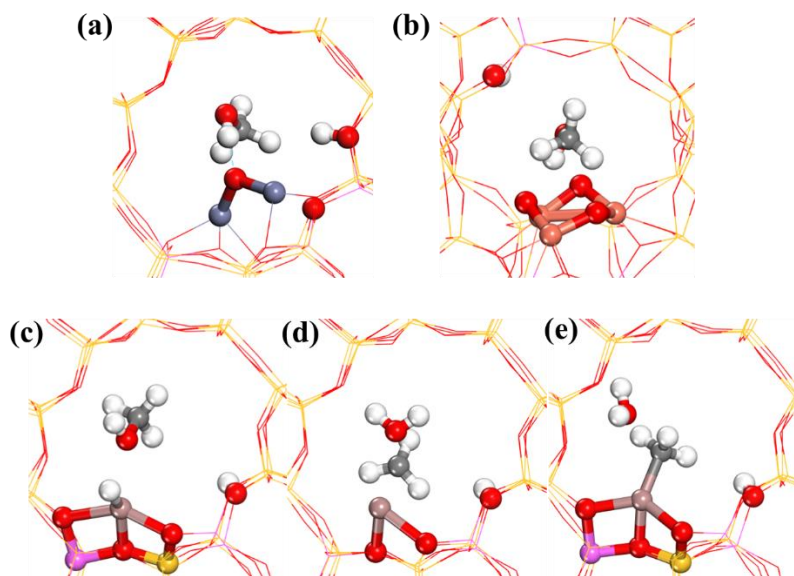


Figure S8. Optimized structure of methanol adsorption state over the metal-Lewis site of (a) Zn/ZSM-5, (b) Cu/ZSM-5, and (c) Ga/ZSM-5; optimized structures of (d) transition state and (e) final state for methanol activation via dehydration over the metal-Lewis site of Ga/ZSM-5.

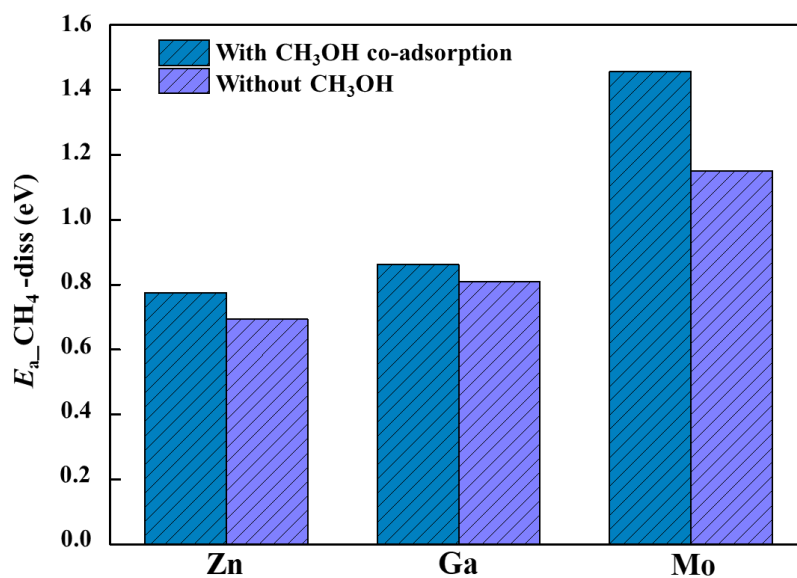


Figure S9. Comparison of activation barriers for methane C-H bond activation without and with methanol co-adsorption nearby over Zn/ZSM-5, Ga/ZSM-5, and Mo/ZSM-5.

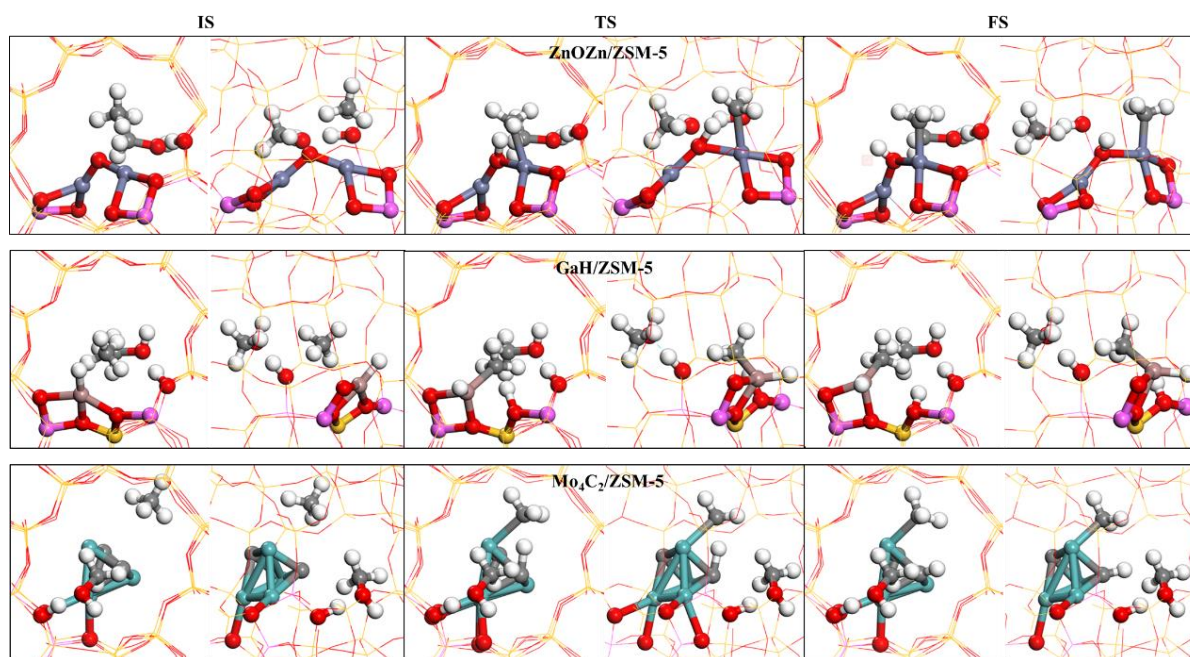


Figure S10. Optimized structures of adsorption state, transition state, and final state for methane activation with methanol co-adsorption nearby over Zn/ZSM-5, Ga/ZSM-5, and Mo/ZSM-5.

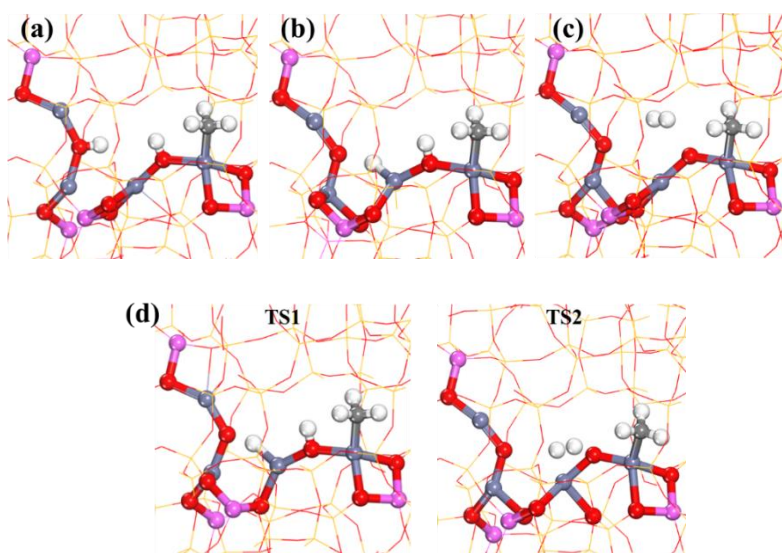


Figure S11. (a), (b), (c) Optimized intermediate structures, (d) optimized transition state structures for H atom on O-site of $[\text{ZnOZn}]^{2+}/\text{ZSM-5}$ transfer to Zn-site and then form H_2 molecule.

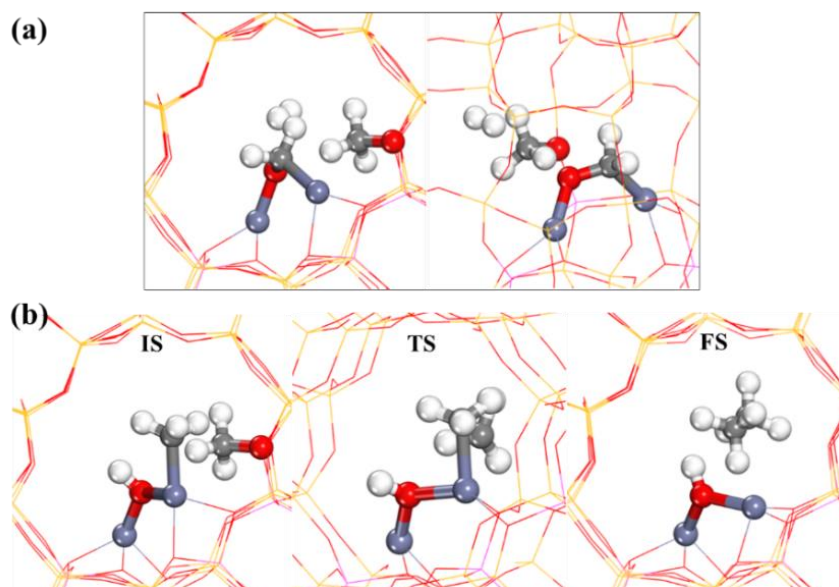


Figure S12. (a) Optimized final state structure of H(O_{Zn}) and H atom dissociated from Zn-CH₃ to form H₂, (b) optimized structures for C-C coupling to form C₂H₆ of Zn-CH₃ and O-CH₃ in the presence of H(O_{Zn}) over Zn/ZSM-5.

(*Note:* In addition, we investigated the case that the H(O_{Zn}) atom generated by methane activation participates in subsequent C-C coupling reaction without removal, and the optimized structures are shown in **Figure S12**. **Figure S12(a)** shows the final state structure of H(O_{Zn}) and H atom dissociated from Zn-CH₃ species to form H₂ molecule. It can be clearly seen that the C atom in the final state structure of Zn-CH₂ bonds to the O_{Zn} atom of [ZnOZn]²⁺ after H₂ generation, which destroyed the original active site structure of [ZnOZn]²⁺. Since the C atom of Zn-CH₂-O bonds to Zn and O atoms at the same time, the barrier of subsequent C-C coupling with O_{fra}-CH₃ species should be high, which is impossible to occur. We also considered another possible route, which is that the Zn-CH₃ and O_{fra}-CH₃ directly go through C-C coupling to form C₂H₆ in the presence of a H(O_{Zn}) nearby, as shown in **Figure S12(b)**. The DFT calculation results show that the activation barrier of this step is 2.27eV, which is much higher than the barrier (1.56 eV) of H transfer from the bridging O_{Zn} of [ZnOZn]²⁺ to form H₂ then desorb. To sum up, our calculation results reveal that the H atom on the bridging O_{Zn} site preferentially transfers to form H₂ then desorb from the active site, so that the bridging O_{Zn} site of [ZnOZn]²⁺ can be regenerated for subsequent C-C coupling reactions.)

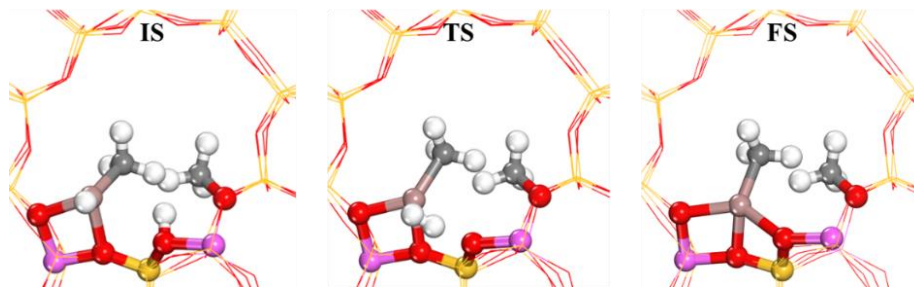
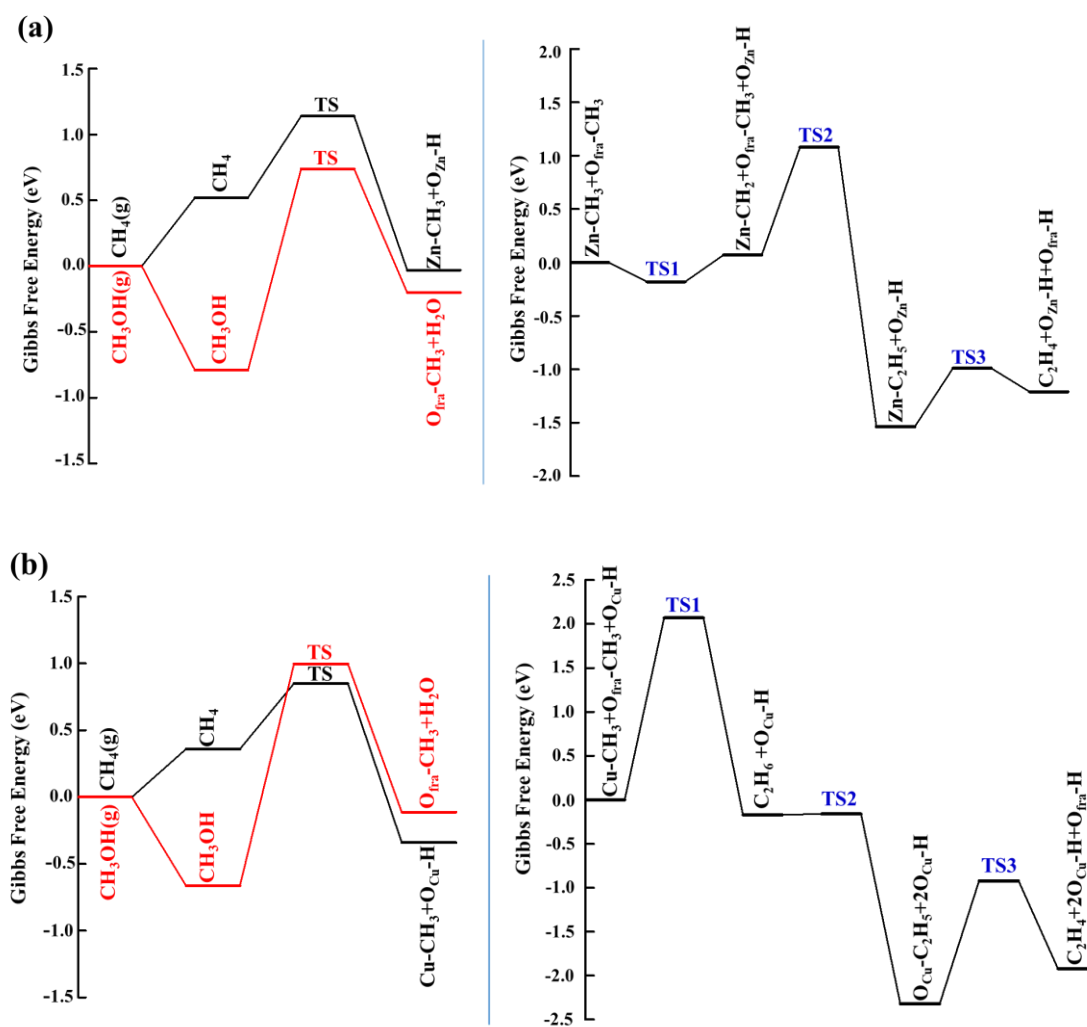


Figure S13. Optimized structures of initial state, transition state, and final state for $H(O_{\text{fra}})$ and $H(\text{Ga})$ to form H_2 over $\text{Ga}/\text{ZSM-5}$.



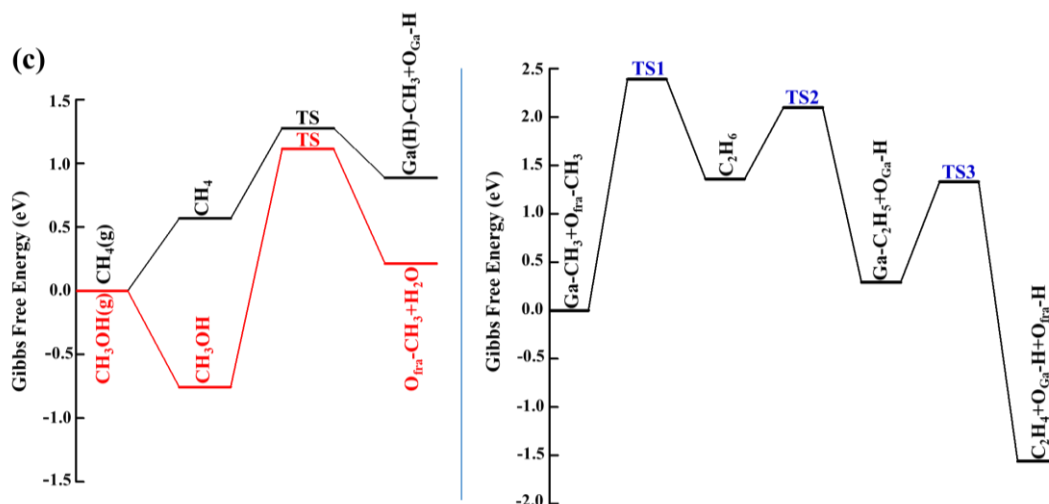


Figure S14. Reaction free energy profiles of methane-methanol coupling to ethylene at the reaction temperature of 873 K over (a) Zn/ZSM-5, (b) Cu/ZSM-5, and (c) Ga/ZSM-5.

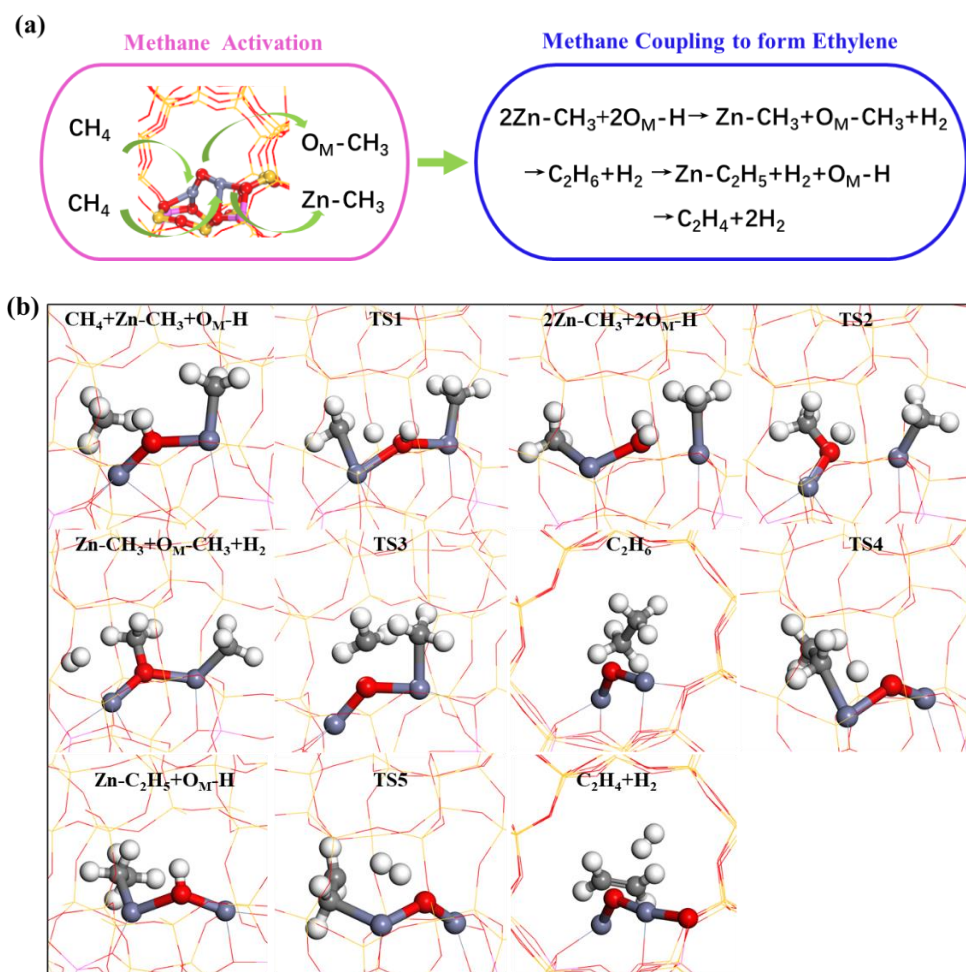


Figure S15. (a) Reaction pathways and (b) optimized structures involved in indirect methane coupling in the absence of methanol to ethylene over Zn/ZSM-5.

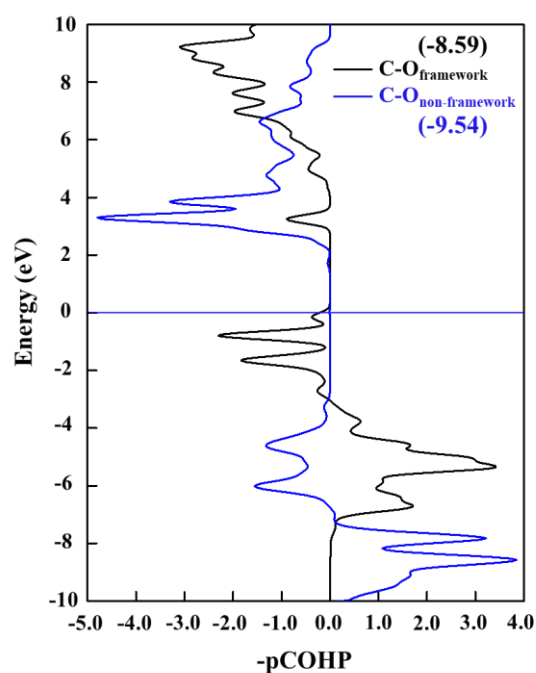
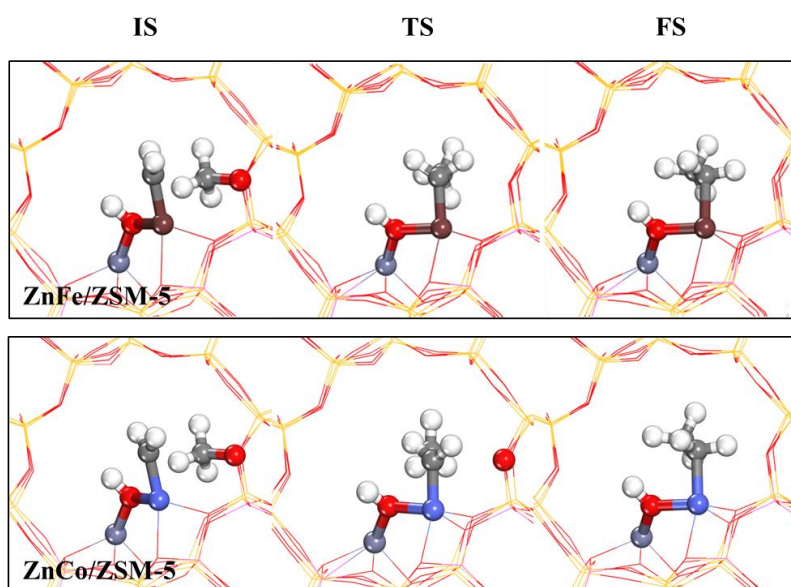


Figure S16. The COHP analysis of the C-O bonding interaction of O-CH₃ species (framework oxygen (O_{fra}) in methane-methanol coupling and non-framework oxygen (O_M) in methane coupling) in the adsorption state for the rate-limiting C-C coupling step over Zn/ZSM-5.



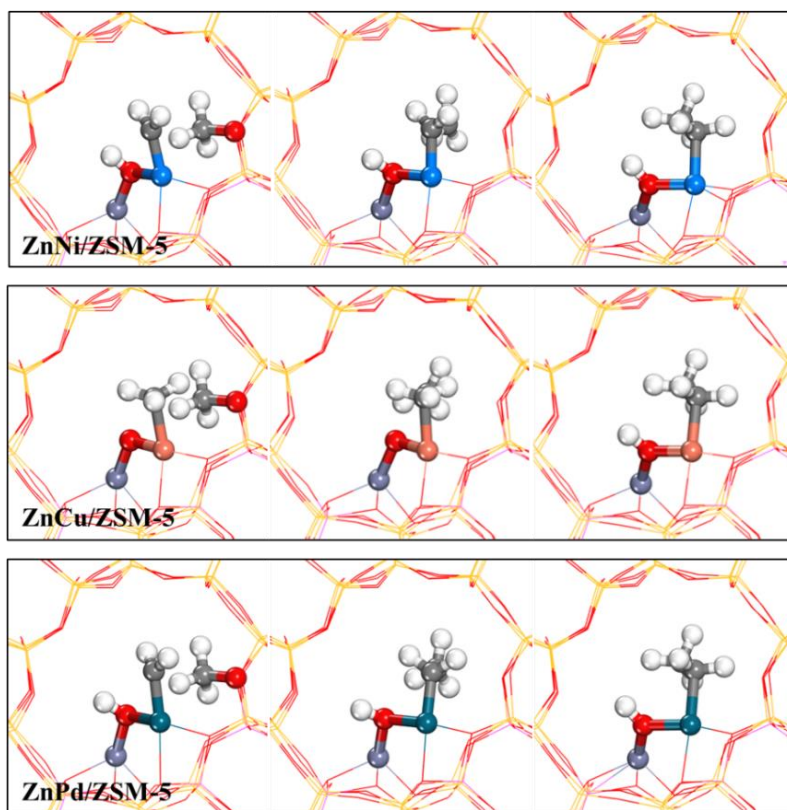


Figure S17. Optimized structures of the rate-limiting C-C coupling step for methane-methanol coupling to ethylene over bimetallic Zn-M/ZSM-5 (M=Fe, Co, Ni, Cu, Pd). (*Note:* The M-CH₂* intermediate is unstable in the Zn-O-Cu/ZSM-5 system, thus the M-CH₃* and O_{fra}-CH₃* intermediates directly go through C-C coupling concerted with dehydrogenation to form the Cu-C₂H₅* species over Zn-Cu/ZSM-5. Therefore, the examined step is Cu-CH₃*+O_{fra}-CH₃*→Cu-C₂H₅*+H* for Zn-Cu/ZSM-5, which is different from other bimetallic Zn-M/ZSM-5 candidates.)

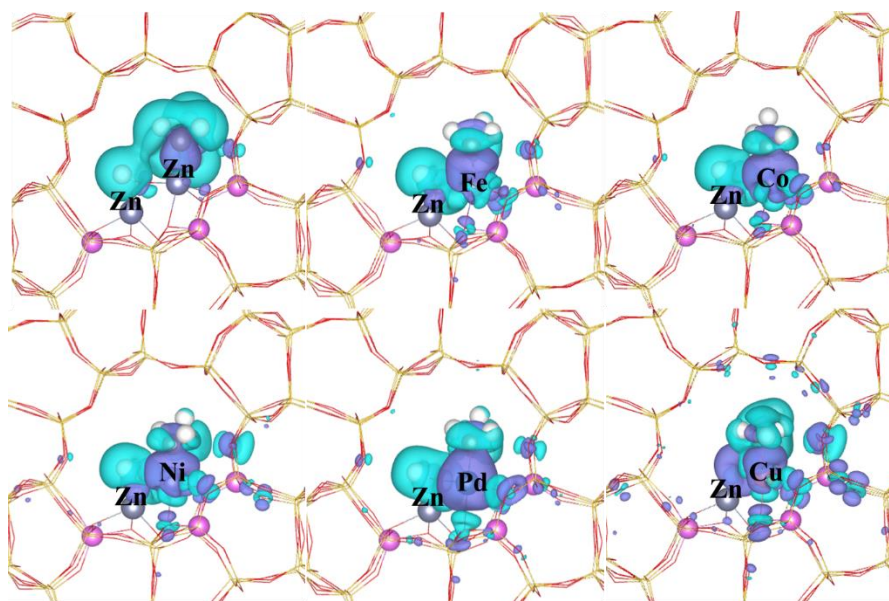


Figure S18. The charge density difference maps of transition state of the rate-limiting C-C coupling step for methane-methanol coupling to ethylene over Zn/ZSM-5 and Zn-M/ZSM-5 (M=Fe, Co, Ni, Cu, Pd).

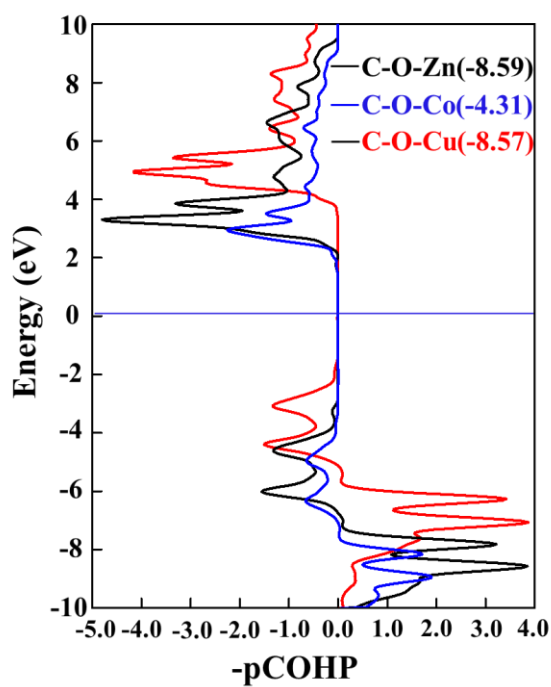


Figure S19. COHP analysis for the interaction between C-O bond of $O_{\text{fra}}\text{-CH}_3$ species in the adsorption state structure for the rate-limiting C-C coupling step over Zn/ZSM-5, Zn-Co/ZSM-5, and Zn-Cu/ZSM-5.

Table S1. Key structural parameters (bond distance (Å)) of the adsorption state, transition state and final state structures involved in methane activation via C-H bond dissociation over M/ZSM-5 (M=Zn, Fe, Ga, Mo, La, Cu).

	$d_{(\text{H-C})\text{TS}}$	$d_{(\text{H-O}/\text{CMo})\text{TS}}$	$d_{(\text{M-C})\text{IS}}$	$d_{(\text{M-C})\text{FS}}$	$d_{(\text{H-O}/\text{CMo})\text{FS}}$
Zn	1.39	1.28	2.77	1.95	0.97
Fe	1.47	1.20	3.52	1.97	0.98
Ga	1.36	1.33	2.59	1.98	0.99
Mo	1.59	1.39	3.83	2.16	1.10
La	1.65	1.11	3.12	2.50	0.97
Cu	1.35	1.22	3.47	1.99	0.98

Table S2. Activation barrier (E_a/eV) of C-C coupling to form ethylene in the presence and absence of H_2O over Zn/ZSM-5.

	$E_a\text{-TS1}$	$E_a\text{-TS2}$	$E_a\text{-TS3}$
With H_2O adsorption	0.87	1.40	1.38
Without H_2O adsorption	0.79	1.36	1.30

Structure files (CONTCAR) involved in this work:**Figure S1 Zn/ZSM-5**

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94 193 2 2

Selective dynamics

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0.1825939083202876	0.9419166752342607	0.4129332947343211	T	T	T
0.2993175567932320	0.9469347628652898	0.5050943721325243	T	T	T
0.4116477774986276	0.9261948789677195	0.4042848799407814	T	T	T
0.3953877857450009	0.9399850935795923	0.2076965096613006	T	T	T
0.2711438603710817	0.9559502170084549	0.2680334287875419	T	T	T
0.1363698910153314	0.1737067946204461	0.2588538115345416	T	T	T
0.1913885845709326	0.1499072253950501	0.4326764081839868	T	T	T
0.3100499900802210	0.1468601946907603	0.5197692430581806	T	T	T
0.4156761142098558	0.1684104945180336	0.4045803106329254	T	T	T
0.3925984012783042	0.1563580781588216	0.2105824693248635	T	T	T
0.2674986455738371	0.1537119103814805	0.2708975154924351	T	T	T
0.1821476534276174	0.0525519367072531	0.2980615597615645	T	T	T
0.4142623348029868	0.0471402421125755	0.3229306303932037	T	T	T
0.0686979264232360	0.8728060517394006	0.0935926922777184	T	T	T
0.0858870373849192	0.0041325306454095	0.0721554721499808	T	T	T
0.1101290593748059	0.1361567326252945	0.0723173081307269	T	T	T
0.3015185120433077	0.8648264370976583	0.1294583101789361	T	T	T
0.3076509341407145	0.9945885284741686	0.0848657071503215	T	T	T
0.2969646435225010	0.1281080554412405	0.0785660800810342	T	T	T
0.5128163421312910	0.9582052858529457	0.2845736411158020	T	T	T
0.5133181960714565	0.1307448557799264	0.2816825261910115	T	T	T
0.6413114458915591	0.5569419638656055	0.2820994343054212	T	T	T
0.6813504291859795	0.5719099147978239	0.0952504233572477	T	T	T
0.7937528609738422	0.5567521352837388	0.9901437773339903	T	T	T
0.9020452652979554	0.5785418717760628	0.0977245136920380	T	T	T
0.8865726549067349	0.5424875062719827	0.2922864475564467	T	T	T
0.7644597963902100	0.5291851789597449	0.2341727166808658	T	T	T
0.6372491397429340	0.3303113652703612	0.2495467117036312	T	T	T
0.6859168752460546	0.3394781917858505	0.0671117136035383	T	T	T
0.8066703827421028	0.3528088678482570	0.9868950971455934	T	T	T
0.9090660286114010	0.3260928781675121	0.1056255049928297	T	T	T
0.9025395166993566	0.3645214747704854	0.2974481301305283	T	T	T
0.7652643253875107	0.3608502500084642	0.2252603827058874	T	T	T

Structure files (CONTCAR) involved in this work:

0.6683710536173817	0.4482067088559434	0.1745503850535602	T	T	T
0.9217331888513819	0.4541332783638423	0.1528991112606786	T	T	T
0.5712504985379528	0.6271472260338311	0.4082975965894231	T	T	T
0.5789340936452924	0.4955816766164514	0.4354234055153125	T	T	T
0.5880809767344468	0.3611665131442766	0.4309919788065735	T	T	T
0.7981994753315504	0.6340270422457965	0.3540095332459303	T	T	T
0.7940644379109512	0.5137404401889173	0.4308136484713007	T	T	T
0.8128945559946273	0.3830200193186009	0.4277718572473150	T	T	T
0.0058952302895863	0.5486666911728688	0.2170339140995683	T	T	T
0.0175711051979979	0.3686895163456747	0.2046748831175172	T	T	T
0.8553811990033983	0.4311234679282471	0.7788784969769389	T	T	T
0.7966573724160037	0.4392283214677962	0.5983167211576558	T	T	T
0.6922490761256472	0.4344741086545156	0.4740885936891736	T	T	T
0.5908841082568991	0.4248601602134111	0.6024148158483996	T	T	T
0.6051252044707924	0.4443442710259535	0.7971926801808562	T	T	T
0.7307036288467795	0.4762444815558993	0.7580432410071015	T	T	T
0.8681251690001071	0.6808552297015843	0.7382836592708164	T	T	T
0.8202663154565252	0.6363542738371758	0.5490548982534126	T	T	T
0.6948862959416947	0.6453881825379316	0.4794520072609829	T	T	T
0.5881570906395073	0.6688966449708860	0.5930160838899698	T	T	T
0.6017611675554571	0.6576761111725657	0.7872824698826854	T	T	T
0.7275501714235723	0.6483551308166073	0.7244311551865434	T	T	T
0.8348382376627389	0.5480765963814992	0.6884631929421484	T	T	T
0.5825685524041589	0.5475753064569722	0.6748249604358898	T	T	T
0.9291068215974662	0.3773522386868105	0.9227774236634837	T	T	T
0.9075195202641091	0.5083030974148368	0.9265824307633466	T	T	T
0.8898360464598577	0.6403504535100634	0.9259358450227528	T	T	T
0.7003727380471400	0.3700080010947039	0.8731507525043881	T	T	T
0.6823512195690173	0.4946506111078326	0.9391321009707351	T	T	T
0.6947873331539142	0.6287532670542031	0.9178877131503363	T	T	T
0.4872524377645499	0.4562203661495922	0.7193437495609434	T	T	T
0.4842354130343130	0.6330527673551397	0.7055055533797306	T	T	T
0.6428830862314433	0.9387545674320212	0.2737006078216667	T	T	T
0.6828421866326818	0.9367492141628742	0.0856570768492251	T	T	T
0.8004245660111752	0.9481377349681106	0.9981135379758336	T	T	T
0.9124228305993738	0.9257780514825318	0.0989851246251278	T	T	T
0.8947164720780991	0.9451889088475072	0.2956747446205581	T	T	T
0.7709287279967443	0.9518938457020993	0.2311406694031641	T	T	T
0.6369898049620022	0.1689624817221136	0.2407890878052983	T	T	T
0.6936167253075178	0.1551397031681865	0.0672308419080794	T	T	T
0.8100995681735240	0.1465549668482972	0.9751325636420466	T	T	T
0.9142333600986795	0.1689835757717257	0.0934926444547126	T	T	T
0.8950853796755222	0.1536203734811258	0.2887105523137655	T	T	T
0.7692711937466965	0.1513728823722160	0.2300271075333580	T	T	T
0.6862035814455523	0.0508799121312066	0.1909328683217303	T	T	T
0.9180331442023173	0.0476462230714321	0.1722354675076707	T	T	T
0.5729722024011223	0.8732765427316317	0.4083271963764053	T	T	T
0.5886475065673287	0.0044797547112339	0.4295790072157705	T	T	T
0.6050133627445691	0.1372501222963465	0.4274557798051774	T	T	T
0.8058065018445290	0.8626132759347340	0.3704570393284846	T	T	T
0.8003553193779270	0.9921279109866447	0.4162613075084263	T	T	T
0.8010098539468993	0.1269018074507572	0.4209708936422452	T	T	T
0.0130823650824854	0.9578561866197383	0.2206629522039389	T	T	T

Structure files (CONTCAR) involved in this work:

0.0145699942199683	0.1351176766085593	0.2124787482429921	T	T	T
0.8586607360177647	0.0636719583396301	0.7745504161017170	T	T	T
0.8184449119842734	0.0563279337258658	0.5862481936538373	T	T	T
0.7004693527028613	0.0573334213404897	0.4977185355586959	T	T	T
0.5875225399878641	0.0750093984036990	0.5973807209023404	T	T	T
0.6058326290577936	0.0544879931884592	0.7927385673840022	T	T	T
0.7306159398747779	0.0430533813439655	0.7325070260774331	T	T	T
0.8667033804692272	0.8271843860603573	0.7427306843971575	T	T	T
0.8136535735184486	0.8506528505519210	0.5671568410948039	T	T	T
0.6954259185383714	0.8516614197780612	0.4787042304401805	T	T	T
0.5897886118361291	0.8292018555686729	0.5942374307529367	T	T	T
0.6101029353135785	0.8484477641064213	0.7882858057991918	T	T	T
0.7350749723586409	0.8454814650464445	0.7256993603184207	T	T	T
0.8201386229719566	0.9473014693930454	0.7037212850137265	T	T	T
0.5825974718256959	0.9520016937415903	0.6687745891970130	T	T	T
0.9325518473258319	0.1286852361745302	0.9053440874647360	T	T	T
0.9134705716241321	0.9984534265832795	0.9321492170391913	T	T	T
0.8934937412766273	0.8658727857093382	0.9280361991394932	T	T	T
0.6974835854304720	0.1319423489797643	0.8719472134949465	T	T	T
0.6944122313722474	0.0022960357622286	0.9155781061972835	T	T	T
0.7077689057663047	0.8690113188441075	0.9190767243737563	T	T	T
0.4873301254611670	0.0414006264368942	0.7186028223540444	T	T	T
0.4890874526717572	0.8624252750657936	0.7138318565524908	T	T	T
0.3567611224005218	0.4340894586867579	0.7253594557877304	T	T	T
0.3155018993737284	0.4406421261323660	0.9128635901836152	T	T	T
0.1985324569742778	0.4554407249865060	0.0033554275558135	T	T	T
0.0858079448233338	0.4265702587883287	0.9076083584897123	T	T	T
0.1036870588309213	0.4392332137964438	0.7114024969767275	T	T	T
0.2286685229435697	0.4573892904254100	0.7672727702754110	T	T	T
0.3640274906662555	0.6733132694307992	0.7599747402143365	T	T	T
0.3079623525616924	0.6481599537208143	0.9322151067751582	T	T	T
0.1909874496179602	0.6449773350542317	0.0248956585246030	T	T	T
0.0901301845642471	0.6697991135172014	0.9026112580231178	T	T	T
0.1072566201583644	0.6525391160137316	0.7087584622480819	T	T	T
0.2327557938433391	0.6509524694901816	0.7692070761304780	T	T	T
0.3200505246281402	0.5512947462598505	0.7974393379173875	T	T	T
0.0820655996387432	0.5469819478698045	0.8259152347391161	T	T	T
0.4311092692713704	0.3750574905424534	0.5870558856692759	T	T	T
0.4126303893770436	0.5064190624331129	0.5767465533469867	T	T	T
0.3849849723625940	0.6373433298188476	0.5716788480139579	T	T	T
0.1990398144159684	0.3658755499145032	0.6302543582194244	T	T	T
0.1885346128317010	0.4954953950161103	0.5858158712444527	T	T	T
0.2032967108339312	0.6285312529531342	0.5763757925346926	T	T	T
0.9849217701919347	0.4568190361937763	0.7870579294125504	T	T	T
0.9870851942336856	0.6359263354001671	0.7885249313811455	T	T	T
0.1372886349847358	0.5642543322095395	0.2282893579739209	T	T	T
0.1807028646676117	0.5570383195558387	0.4131284396866799	T	T	T
0.2971969259600059	0.5472780085894720	0.5054137927809035	T	T	T
0.4092431839003950	0.5725511047488582	0.4054819654738199	T	T	T
0.3926870458513123	0.5572477722107048	0.2093281358801510	T	T	T
0.2666863819155393	0.5449041713813286	0.2646682672552083	T	T	T
0.1343460470386988	0.3252867453919593	0.2628124716319471	T	T	T
0.1897418071750559	0.3528568736184311	0.4348134330944912	T	T	T

Structure files (CONTCAR) involved in this work:

0.3092002643096950	0.3546061031572362	0.5186793456692841	T	T	T
0.4131182006932093	0.3295228192764323	0.4005413576660261	T	T	T
0.3882059369777557	0.3481958861323934	0.2061925329830991	T	T	T
0.2649973467608135	0.3454965039348296	0.2719188775971027	T	T	T
0.1794037028712284	0.4474478932590262	0.2954732144982645	T	T	T
0.4165797829138767	0.4514772844732953	0.3263456321277315	T	T	T
0.0675193221282731	0.6252366115643960	0.0868653535533474	T	T	T
0.0822084112082420	0.4923847483252822	0.0795492368306308	T	T	T
0.1162026190760665	0.3625708862015030	0.0727034076351671	T	T	T
0.3029149337318588	0.6353731710234513	0.1287825288984508	T	T	T
0.3070060414010299	0.5051122233774631	0.0836136445054980	T	T	T
0.2895367822495292	0.3719443011121197	0.0782815049102876	T	T	T
0.5104482162934266	0.5434095085768302	0.2834985893856605	T	T	T
0.5096695157566522	0.3620615087615152	0.2720178002030523	T	T	T
0.4369986860767407	0.7497320636392316	0.6407139596143642	T	T	T
0.1910423732759366	0.7490704437254967	0.6480934378393918	T	T	T
0.2719930396722025	0.7500355737688097	0.0483882861831553	T	T	T
0.1099112840644347	0.7493992519865545	0.0577587655400228	T	T	T
0.0626202578424397	0.2501476469229899	0.1407786062069513	T	T	T
0.3070042932883686	0.2501652342900733	0.1461467238723706	T	T	T
0.2282995629262985	0.2507241765935677	0.5500529819912501	T	T	T
0.3908151968231526	0.2509061589210573	0.5549908623209839	T	T	T
0.5574708135191572	0.2475817259601466	0.3470767317634481	T	T	T
0.8131120070724552	0.2498573755550618	0.3487646592644065	T	T	T
0.7290128412991445	0.2496978823269113	0.9359904941696969	T	T	T
0.8906703346316828	0.2515952155449943	0.9445127965050099	T	T	T
0.9434482188832538	0.7526380602836824	0.8611415350335611	T	T	T
0.6906796081451798	0.7490915804992906	0.8461398578065649	T	T	T
0.7787553103426739	0.7472941323114278	0.4539814036870960	T	T	T
0.6142795954884736	0.7494417463270391	0.4408892816722933	T	T	T
0.9417575930155437	0.4899457819661792	0.4990451548495333	T	T	T
0.8171260194373967	0.3329150093540418	0.3189451464675356	T	T	T
0.8072977946478551	0.6338209065656726	0.6830253666437422	T	T	T
0.9137205811912018	0.4267750905195370	0.4118535386903046	T	T	T
0.8813957902597264	0.5510515141027812	0.5463799577271241	T	T	T

Figure S1 Fe/ZSM-5

1.0000000000000000

20.0219993591000005 0.0000000000000000 0.0000000000000000

0.0000000000000000 19.8990001678000006 0.0000000000000000

0.0000000000000000 0.0000000000000000 13.3830003737999998

Si O Al Fe

94 193 2 2

Direct

0.4215551130546175 0.0565724124945917 0.6505401436922217

0.3061892262011225 0.0287373189438237 0.7993281579746476

0.2795477902722761 0.0593903253732192 0.0195652636240726

0.1199860785678873 0.0658819544934472 0.0130252962306855

0.0657578419822455 0.0303535244874677 0.8027006590069299

0.1825049856946031 0.0608663015889563 0.6693333769056565

0.4176295814418585 0.8267943580420495 0.6688565653553491

0.3043820695883894 0.8694112115176613 0.8120515467972548

0.2686057001586401 0.8298402711671032 0.0307615351544156

0.1144663103484649 0.8263396287144261 0.0178365889200574

Structure files (CONTCAR) involved in this work:

0.0663715408506379	0.8717910390235414	0.8050379629294827
0.1832213312665389	0.8290007110232196	0.6758153895386141
0.0778770020633109	0.9420373555854273	0.1512717899038710
0.1936034841253187	0.9699391213134732	0.2995868366818405
0.2186763022432283	0.9414768068385763	0.5194288503430923
0.3773624654897580	0.9333606794712112	0.5126554284178935
0.4337082397531202	0.9695074580268164	0.3043347085280289
0.3174923183554744	0.9396921835056247	0.1697449442698580
0.0802429113461935	0.1725054742819695	0.1725209222041126
0.1956725118316965	0.1294079431520861	0.3126443009441752
0.2322207187102655	0.1703225680204329	0.5294177768686863
0.3867508063269169	0.1729951807369620	0.5148899317479456
0.4348421980115056	0.1272309509827625	0.3034141626373058
0.3166758174675355	0.1705991467541621	0.1761384657468291
0.5778534702938034	0.5564680633402153	0.3488332067294048
0.6925738494626390	0.5281574473397882	0.1978747692232275
0.7183788434207227	0.5548295121146753	0.9796061835518772
0.8763242385319242	0.5662312926362879	0.9904188825581303
0.9329473764115813	0.5302652013909206	0.1979945895605203
0.8151969987851109	0.5588321561559170	0.3293222975020142
0.5788055668444689	0.3274959362444363	0.3286407074538952
0.6947771346193613	0.3685538498138898	0.1867751524187270
0.7316587737039810	0.3247958971068032	0.9699530706988209
0.8861575276342767	0.3278021221999573	0.9852552024418197
0.9348911352654827	0.3727884299115723	0.1963876013595895
0.8168615209442314	0.3305987061430741	0.3254043024289061
0.9224419799020731	0.4458093769289891	0.8506316537381416
0.8050686184448880	0.4716312808934129	0.7028133510381690
0.7794359667695031	0.4407205899828011	0.4831853342039023
0.6199272170154431	0.4331677658392556	0.4892366563830453
0.5655040942507176	0.4680596148858781	0.6993310997786599
0.6815579395895709	0.4349997516275588	0.8321650954362108
0.8012202114209208	0.6311119566575765	0.6824742158272481
0.7656496067803866	0.6686253595597887	0.4640104623148549
0.6115105451778154	0.6728350891559038	0.4805328142099460
0.5652913207169610	0.6262150871314173	0.6951960532596232
0.6823160763575843	0.6684556394001119	0.8212127402174060
0.5783072682592252	0.9430038243646458	0.3502159786192399
0.6927980537241497	0.9718560632694407	0.2017500882984123
0.7204174947172718	0.9387890329792589	0.9834029531701003
0.8776440832997982	0.9409953945711386	0.9881241698312883
0.9337025493332189	0.9690799077573115	0.1977750837174572
0.8159155283744728	0.9387177641515718	0.3283997848213736
0.5794520142067939	0.1740715128505975	0.3258943277852926
0.6947974341891630	0.1305729744953572	0.1883105353884920
0.7352560571540034	0.1650390165920464	0.9702776121412443
0.8900743944082253	0.1740591976671788	0.9812322672974387
0.9365544313431541	0.1273124499128202	0.1952494105166205
0.8174183808980107	0.1730623127453489	0.3219924904896500
0.9219122257382982	0.0601511782447436	0.8449723491945397
0.8080354508168341	0.0283983038994980	0.6956644501794357
0.7813015681168783	0.0601164802663363	0.4773513937007522
0.6217134064388082	0.0681294659771831	0.4850553245999641

Structure files (CONTCAR) involved in this work:

0.5660396886590690	0.0317972891704829	0.6927990999840890
0.6837593132578954	0.0536933044724359	0.8259166060497867
0.9170695789662586	0.8305307210226196	0.8293016779652435
0.8065994294674284	0.8703859513012621	0.6816568256915890
0.7670234984376451	0.8291809395056616	0.4684589030894988
0.6121950769023424	0.8269108711353748	0.4870907595063721
0.5622044209133257	0.8747360498581065	0.6965766581714694
0.4217543970111177	0.4426355955020954	0.6529433195714104
0.3062254823698463	0.4714192535335623	0.8005625136526817
0.2810888855973546	0.4404919844885042	0.0209513341052925
0.1214749734942524	0.4328360555243734	0.0151748754773529
0.0677017786679580	0.4685085175204456	0.8053371196210884
0.1829585026727156	0.4396098410471814	0.6712174285122083
0.4197712482315053	0.6731098787478531	0.6709814828106595
0.3067783827893238	0.6308114362767137	0.8138991737095077
0.2688224443274373	0.6694812664352267	0.0313856962181117
0.1148061157463500	0.6721512046563151	0.0150017814733219
0.0680714740425249	0.6257154147006951	0.8022410148268087
0.1863928803001380	0.6714191468518740	0.6753312715277016
0.0778911343606439	0.5574471953093305	0.1514154384965266
0.1929205144417389	0.5299852525651660	0.3006441825243216
0.2204091855793665	0.5587519682202579	0.5205950725814090
0.3786248930879483	0.5651599922518810	0.5143434123910264
0.4333437881739220	0.5298185589276804	0.3055542836874208
0.3172903055871270	0.5604237005727954	0.1715252164315702
0.0799772974330050	0.3262268556586983	0.1732680370176094
0.1948860736321298	0.3707355643916432	0.3126209956652306
0.2334112865651541	0.3306615404469365	0.5295332920906695
0.3880393575797124	0.3265273853349032	0.5172109799089437
0.4348074268517794	0.3727017586465399	0.3049493301325101
0.3168125589932409	0.3285821017599911	0.1764909102122924
0.3574554945263482	0.0658190640013602	0.7235835935458926
0.3165425724802828	0.0578298129619792	0.9115293852006946
0.1995585969872743	0.0535879201016902	0.0041494110353109
0.0870112190006091	0.0712212990679599	0.9028085533078808
0.1055484274963645	0.0593005752623225	0.7065617726123036
0.2297513179275003	0.0436245883681005	0.7648375282993835
0.3602746670501605	0.8252790990848358	0.7547127331155127
0.3076982725476576	0.8521897351659584	0.9300440167038888
0.1909133591693884	0.8538270283728872	0.0237287507334384
0.0887018065389755	0.8300665487588496	0.9033341553390014
0.1058213088213885	0.8429051385742892	0.7078877305827237
0.2302000617639904	0.8510877526632592	0.7699155118071054
0.3203579551783698	0.9484373367990765	0.7942865423747014
0.0822935443989439	0.9510406391844740	0.8202954008065906
0.4315209252675105	0.1250016845849371	0.5859483574755733
0.4130411899073060	0.9935000777386895	0.5745943739543347
0.3879699681475878	0.8617852291221914	0.5683350361922218
0.1992255634665583	0.1353273431890525	0.6269745589896218
0.1918898671612027	0.0056711618613872	0.5816530877923465
0.2017688296480706	0.8718450585470771	0.5766706543281015
0.9869557999231082	0.0412437820079136	0.7786008098538255
0.9867320567748723	0.8607780572054683	0.7882823333829817

Structure files (CONTCAR) involved in this work:

0.1422826979172369 0.9333670151652557 0.2234272856102825
0.1816590617804011 0.9409326784921802 0.4113698419337797
0.2983724144826467 0.9496535352764777 0.5035849153553819
0.4102778069914677 0.9276141577261199 0.4024015851940821
0.3945938379731307 0.9434143351595895 0.2056516816403212
0.2699914953735502 0.9540895433167979 0.2660783455862005
0.1394233834183055 0.1728624225616421 0.2549769480744839
0.1914545252650575 0.1470045877499836 0.4304557494572568
0.3096728146363377 0.1468824704963277 0.5176737792751714
0.4141272653572431 0.1708704522872710 0.4009919354578149
0.3938636925322329 0.1550648201877562 0.2068337091839280
0.2694658285059613 0.1484358699982875 0.2699929818293539
0.1802053657432133 0.0503386302978256 0.2943759384597890
0.4175438502195005 0.0486529063070992 0.3236247954859879
0.0674010229208060 0.8724320417483407 0.0891595348602153
0.0863284759005038 0.0035313883465820 0.0727834365656632
0.1050507760394132 0.1358864497325001 0.0706764261109325
0.3036629692187292 0.8649125162035665 0.1264343368122565
0.3045989489033681 0.9951587685222094 0.0835102593504902
0.2976574236051241 0.1291965956387162 0.0757127013307950
0.5124634354283553 0.9568675649633754 0.2825698653003036
0.5142455369719149 0.1353934365155468 0.2816082772366795
0.6417323332947253 0.5642843524043020 0.2750426279606440
0.6816313283910844 0.5605695373262134 0.0874088843520087
0.7980643329787176 0.5466789461957161 0.9961649100166194
0.9077922262695621 0.5731126939935850 0.1013727195143412
0.8931739869872179 0.5541584993634563 0.2971274116140799
0.7694493301226255 0.5407715694467210 0.2322276439798115
0.6382819775644250 0.3270970953691644 0.2467714681165099
0.6918650932820145 0.3447912187100117 0.0712655631865982
0.8083399781546351 0.3512983900480371 0.9807680385735007
0.9128361883280962 0.3291766759171658 0.0995422316971326
0.8938084916207691 0.3460511526940300 0.2933201852716998
0.7684853170308298 0.3532783441113735 0.2331522952839214
0.6777199787945289 0.4480349179902265 0.1958839026965547
0.9183675352734193 0.4514257458227722 0.1749592120463926
0.5653724734306580 0.6269447087448667 0.4075478564084294
0.5888518225052973 0.4969926325037209 0.4300354046191215
0.6038109878236930 0.3639086996549735 0.4303924708226501
0.7997102521360785 0.6348069610496706 0.3661568294292851
0.8009786132353190 0.5058820173709195 0.4185262671896455
0.7997292221460715 0.3717359070729536 0.4265846125111581
0.0114851012437180 0.5445688399182254 0.2183688267231444
0.0142298835231285 0.3640833160428152 0.2174615498630455
0.8581898233850583 0.4369315701030252 0.7783667933815483
0.8172407075568316 0.4432691774016360 0.5905358861187793
0.6996014289581918 0.4430507587335029 0.5006039036201015
0.5860993029313839 0.4276070412284496 0.5986491683133237
0.6047657308628455 0.4375530969270613 0.7949406338711478
0.7297067915169022 0.4521415260298042 0.7378149759424441
0.8561995968874094 0.6765636544533047 0.7351953955362928
0.8036371951527878 0.6411442790211798 0.5624719878168190
0.6878065134217878 0.6458531058906578 0.4709798392958821

Structure files (CONTCAR) involved in this work:

0.5870426299999817	0.6666763303794093	0.5955302926926386
0.6041852695200871	0.6582429547462223	0.7918585488743139
0.7262407187632599	0.6514918142090892	0.7227522052432999
0.8145139876380261	0.5522676338659472	0.7090932157623936
0.5843494217524234	0.5471647292944395	0.6847293426078540
0.9307898979066397	0.3778132094891818	0.9167704258236669
0.9153194461093443	0.5101786673466481	0.9253551447415534
0.8855025946851828	0.6402431718250335	0.9381782467417593
0.6969194296587435	0.3603323964649142	0.8743127721872820
0.6911175977596236	0.4894790273845893	0.9213893787562358
0.7032470144577062	0.6232576349329618	0.9175256572191558
0.4866230390922033	0.4572903043000338	0.7222450183822994
0.4855687561826094	0.6340462874170556	0.7123219591616329
0.6422140987396191	0.9331746455979012	0.2766361765490615
0.6802402502114840	0.9453854005203243	0.0883256716045280
0.7986902574396177	0.9558436681488216	0.0014321385860729
0.9121983508612904	0.9295284502158909	0.0960356935846823
0.8934064412513580	0.9393781350820738	0.2929527088055794
0.7698179166223357	0.9557190811731205	0.2312808627267524
0.6368232277805371	0.1752271915332830	0.2400879826032298
0.6936353526113830	0.1431765376742850	0.0690460380786847
0.8137196601300053	0.1455596463603015	0.9836850744637864
0.9210769648777407	0.1675921734877158	0.0925095646749781
0.8940775416407587	0.1601993001367076	0.2865037869874716
0.7680250643818949	0.1518600033004403	0.2304363873901552
0.6792834750416532	0.0520284069825512	0.2120125486445670
0.9169796681665485	0.0484724233703881	0.1826293438796997
0.5677543005354420	0.8746832896052132	0.4144425738474193
0.5879447100327545	0.0057412546277718	0.4259220576198482
0.6073634189931649	0.1377670940833230	0.4259373102317764
0.7974357282089576	0.8645297684249842	0.3691684547002507
0.8051677399968126	0.9948857149534459	0.4143995340267169
0.8011598869859059	0.1292400555136750	0.4208469243843182
0.0123757029484168	0.9562032398922052	0.2195391414024382
0.0157182717095176	0.1341516485033402	0.2201132884060284
0.8570669755238948	0.0669086844420117	0.7734809650305229
0.8187350189632794	0.0596265781443099	0.5848918715843417
0.7013646191972511	0.0559066931616177	0.4934262869912131
0.5887326959589361	0.0747245556321171	0.5950051103656652
0.6067860605237062	0.0580389707631618	0.7901266091985777
0.7308234831561888	0.0400475487243268	0.7290524754661845
0.8649343542018886	0.8275786591882721	0.7381774031258240
0.8113815096380650	0.8527970635251738	0.5633959602362857
0.6896129787732234	0.8521687136816007	0.4836288712488724
0.5845365954969789	0.8293017091297676	0.6004911775401980
0.5994923730119885	0.8494611314339533	0.7960507194079015
0.7342998412144497	0.8529585192803192	0.7253621731184607
0.8261625870727511	0.9491826520106156	0.6985430189339863
0.5804506614505333	0.9528865011654479	0.6708967583368817
0.9338790291468099	0.1311966987567683	0.9016372867253771
0.9127665621747797	0.0027270725810905	0.9304932993181740
0.8874131491891045	0.8720469011956892	0.9245913019486763
0.7043492514106919	0.1245515051888849	0.8765071484570163

Structure files (CONTCAR) involved in this work:

0.6899200694591614	0.9909428104179763	0.9032714817512107
0.7121778277874169	0.8618780706100717	0.9397816357871409
0.4877154320704838	0.0449025694926139	0.7179314152555814
0.4814821874620751	0.8681645701126975	0.7105320030711674
0.3567937785150485	0.4339952716027841	0.7241224800354803
0.3178105403417421	0.4430092972043536	0.9127958834049219
0.2010033560248532	0.4457230655614359	0.0067746143696791
0.0888784933534437	0.4268516195049339	0.9049505718691653
0.1059346751667476	0.4386855673999760	0.7080590733811462
0.2296850006684613	0.4559106994282587	0.7677350749989245
0.3650816590868459	0.6737438397848230	0.7601638736092146
0.3094934300323246	0.6464663795670227	0.9323899186644450
0.1914397716529873	0.6451415985015432	0.0221255670688445
0.0899892116369344	0.6693973095228546	0.9002923391158246
0.1102295235821135	0.6533115605163865	0.7062056348550593
0.2343153358069306	0.6525102818212974	0.7697849400993766
0.3204379061823254	0.5516214814334611	0.7937928156364197
0.0869466508365755	0.5470324589777831	0.8226640005437035
0.4325067774507633	0.3731395676894669	0.5911114657018010
0.4145231659845249	0.5043978809563638	0.5744598963682181
0.3895375348639387	0.6358040877538689	0.5727658831188707
0.2011311175944524	0.3660727565548564	0.6269851581716693
0.1920820499393037	0.4967656248494215	0.5861925572099290
0.2074752011484485	0.6300588417024171	0.5756718073439872
0.9885903026300089	0.4576135013417817	0.7834120959963712
0.9900682304409669	0.6348955173712202	0.7813478146768277
0.1412309739617705	0.5673691609462974	0.2256505961820469
0.1822815832927125	0.5581291859727762	0.4132940190582591
0.2998773141950957	0.5481934281734387	0.5036634960013793
0.4121326255057607	0.5719908927907953	0.4045818299143593
0.3942643558737576	0.5581139652480230	0.2083216520111727
0.2693677568927416	0.5454185020347637	0.2670846769648198
0.1375572308605864	0.3265540167026029	0.2584069692210917
0.1927413695447888	0.3545514171831795	0.4309379865682650
0.3111346626868243	0.3531887892793517	0.5178217367659755
0.4169002577099518	0.3297830167772754	0.4043096386761998
0.3936695885744863	0.3426134253654985	0.2102084024346748
0.2681335582527414	0.3514500854167804	0.2681557407325850
0.1789272422456832	0.4496813802714028	0.2935350155724268
0.4151910392966554	0.4509476856616613	0.3235400523078304
0.0677733747779541	0.6257043868150237	0.0860824777428397
0.0873206396969958	0.4945600446327410	0.0757456886710975
0.1070218071531707	0.3626513069349218	0.0726737884529441
0.3026696171078493	0.6350644136285442	0.1284848108925269
0.3060537734901653	0.5045406694834798	0.0853923678604673
0.3002926513272163	0.3703975562093869	0.0755013336112244
0.5123357136917606	0.5393770764047571	0.2823241221410885
0.5142507118345885	0.3660460249045772	0.2817304522399909
0.4380924234331844	0.7499399439672788	0.6414875332826991
0.1939183275773295	0.7505308729623714	0.6487157789858461
0.2728496812060802	0.7497098613755568	0.0458518316772378
0.1094687239916219	0.7490275187031441	0.0554730367206447
0.0612178029182673	0.2493895626745212	0.1448328002916399

Structure files (CONTCAR) involved in this work:

0.3063386277920053 0.2496294823147085 0.1515734531152505
0.2272045594624601 0.2505147583121367 0.5441991644148910
0.3916792496151956 0.2494599789720116 0.5562483228552986
0.5597232141430449 0.2504856127545108 0.3554135700538819
0.8068016374254804 0.2515239466795872 0.3499671678082631
0.7281261730804321 0.2447798183589050 0.9505656271177615
0.8926461973433029 0.2515188626194222 0.9441662821897997
0.9250359569435097 0.7545191087452155 0.8769859884195416
0.6954614574964019 0.7457911249406719 0.8613022383978275
0.7717677922530699 0.7489670700666723 0.4532748120872824
0.6061206768173846 0.7504868830191098 0.4453461774062347
0.8023602443487572 0.7511889362112586 0.0887187505828847
0.9184736864121413 0.6718251108033720 0.8217566799833483
0.6814615970939811 0.8315279122746958 0.8208923022034886
0.8646345972562299 0.7344193950046868 0.9952755354327741
0.7469311350699317 0.7679871064378923 -0.0133587105071988

Figure S1 Ga/ZSM-5

1.0000000000000000

20.0219993591000005 0.0000000000000000 0.0000000000000000

0.0000000000000000 19.8990001678000006 0.0000000000000000

0.0000000000000000 0.0000000000000000 13.3830003737999998

Si O Al Ga H

94 192 2 1 1

Direct

0.4215988573438575 0.0586802642008117 0.6503754141180886

0.3057837784988079 0.0300751137048940 0.7975997213935381

0.2808386827526301 0.0578622242011981 0.0192480782132676

0.1211295451909348 0.0641372975907686 0.0131134569228907

0.0663851200373345 0.0301303555696156 0.8010878719193447

0.1821626297212952 0.0607616781425822 0.6677447802962562

0.4208731137132491 0.8276029795536324 0.6741423644776674

0.3035139094382814 0.8710347130576148 0.8101617452182069

0.2668530099334541 0.8302916027514808 0.0284240179968314

0.1122059737320055 0.8271226328826082 0.0175596426472350

0.0639784111590990 0.8715668326249958 0.8032713847941930

0.1814867881123789 0.8276061430189630 0.6752979162432535

0.0769786536910187 0.9421634530453007 0.1529163024271764

0.1940669384717698 0.9705699802801665 0.2983505561803902

0.2182692188936985 0.9393245054377659 0.5203998269200758

0.3786395989836860 0.9333899680922791 0.5154634793663316

0.4338474532976512 0.9678190769365218 0.3041645418331260

0.3183550080653628 0.9384548341414894 0.1686317617537308

0.0810367924396914 0.1736177547824150 0.1678574723859179

0.1960043591359210 0.1300312965843662 0.3088240939687376

0.2325977974922947 0.1701556873319178 0.5258141603576070

0.3873314299667655 0.1732975858502790 0.5115012352738141

0.4366785276311608 0.1262372212248083 0.3000959760935504

0.3179325592944469 0.1698965558110027 0.1737882357253015

0.5795252675311524 0.5581751011244166 0.3468385297409294

0.6902468728510677 0.5338307787064300 0.1897583137325660

0.7147032119145378 0.5634065695567215 0.9737715448360011

0.8725880392914634 0.5601225121246780 0.9724768441688426

0.9314917361988571 0.5290352657292129 0.1858791446687498

Structure files (CONTCAR) involved in this work:

0.8144471241863960	0.5613382740101376	0.3172821476656136
0.5774612342656978	0.3285577881714269	0.3271851869153266
0.7017523460562930	0.3764718820924262	0.2066531247052875
0.7355750710552389	0.3294245359802394	0.9840723040545333
0.8877786264288950	0.3269184631593856	0.9757087711332292
0.9364440302376648	0.3713701144128843	0.1922919188299109
0.9242565165328185	0.4372472525406090	0.8324446342033187
0.7809541942907751	0.4425448139476825	0.4724030885928637
0.6207038730270276	0.4327476329336566	0.4861282674515355
0.5658220542482955	0.4687563229744490	0.7003264237625115
0.6739830420736646	0.4359742036834522	0.8438002304300701
0.9174886775511490	0.6741607733966880	0.8258234488932598
0.8013354287060999	0.6365870331467712	0.6919628270607532
0.7658995968211582	0.6658266868048380	0.4723811072123052
0.6111697202761087	0.6716067211617095	0.4861806346304878
0.5639828849433705	0.6270502717224009	0.7021057885514997
0.6823401729241081	0.6795712699335128	0.8222328560653512
0.5780391988516220	0.9425604383706463	0.3555477083924087
0.6949413916732128	0.9709810640793998	0.2099380957567644
0.7205983503111868	0.9439528974869866	0.9884274720934331
0.8797721495640596	0.9354068181703207	0.9924127279229823
0.9327161967622033	0.9702195589722209	0.2029028239211297
0.8186654619863845	0.9392352844200488	0.3433058268715298
0.5802972594381192	0.1738770478000706	0.3270176814638818
0.6969294968076413	0.1289675033213932	0.1914358746926359
0.7338549497430928	0.1701357626302481	0.9732330649472608
0.8883182735017503	0.1727099326518857	0.9846582366848687
0.9361107136906153	0.1285984575741515	0.1979888647278865
0.8183200851078168	0.1692869043719613	0.3290492955253925
0.9234421998225203	0.0556118300986137	0.8532142204156897
0.8047867113339511	0.0268250035662102	0.7083826983619443
0.7809683148549198	0.0578168772680034	0.4880190612381703
0.6205318358034968	0.0683915864663750	0.4881301573983512
0.5665572029003514	0.0335370542966723	0.6978059935075366
0.6806015612309957	0.0594478901915000	0.8404472503211623
0.9188103808380547	0.8264551712291859	0.8358595898842748
0.8044844683705165	0.8682391467991837	0.6909789538688244
0.7686459511654300	0.8262089038918020	0.4743949704695447
0.6140234716704785	0.8264069697834495	0.4913117737312761
0.5646563591653002	0.8762771325815285	0.6998991262187689
0.6821016398906418	0.8349147148360085	0.8289513490497151
0.4196659670814453	0.4424502704210115	0.6458722559539375
0.3078211463554895	0.4685504744231417	0.7976127377498895
0.2822418065895961	0.4405237107735311	0.0182741301379826
0.1243639241367178	0.4346740851610856	0.0075998961122694
0.0709734313803943	0.4716760645918570	0.7984423145050807
0.1864512814126708	0.4422452780126380	0.6632198041060429
0.4214632450656901	0.6734669744858983	0.6720547150771012
0.3034087293345058	0.6271779248073220	0.8053592370567353
0.2667486211301822	0.6698373280690371	0.0236546173365009
0.1122956283685412	0.6736201735876834	0.0130273334624979
0.0635530421965819	0.6294416866583451	0.8019019191555254
0.1807089041323447	0.6695985769764596	0.6707763095384831

Structure files (CONTCAR) involved in this work:

0.0762345147198733 0.5556890594266762 0.1441754288629964
0.1935392806453658 0.5283724202857523 0.2921692666105721
0.2197630806392563 0.5629655493713792 0.5114168623938714
0.3795244368286168 0.5698741688263131 0.5095707921880677
0.4348049302169106 0.5310348843083313 0.3009196249102372
0.3196698338592712 0.5605726203795457 0.1649223290645953
0.0828382206965063 0.3273235227912762 0.1616833748243313
0.1955636755923546 0.3687396064240466 0.3076920352346472
0.2320135031032804 0.3302216667276666 0.5251772406475531
0.3865096615764703 0.3273308770304802 0.5093970506121351
0.4335960178770544 0.3736002445395529 0.2970692257340737
0.3161208565801364 0.3276142614283539 0.1721804549065758
0.3572865641035727 0.0677895946209365 0.7229317771148464
0.3164117852489964 0.0577113558944655 0.9102829476797734
0.2006986939048927 0.0501122165496739 0.0075690079059001
0.0900114016088463 0.0687560864222858 0.9018029567219416
0.1051163295899821 0.0608428486807162 0.7048701988315450
0.2293673930972218 0.0457257402604313 0.7641074598371040
0.3610650588261662 0.8270579551885607 0.7559476922070976
0.3055598925872152 0.8550413752257952 0.9285554255957377
0.1890816914505201 0.8536686998385208 0.0219220740112744
0.0856552425557939 0.8316410849357567 0.9036811451542908
0.1040905092264217 0.8393959179550704 0.7086874586106643
0.2299743824916311 0.8519044345904411 0.7664056008966335
0.3196594575421175 0.9497668729643785 0.7903250043576587
0.0830476115645993 0.9505177778294864 0.8134858281414623
0.4316849069708645 0.1272165749226382 0.5861049050979565
0.4127100934338069 0.9959299955093464 0.5739959975368368
0.3958473707087454 0.8632822167683185 0.5716770111429400
0.1995713957924441 0.1341600814489377 0.6223070863777340
0.1916395530235288 0.0033555934553541 0.5832847350900390
0.1972922142908752 0.8692546345615793 0.5738456631617447
0.9873081322818484 0.0424392550642648 0.7811150189063230
0.9840183750373802 0.8629149944830542 0.7868725026501128
0.1418550556851226 0.9332792329181585 0.2243648176104365
0.1840129211793652 0.9418083968224029 0.4106026088007347
0.2986632488929810 0.9444910329156796 0.5111263141683724
0.4086489879790830 0.9285021079856222 0.4035471235733039
0.3951652504842514 0.9390476640920520 0.2066362219305192
0.2702837126358939 0.9551975717421860 0.2635143416946806
0.1403893277890177 0.1739507796848494 0.2504520604295112
0.1916631472314460 0.1480429672879142 0.4265500136593162
0.3101769943784937 0.1471053290127572 0.5136750412129036
0.4161351382544205 0.1689219151568992 0.3987503709135599
0.3952315992286110 0.1552365604742645 0.2046334986597241
0.2704182749483837 0.1481250637502635 0.2675228403060796
0.1800173264311104 0.0508790609006875 0.2921401154720393
0.4185907598160307 0.0476017401861676 0.3180254180306241
0.0662530780963906 0.8727827122184098 0.0906604549666852
0.0856928250794467 0.0034802320687111 0.0741010667902612
0.1062294527268347 0.1351848215893995 0.0677255100424806
0.3017493962512408 0.8641943598663916 0.1252495749198058
0.3090571175181649 0.9943836006991477 0.0818869039448250

Structure files (CONTCAR) involved in this work:

0.2986364684210868	0.1281177096340421	0.0740521241743805
0.5127613463437052	0.9540359596258644	0.2857518876993363
0.5161337177110973	0.1348755513736537	0.2790555263299290
0.6420516030544343	0.5689202973761598	0.2719466635254823
0.6776239297679919	0.5686080748692317	0.0817433431596956
0.7936993090398522	0.5477204346370298	0.9907557402516610
0.9121219884822070	0.5615917291563235	0.0781252733520406
0.8909298566907955	0.5634449919546332	0.2782681602571708
0.7672625638596966	0.5493422549824866	0.2210039437742271
0.6385398805206967	0.3338763604300333	0.2493398204792919
0.7212842114810062	0.3410729403405348	0.1013432177664096
0.8118120275558982	0.3550129957062024	0.9603517070546349
0.9125044483236212	0.3334822151249963	0.0898370193254319
0.9035307967780039	0.3387287677176176	0.2895644147521551
0.7631109228589019	0.3758439604101937	0.2843919500697315
0.6765644457278213	0.4534900989093682	0.1858421869024963
0.9145087852192244	0.4498479674185727	0.1806993603260072
0.5667639332365438	0.6272868939806586	0.4087175329782416
0.5942739621588632	0.4982369770611819	0.4264939964771043
0.5960327578643793	0.3641602490498311	0.4333686900284822
0.7978308065889809	0.6310609014208356	0.3737629295012536
0.8039576866116229	0.4994539454345243	0.3958535928086523
0.8259609074669283	0.3721919619887978	0.4649622856351424
0.0097315004968381	0.5430829435855142	0.2106456801981136
0.0178172106600350	0.3684346818271909	0.1994287715331091
0.8696788515604116	0.4244890102305957	0.7396513650761268
0.8151329956491379	0.4632438459668475	0.5831974011834461
0.7024152375769315	0.4341243207484549	0.4869523307344643
0.5938554051494632	0.4329787980238807	0.5995277690773078
0.5986215510849145	0.4337516626256200	0.7979761594406006
0.7275585223217768	0.4377634048758006	0.7538229536959902
0.8631490336731225	0.6804379226103804	0.7363863033020177
0.8062638625757997	0.6392040943201485	0.5702443031717336
0.6878393568438849	0.6438069683512158	0.4838347603724920
0.5812685648466893	0.6648441173860337	0.5979399844371928
0.6054713440260865	0.6617002850763291	0.7928091033498342
0.7295764047206456	0.6696110001030827	0.7237643479787176
0.8067769567320192	0.5613929853307330	0.7355651163935328
0.5846244559269215	0.5482863864376668	0.6943581817011512
0.9347012234466772	0.3701466985644219	0.8989091095560056
0.8989072276165605	0.4985624725666474	0.9016608664536834
0.8869519271210135	0.6316364053878079	0.9188340707223783
0.6836312872638028	0.3700634837397217	0.9140073526354489
0.6801171970852163	0.5032525986148287	0.9120285697585677
0.7070394287325821	0.6339470267483218	0.9151070470483649
0.4858157867235391	0.4591740829269420	0.7103567654618316
0.4843798343375103	0.6349507820478929	0.7241530857425107
0.6430240182815583	0.9336993110331027	0.2844632012857891
0.6896116049157760	0.9372111008814829	0.0999137698100841
0.8009959904884287	0.9542296102737905	0.9922908735810448
0.9067793689961037	0.9282232405581943	0.1060222610696399
0.8949953280105549	0.9445635583442695	0.3033475478102230
0.7706137567208939	0.9610811659653073	0.2508875974836184

Structure files (CONTCAR) involved in this work:

0.6407783741576453	0.1742736001896563	0.2467634093283169
0.6949497865461810	0.1472271919942505	0.0736513394813467
0.8114792779986146	0.1461372778676886	0.9813453325950704
0.9156520885097761	0.1705047754184885	0.0983219716209633
0.8958033540549748	0.1578762348496373	0.2934153851300736
0.7707218760594845	0.1434295558774148	0.2367233402190546
0.6768053011822792	0.0504090346927006	0.2065603454443671
0.9186341123917291	0.0494642665610459	0.1819957450954095
0.5684990544241535	0.8741019649248061	0.4204013586061258
0.5846196590529616	0.0058373256893855	0.4316186902308971
0.6039629634610046	0.1380164128191994	0.4302376060312287
0.8029989541267024	0.8625442634700747	0.3785637296512981
0.8081422687329964	0.9883958439755347	0.4387006543307758
0.8057109892907861	0.1226910580481751	0.4270294303138792
0.0117549971335429	0.9562656825579718	0.2215079994984286
0.0160219866799156	0.1373017288763291	0.2167922741167580
0.8566764833198159	0.0616579511433052	0.7854313917218364
0.8109692125854958	0.0633173304114408	0.6006174968507784
0.7000946466149982	0.0547793094358061	0.4909717725205787
0.5916642406913567	0.0757658140099161	0.6008669106363710
0.6047168967280727	0.0583126288845756	0.7982250954807008
0.7290675005867849	0.0354215955317805	0.7496770396345898
0.8595380835950025	0.8265904884129743	0.7537605252714578
0.8092706840613587	0.8452106059009460	0.5753415918830083
0.6914782397149657	0.8512725872355438	0.4857910514344287
0.5874528724017760	0.8300279924724479	0.6057438197872764
0.6053855049492989	0.8530287581969458	0.7991282820952937
0.7298345254318147	0.8528661432383301	0.7337223606910269
0.8221062599138754	0.9474688976363855	0.7003256075746567
0.5810678506544436	0.9544135726715849	0.6754691857604592
0.9340858955626508	0.1259630717973404	0.9126526606879004
0.9195448497599114	0.9949249232084545	0.9344317029510933
0.8939681290643109	0.8643030283770879	0.9368004010378033
0.6992391660290554	0.1350667551711119	0.8765152607529421
0.6868422153380713	0.0086935629552320	0.9349590257445702
0.7042212691541655	0.8758938649366270	0.9275994685187137
0.4875962359280848	0.0464072915961735	0.7180771447351502
0.4851805317523698	0.8667388042604338	0.7206631002055092
0.3579425821827213	0.4296739316724025	0.7221924635007867
0.3177105871873189	0.4387546476921688	0.9092235857381611
0.2028413204179911	0.4544643098489173	0.0057683600759407
0.0959436497855950	0.4284530867442726	0.8941516535131255
0.1087703690346872	0.4493909169140247	0.6964698204052078
0.2310678286041263	0.4556674363426900	0.7626882040011512
0.3583678422335161	0.6723516569512640	0.7478815716731800
0.3047042402707238	0.6478305100988576	0.9219705841558353
0.1890026885657053	0.6464877010509026	0.0161785809117920
0.0854962444108933	0.6730452897371118	0.8987237914937172
0.1035591446938264	0.6570596817974255	0.7045357962128768
0.2294011058040820	0.6405789248318114	0.7586531350333408
0.3236651463167659	0.5486075034850896	0.7930334973815469
0.0818799596806962	0.5509035733015962	0.8218712735330941
0.4322093964099540	0.3747023556712580	0.5806915467013065

Structure files (CONTCAR) involved in this work:

0.4039063883986899 0.5041900983292090 0.5707197666957452
0.4012157816599737 0.6378864505760060 0.5673529301314012
0.1986546539529089 0.3668341398055497 0.6213603159346982
0.2034150403627830 0.4963575151506183 0.5766876788069539
0.1934547922624403 0.6305104530090043 0.5662667395392801
0.9927649103181915 0.4558347197037047 0.7750174191206046
0.9839556469125129 0.6368968120993618 0.7822016980956421
0.1405234283094591 0.5635435342303777 0.2171054236124520
0.1820633571688983 0.5569603893556389 0.4044080928345278
0.2994868328010509 0.5675361088568406 0.4950343950732513
0.4149248077778660 0.5717723381054024 0.4013139834415476
0.3958066850519697 0.5627881366334592 0.2058659602987528
0.2695530818786452 0.5452457478947489 0.2579869834960504
0.1386144906010724 0.3264241613144502 0.2498262977729864
0.1906526582297478 0.3520240426651307 0.4259179129887342
0.3094694035475118 0.3538134244957039 0.5137321864360619
0.4128471323293582 0.3305304817036034 0.3952314926048980
0.3932734482507978 0.3447685965251450 0.2005868385337911
0.2695622988274305 0.3482335764130602 0.2675537180853400
0.1815779630751945 0.4478662234577200 0.2880417814833297
0.4149929361038178 0.4522603980372561 0.3149499896933206
0.0665152554312885 0.6252212540784705 0.0821189989916633
0.0841289984544844 0.4936201195596863 0.0659601020869424
0.1136116899102414 0.3625290994651035 0.0617108564145654
0.3022677140338483 0.6333438339489961 0.1176121599076174
0.3143901283125158 0.5018091119520461 0.0815127045934817
0.2942697445191257 0.3689607148972252 0.0729935576251655
0.5142663231707729 0.5395461432035440 0.2807254519923554
0.5129944069128424 0.3654095910046787 0.2769586885760247
0.4410066840174630 0.7507362457914728 0.6479563256912413
0.1944689626875894 0.7487325005881044 0.6519772763542344
0.2722526402332727 0.7498336329579004 0.0403912172018449
0.1078783588719056 0.7497703124482122 0.0554426797726719
0.0632778132273377 0.2502127621712898 0.1356721850952164
0.3074805624603403 0.2485889192543911 0.1474237456859367
0.2271018092349940 0.2502701841181285 0.5428924022358473
0.3915153081278737 0.2506349017954704 0.5493721260990425
0.5600047462049099 0.2508688748011879 0.3520769219630662
0.8038796228979017 0.2455545084755558 0.3588022400102304
0.7291144084284658 0.2504223391633071 0.9573839663223561
0.8926412804913573 0.2489009018051261 0.9419085812387853
0.9363984477643256 0.7491006574729958 0.8649996654722240
0.6878170938658338 0.7565941287374132 0.8589783922070920
0.7720988720414129 0.7459704018395519 0.4570456756719388
0.6079156700941182 0.7495938958258208 0.4517540068750617
0.8254325448896837 0.3281678121301780 0.3420490208556460
0.7975539080892488 0.4778108801715653 0.7141952727116185
0.8817485571028997 0.3943487534213300 0.5922363080895073
0.9496856977722237 0.3588301523258075 0.5831914512548976

Figure S1 Mn/ZSM-5

1.0000000000000000
20.0219993591000005 0.0000000000000000 0.0000000000000000
0.0000000000000000 19.8990001678000006 0.0000000000000000

Structure files (CONTCAR) involved in this work:

```
0.0000000000000000 0.0000000000000000 13.3830003737999998
Si O Al C Mo
94 192 2 2 4
Direct
0.4236882982128091 0.0572890417265526 0.6509802815660809
0.3060258975753334 0.0294188671986075 0.7969349981040565
0.2810209771346244 0.0597435781119435 0.0188893422734555
0.1208043541403034 0.0669946809794368 0.0151647267950513
0.0658106205874458 0.0319492926751955 0.8046031048878237
0.1808379394706887 0.0624561905691111 0.6690354920785270
0.4178458908454785 0.8276580615606938 0.6676580986391090
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0.1155357047830179 0.8270582294630204 0.0144367943468895
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0.3186125710054011 0.9395967036421946 0.1687839207879918
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0.9325247757779107 0.5350519679173328 0.1911996885814252
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0.6121179858629886 0.6730086653146412 0.4889994270542983
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0.6759658964514064 0.6733903003545324 0.8314126187454520
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Structure files (CONTCAR) involved in this work:

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0.8184854559342785	0.9425017296624628	0.3320357460309789
0.5815041950481051	0.1741668425887933	0.3316575071069814
0.6956495073559376	0.1331637975767515	0.1915054572001434
0.7329034273775121	0.1690608733785477	0.9745812189327289
0.8876496844743915	0.1724983490838058	0.9881631313548410
0.9360902437165650	0.1260355662605637	0.2006480939457744
0.8175148228078579	0.1739612988280496	0.3228951112895280
0.9191142849247993	0.0579328084932223	0.8493347553452040
0.8063426973164686	0.0345634286271610	0.6977710364038262
0.7815283057148454	0.0624895724831578	0.4786199590662285
0.6227914163822862	0.0655050577574851	0.4882693128756292
0.5686369871144983	0.0316747591321845	0.6988097056659982
0.6848252403868177	0.0615966517794915	0.8313559877572095
0.9230384309494097	0.8265082175503087	0.8283701350306444
0.7661736723174448	0.8281876220045580	0.4680654642717010
0.6133312181800010	0.8270769297374169	0.4901255272174261
0.5622807499853846	0.8743866642225954	0.6990777524657191
0.6732537500894179	0.8293735651686149	0.8357647545001212
0.4220454591245748	0.4427611488883550	0.6494189088111947
0.3044102996731391	0.4706029420559630	0.7948627117115415
0.2812397662584472	0.4396214577545624	0.0172940137867094
0.1208172636132296	0.4331326904072358	0.0131019309419221
0.0671844341097943	0.4693779609813219	0.7997007387999494
0.1806759546828098	0.4376977534839552	0.6651659346811176
0.4179019266022360	0.6738565536568139	0.6667925716810970
0.3017587556651443	0.6303403335850762	0.8060763678042455
0.2706347850753500	0.6702765910059069	0.0262494551213533
0.1171193997550005	0.6726161520067577	0.0111586493211735
0.0680869245008555	0.6266823912321889	0.8002448368059131
0.1823136395918693	0.6723663462213146	0.6703486818906869
0.0778898008402450	0.5588988128479188	0.1478631656661762
0.1940609360785014	0.5315358022902046	0.2946719629936023
0.2180992826286531	0.5582647774459291	0.5173940616499429
0.3781871036684564	0.5658720125715645	0.5116427053176406
0.4342527563787438	0.5298172992243297	0.3018961283574523
0.3193059555656442	0.5603532623838183	0.1654220373627042
0.0788210870722010	0.3277199727427006	0.1703984654031946
0.1967609254290927	0.3720761246499252	0.3062441379342138
0.2332125912292032	0.3300661789529087	0.5234960963831119
0.3878979049894078	0.3266041771475630	0.5135725019270987
0.4370213962055111	0.3717794221451710	0.3018424858036485
0.3193799014740332	0.3288919656941107	0.1723147619905359
0.3589206176747878	0.0658413302424704	0.7231028109357536
0.3165052811380931	0.0568000310646831	0.9099183704329392
0.2006383125146129	0.0561131644851149	0.0069642309406395
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Structure files (CONTCAR) involved in this work:

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0.1075676213334401 0.8434574182396929 0.7064565018153135
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0.3183173923698424 0.9488068452636630 0.7893717625706409
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0.4333496046943016 0.1261062939872630 0.5870363472861225
0.4156338563998064 0.9945593707183334 0.5741675576462725
0.3877004989276691 0.8634864984049642 0.5680433014801932
0.1984279494313671 0.1358980829062792 0.6236074134835377
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0.9863313902650925 0.0404420528840905 0.7860405501066360
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0.1400123046420373 0.1736565777431307 0.2548609725738113
0.1943506666849524 0.1433907404139846 0.4273024594967472
0.3109926436338017 0.1463022966675783 0.5192628582322588
0.4148736930170933 0.1698516925227289 0.4011886522714587
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0.2705765487531993 0.1478975105305670 0.2655135684790053
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0.4191781795880303 0.0488897653755077 0.3195612741294012
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0.0880211846785021 0.0040491741644792 0.0749428583224700
0.1041261872304070 0.1368893361141875 0.0719625253984284
0.3040157806041660 0.8649258666447489 0.1253727210589456
0.3054968866847310 0.9952354196668892 0.0827758378961879
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0.6435653745142614 0.5653034109738274 0.2830681582120063
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0.7957114138837552 0.5549549914227551 0.9967832529091578
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0.9146273778591573 0.3312577240791086 0.1004627005793187
0.8940909782216857 0.3527063260056696 0.2936190004584442
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Structure files (CONTCAR) involved in this work:

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0.0150575132945555	0.3673823584582561	0.2176496408533477
0.8580995025002376	0.4303247495182740	0.7768299821635567
0.8142649033537822	0.4364540861560692	0.5920454735437319
0.7003304974317681	0.4520202259798789	0.4908322725146200
0.5917224437323326	0.4278018199872969	0.6010043181821846
0.6041947768777036	0.4404292933776547	0.7980606276966513
0.7289203801241082	0.4524994717747071	0.7394408243779409
0.8731187583438007	0.6735081591287452	0.7280713675183808
0.8110482968697106	0.6543314155379983	0.5612975444096292
0.6890272822987779	0.6456024219176515	0.4873203000845355
0.5828552781920135	0.6687782097500521	0.6013606001423952
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0.5802669815244786	0.5478910099608402	0.6826064964426068
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0.6974141951663111	0.3632203166465275	0.8773771080038945
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0.4871201564844403	0.4549636514421396	0.7186366869707653
0.4808435244585962	0.6343835322982325	0.7160978862110132
0.6442281332383720	0.9358486694459022	0.2824471190081225
0.6811578471268626	0.9514425396112094	0.0932069090695741
0.7967628319856188	0.9353149921726337	0.0010107991593436
0.9126636651269994	0.9288495195861060	0.0950973906380881
0.8952961995964011	0.9355731113787211	0.2923765841679931
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0.6393889759267095	0.1780080606930355	0.2470050667860446
0.6910564890058746	0.1446648621104637	0.0721533059875821
0.8106585875814309	0.1458209674931606	0.9861647155194307
0.9160701357649332	0.1683302896937026	0.1015682154843046
0.8945328911427960	0.1546572245861889	0.2959152513611691
0.7703887476110226	0.1545983736830745	0.2276334625545904
0.6798409111495843	0.0554437203774238	0.2197614396442978
0.9186704271599980	0.0468840232925115	0.1848908521383744
0.5689197402645987	0.8734288660740234	0.4156412442433342
0.5840984510637561	0.0047800679923587	0.4316143010826798
0.6087321656910811	0.1358276817621940	0.4305844444220809
0.7983743907337530	0.8692503296484315	0.3751829521828491
0.8147758774350069	0.0001537750167942	0.4171277244711054
0.7935531234311474	0.1331552831903352	0.4210961395705022
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0.8580516582710789	0.0726478519573298	0.7733985336106107
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0.5941429615406250	0.0730167619235548	0.6009966637925955

Structure files (CONTCAR) involved in this work:

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0.6904239147671709	0.8541332935517933	0.4891864894983666
0.5851464537232307	0.8300778677958788	0.6030996114034379
0.5964286560902271	0.8454719357150580	0.7999211560529343
0.7239772337680972	0.8489571298838439	0.7474088475800094
0.8190619879340317	0.9554756579601174	0.6985995928169387
0.5827954444242768	0.9522742073737348	0.6795084690411569
0.9326604410969708	0.1252468926215708	0.9156821347053156
0.9034229174193785	0.9958201030883053	0.9244637458393410
0.8961402002539125	0.8622485188988324	0.9295016070354074
0.6990390849013346	0.1357574079588134	0.8769192504275047
0.7013391457729947	0.0053023816559049	0.9152024623186422
0.6875260108689344	0.8723188268894174	0.9374672628240349
0.4896519166363117	0.0454208182865233	0.7186319880554731
0.4815012296118064	0.8689310691679223	0.7103615557269635
0.3566927219217900	0.4341630079388612	0.7202626255448092
0.3153471650498357	0.4428259446220873	0.9073730165646922
0.2007794938396530	0.4435795735588124	0.0082200405252637
0.0906644261395848	0.4319808815893665	0.9011336315502901
0.1037614694801619	0.4362503879333052	0.7033067844164993
0.2282905746356252	0.4542218606832703	0.7606144609714670
0.3558564511973740	0.6743877989769529	0.7454406992310928
0.3073596563669022	0.6486656248267924	0.9231584837649989
0.1932710012215143	0.6452812126225925	0.0212064095270153
0.0960629019699355	0.6695209207765028	0.8937063503499755
0.1004548706506978	0.6624904204603839	0.6965269933870373
0.2260428327750091	0.6486521499727002	0.7659689210121018
0.3164718708483036	0.5513318101512926	0.7883025216741046
0.0903397058189353	0.5486681510990711	0.8050626243805727
0.4326232405090847	0.3741225833151658	0.5855925206411344
0.4139768861110181	0.5054546273289171	0.5725862607143813
0.3931617298826742	0.6375657697846303	0.5644811672167941
0.1987765480844588	0.3644913427817242	0.6202930363809928
0.1888122014775189	0.4955461640277404	0.5803996541551503
0.1979491376228185	0.6290068238624587	0.5713189891792841
0.9874383003617523	0.4607506970596278	0.7847490128042507
0.9880211282359208	0.6305518378763760	0.7941491070076498
0.1414570705747576	0.5693958576597649	0.2216694713486803
0.1837025510073280	0.5589349485954745	0.4078378480637950
0.2982773136952410	0.5517303922236098	0.5092226003553814
0.4074998049629164	0.5702558152995812	0.3993740946412070
0.3959215104071933	0.5562373274628992	0.2027456718432002
0.2701432666719864	0.5480512553710860	0.2605982608681263
0.1395438726194667	0.3287920905358351	0.2505559087150544
0.1939310071897427	0.3551791644568028	0.4243166176846601
0.3109072411183635	0.3532516889233493	0.5157865755723202
0.4154079248932561	0.3291213256318284	0.3999380671335753
0.3963109485784387	0.3428722043550196	0.2056192277988545
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0.1809913252750950	0.4511836216604727	0.2879434676794598

Structure files (CONTCAR) involved in this work:

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0.1026174401301813	0.3621883187240919	0.0660312846328284
0.3071915672407065	0.6349039510885934	0.1200482581812080
0.3065547379527143	0.5041478023292734	0.0802543531880761
0.3030911042869227	0.3698316344696516	0.0703215568874916
0.5128693980523510	0.5443056402289337	0.2827839172674900
0.5166079257039862	0.3634843834988727	0.2825836621771174
0.4377665702204832	0.7507974115990128	0.6400881188567953
0.1923386130817573	0.7507616049467545	0.6434794262559393
0.2745109170949313	0.7503200419438939	0.0419480001674304
0.1107633741122493	0.7493128931115021	0.0505332845048160
0.0596370607369805	0.2502060533505920	0.1470205876233759
0.3079197091395404	0.2498602293212096	0.1493570167450970
0.2272996039304001	0.2498310963981863	0.5363867897556569
0.3922150614832815	0.2499904497959200	0.5543178601201854
0.5614391124244338	0.2501837960575493	0.3636999986242811
0.8116375514045386	0.2533032955938344	0.3463981476949008
0.7288651647960485	0.2492420947466928	0.9613814000870323
0.8925387147807294	0.2497408163768725	0.9494783165907779
0.9423968187588275	0.7493062922388536	0.8583753883813480
0.6785196894132728	0.7509931774632809	0.8682591347724795
0.7653543344797809	0.7498179775400712	0.4366625383267977
0.6088595343500370	0.7502175663495972	0.4505281428597878
0.7988442646148007	0.6302597878363236	0.6880433548326839
0.7983277338465410	0.8719855031163311	0.6948967246955711
0.0209784241327557	0.8100920585392299	0.5215288756675009
0.9818327391673400	0.6898328921337102	0.4505852425695104
0.9597544012390506	0.7797187762652028	0.4161690297446280
0.0318252218236619	0.7206000160443096	0.5703868892187216
0.9146093351701716	0.8065562008673218	0.5710167539480574
0.9176249325383423	0.7007778325334688	0.5852274498071088

Figure S1 La/ZSM-5

1.00000000000000

20.0219993591000005 0.0000000000000000 0.0000000000000000

0.0000000000000000 19.8990001678000006 0.0000000000000000

0.0000000000000000 0.0000000000000000 13.3830003737999998

Si Al O La H

95 1 194 1 2

Direct

0.4219298022682870 0.0576416925868555 0.6495056956248796

0.3060773151120852 0.0303083967152425 0.7979258631110954

0.2801973415574439 0.0624300153129417 0.0181864321664942

0.1200149777357238 0.0680562569268514 0.0115569709127587

0.0659099768395656 0.0309809627638235 0.8002850961503186

0.1825758068372066 0.0604915842844504 0.6671347204426796

0.4196128572698731 0.8268209916815580 0.6687143110055033

0.3033322468594869 0.8708295737760274 0.8081212696648484

0.2667837735434307 0.8307139824812882 0.0255338678028357

0.1123886699208982 0.8283545627506382 0.0114670196330126

0.0635354329643885 0.8732115737545786 0.7993347776237519

0.1815612302060054 0.8291310718091113 0.6734831721680881

Structure files (CONTCAR) involved in this work:

0.0782463802832655	0.9433186549796347	0.1493354637224631
0.1939138120269085	0.9702349503817269	0.2971036467927064
0.2191034853713921	0.9397384147848497	0.5180558094461959
0.3792768896017373	0.9338578559310088	0.5108915794360133
0.4339154590418771	0.9698748795965370	0.2995919484915857
0.3172064860065565	0.9410304650477290	0.1663345491364299
0.0793380421628493	0.1740372651821453	0.1702505050318395
0.1958335193398284	0.1293749264830090	0.3085413713995850
0.2329624894144477	0.1696471201148804	0.5257739657907189
0.3874130787531270	0.1728542536783732	0.5127998700063329
0.4361688180642004	0.1283651271718778	0.2998416081719423
0.3174530016957762	0.1724272277522879	0.1745149894647776
0.5750567251081248	0.5580493816329288	0.3463345590951663
0.6916216560245217	0.5282184864506493	0.1990631733607358
0.7183234614805331	0.5599391914946330	0.9801819539103019
0.8775360479409267	0.5666598116263365	0.9817346415261757
0.9320100118202278	0.5346909464621838	0.1887536751554079
0.8173335293953246	0.5568311661540275	0.3277036536247606
0.5823207518136434	0.3277064392566055	0.3290115342992763
0.6961211461026121	0.3702463756328828	0.1873572106552277
0.7336946906864662	0.3280171014014514	0.9692219808463611
0.8878607827717981	0.3234948867425550	0.9831735454207126
0.8148979335012778	0.3322755491627307	0.3302454200072996
0.9212770127174666	0.4411635813716696	0.8490033290904470
0.8048996355341483	0.4716902452448820	0.7031730824411487
0.7778129272327874	0.4418707358176260	0.4807552890250414
0.6199843151242608	0.4374144962038210	0.4845072302851683
0.5661123811198732	0.4691788598959712	0.6968529759313673
0.6807945751833749	0.4396206432074576	0.8338878252285032
0.9182369637242299	0.6729758362421150	0.8211345380978903
0.8036880152470337	0.6301213885569871	0.6846593108302769
0.7633128218338491	0.6672086290520741	0.4676405870568183
0.6090988676964610	0.6729569460734114	0.4838872402635026
0.5628214699925044	0.6273891483106341	0.6976986712788672
0.6827672027272901	0.6715146358466328	0.8221003931644305
0.5776627517665891	0.9430166358423467	0.3491193732700569
0.6951473954955134	0.9708359140559764	0.2035356536618529
0.7193966299444270	0.9387770899383073	0.9818917404232594
0.8798728805105067	0.9318947263238725	0.9874339733501850
0.9337161493311665	0.9689928141507467	0.1988514850771071
0.8188080671918425	0.9395477426963700	0.3350971924922016
0.5806276624395438	0.1742103455287387	0.3282391926908121
0.6959826877827932	0.1303249229264952	0.1871185821385211
0.7329019322507548	0.1682994030974596	0.9697655003642632
0.8872880631685326	0.1713708075490061	0.9818036899700336
0.8174509670718105	0.1732122931467418	0.3205807531331570
0.9213956106470114	0.0547342896207623	0.8469311841038096
0.8051754637071818	0.0286571280542457	0.6968196798714550
0.7807509399728698	0.0617839265021106	0.4783349425465556
0.6207918387827284	0.0665420908264712	0.4857456499889917
0.5666590717266748	0.0307047420376068	0.6966799854243649
0.6827660796647729	0.0578244092504251	0.8312411343784546
0.9199868975445221	0.8265742523616135	0.8293868878843454

Structure files (CONTCAR) involved in this work:

0.8029047350991888	0.8694002598579278	0.6876345580413460
0.7660589034635088	0.8264961818015648	0.4709122408521540
0.6114900515265036	0.8267777505461554	0.4849750571200218
0.5635774105979890	0.8726073875801276	0.6975304240394111
0.6815234473527607	0.8295909485120420	0.8254882201704816
0.4217271758376542	0.4428139980309429	0.6478635392121280
0.3049653530048269	0.4711203489905610	0.7952652088635404
0.2794574443907306	0.4381661974270076	0.0157097886824316
0.1183577769197618	0.4337246704192948	0.0125046263584988
0.0650540667307615	0.4681776137220733	0.8001092196475833
0.1810013708494657	0.4399165659763887	0.6644908096722646
0.4192897883530448	0.6728881944215325	0.6697557410301014
0.3032451400854365	0.6302747379689175	0.8098156131518285
0.2659921218681894	0.6707844764590564	0.0259934741827142
0.1115803081800422	0.6742722143503159	0.0109359574773636
0.0626349479256339	0.6264255158206181	0.7992726425945104
0.1815548621157334	0.6712451320933039	0.6752521618787310
0.0775139976740052	0.5599073694236550	0.1484093289891798
0.1923208642750669	0.5306317191896891	0.2975943114056380
0.2183619457599872	0.5604697619277935	0.5183693368971851
0.3785290161770660	0.5659571871616585	0.5105190231025774
0.4314683254122720	0.5313106244597701	0.2985305272042842
0.3147598789576597	0.5591307186176619	0.1637637784639083
0.0783681802899611	0.3282845763232086	0.1758724522970008
0.1977191336006699	0.3722095892308535	0.3081590634351096
0.2332329805871773	0.3299134760080055	0.5254635670962120
0.3877191236577514	0.3268132534619793	0.5130102010110812
0.4375791513832438	0.3732530646229267	0.3016925561185803
0.3197793821198622	0.3307482485032099	0.1747071601871490
0.9358222280145879	0.1273413106687666	0.1956735051344518
0.9322676119932261	0.3734955443136813	0.1945299882467506
0.3577864830072860	0.0669593051943480	0.7223248392900309
0.3164992054309710	0.0597842374563988	0.9097553659110343
0.2000267475366483	0.0571414133481847	0.0050721504523277
0.0883170745274126	0.0712155279295762	0.9004034082146192
0.1054526274805818	0.0600590974948520	0.7037240451076926
0.2297089496581630	0.0453716826939241	0.7636010638457623
0.3588547915441616	0.8274862610954349	0.7486898499684569
0.3074322638120127	0.8512920905347674	0.9252605831658427
0.1894257117678051	0.8548033280415265	0.0139236489063054
0.0842770169968253	0.8311114369673799	0.8982739677934355
0.1040199874888849	0.8430013580426684	0.7038053622446939
0.2289828659657253	0.8535801205219659	0.7658469515178733
0.3200420098605570	0.9499461283119454	0.7933077003482043
0.0828695030786590	0.9516570002184234	0.8156603876637684
0.4324389928038005	0.1265464318906599	0.5861902987894801
0.4126131202566829	0.9957676947525058	0.5718037098223778
0.3967891367221609	0.8634129469430584	0.5658323710693944
0.1994564800490119	0.1342515436700493	0.6223911650120125
0.1932123495258737	0.0035503301544783	0.5821640340913219
0.1994985708070810	0.8695342565259766	0.5718463036345245
0.9869594043889809	0.0419243509662611	0.7781692898022127
0.9838059254635155	0.8651076484137159	0.7798931517906140

Structure files (CONTCAR) involved in this work:

0.1426923095073495	0.9330276984556943	0.2213930733108522
0.1831388091445410	0.9418331431985381	0.4093938661243794
0.2993364240955280	0.9449608582761018	0.5056212965924179
0.4100568555118312	0.9301700473489010	0.3993184939120771
0.3944755862040202	0.9417898341147288	0.2023013538526747
0.2704327388615748	0.9550106792882532	0.2635886845676819
0.1398447541173523	0.1730978639478560	0.2508752351558278
0.1922862896416281	0.1474236242493905	0.4263043082068760
0.3105069343037247	0.1460530146665730	0.5147911751081720
0.4154903261813900	0.1697319632720442	0.3995570196672120
0.3949231901052804	0.1584130970559263	0.2049643701614783
0.2700527621229629	0.1471912560327669	0.2662995336202281
0.1794989281028478	0.0504412493507910	0.2913100805700909
0.4184297207723658	0.0494591567387152	0.3150698012956025
0.0674622805211084	0.8750601107681161	0.0845280022213707
0.0873135577926121	0.0060969548854657	0.0732167809191442
0.1029495200689306	0.1386652762217557	0.0666067211184206
0.3007028716000195	0.8675697201702233	0.1205780539351576
0.3058430450808650	0.9987854939880673	0.0829307601972942
0.2997583839843672	0.1328376562491022	0.0719175581977569
0.5127476166477587	0.9564506112414692	0.2792994764409175
0.5155817641536670	0.1375722868353511	0.2794278433025829
0.6409905256025238	0.5647607205707890	0.2766109713789615
0.6834417077847311	0.5626303623242916	0.0898179022276022
0.7983432822175669	0.5509523583814100	0.9915997739081394
0.9109152604401954	0.5785523000137376	0.0905450593616656
0.8930258362301525	0.5637925182323271	0.2870006821198343
0.7683660273771582	0.5369874022874451	0.2356213727175865
0.6409586137754280	0.3255427019054306	0.2457665813352713
0.6952482390875980	0.3481917041446511	0.0715170155039702
0.8110233961570604	0.3515421351275412	0.9764086013799339
0.9137817776337536	0.3222563845644650	0.0961472512953955
0.8924216173225008	0.3539845323176526	0.3108175849663675
0.7699671452728877	0.3576909111775112	0.2354363921928183
0.6740663291108320	0.4485647852420100	0.1966959413001423
0.9162376756541230	0.4569144983442398	0.1711452365372604
0.5647397217037181	0.6273409044289373	0.4086331770707198
0.5800875269304722	0.4959926178758339	0.4251315609279340
0.6092541144533756	0.3658137012985659	0.4288067923752171
0.7944613576462534	0.6287714028863196	0.3722255978543650
0.8156384149900845	0.4980931334730820	0.4129563975778919
0.7894674183544542	0.3676104762724707	0.4334914411426953
0.0112048249603969	0.5460020490278956	0.2141354864956343
0.0170298825467597	0.3640408251845278	0.2365033598994791
0.8568123570751193	0.4331635190505902	0.7759820678911277
0.8129533054830688	0.4430876972421098	0.5901060747025619
0.6986304523402170	0.4582537260567992	0.4873469693606788
0.5908551919916805	0.4300625889831217	0.5967716231589305
0.6042737923053974	0.4398269252600313	0.7942432119851770
0.7287491753038275	0.4580652044999797	0.7394319709059769
0.8613435731524224	0.6760835081218239	0.7348279050472357
0.8050518654390226	0.6443521681457954	0.5657767745380156
0.6856699882112764	0.6455075844168746	0.4829144170042918

Structure files (CONTCAR) involved in this work:

0.5802915046851258	0.6688094859582591	0.5966931322937286
0.6052656485107298	0.6580903261476319	0.7908224337097427
0.7303197871322624	0.6492276153624289	0.7287733823865287
0.8207081969121075	0.5517789173966061	0.7073654887411208
0.5819075160262344	0.5488053459410799	0.6824399204213430
0.9325850607373104	0.3720102876976193	0.9108771043164449
0.9134364176952169	0.5040574852747099	0.9254986846167687
0.8882655656052663	0.6354540624264043	0.9187264368213750
0.6977182699248303	0.3652731887618537	0.8757718082026065
0.6887212870200295	0.4952617021154871	0.9214859803423612
0.7012902404905583	0.6292721235755613	0.9218270742408726
0.4870285671961593	0.4566759294523865	0.7163043349342151
0.4833496554064594	0.6353456408761357	0.7203914855369647
0.6428606363082751	0.9343764658699245	0.2784445156374342
0.6853758579166145	0.9410760882048693	0.0918637773114427
0.7999057497031751	0.9433096863466586	0.9905132855300716
0.9096017960600888	0.9289706014639100	0.0996029817267045
0.8955668023414693	0.9398109947677774	0.2966121016868851
0.7710401868122081	0.9553912750632123	0.2395290282460328
0.6398535202291368	0.1735695759750783	0.2457666891491793
0.6911150382186736	0.1465153895132816	0.0688079248635277
0.8101997982429067	0.1445832895085199	0.9833426673277562
0.9171613933236071	0.1673951262065851	0.0941575613667250
0.8947872324825763	0.1593536468245329	0.2893707684774339
0.7700673063581160	0.1507006501450853	0.2272103812606369
0.6814939537315524	0.0512141974605549	0.2072956182523353
0.9169552135399658	0.0483405545974459	0.1838085104203350
0.5668761663705842	0.8741663414502431	0.4124325990524017
0.5849183715654817	0.0050285433881233	0.4271104357743865
0.6043265868053552	0.1369369085331234	0.4300593307017143
0.8019733541209990	0.8657636371985322	0.3797415406978761
0.8098485258885757	0.9964915178637733	0.4205757166630671
0.7989200461129404	0.1308089682618991	0.4203053413533344
0.0128787102423883	0.9566609542706854	0.2179769124506584
0.0153166256964289	0.1351452591430506	0.2180918509584902
0.8563796391332787	0.0624289508828759	0.7757273191798366
0.8142021363176176	0.0646044826080801	0.5888666856472579
0.7004899053716710	0.0534403364788066	0.4877651787779665
0.5914795333762025	0.0714388645183288	0.5982676829231574
0.6054505500209341	0.0574200045583655	0.7952752088389644
0.7289033434252135	0.0394959112437058	0.7349530197802785
0.8584043471948577	0.8290800263856380	0.7512971996598391
0.8054891549341140	0.8418498108432885	0.5740876121961239
0.6889940193030003	0.8517558413641420	0.4816833934154147
0.5842346802324726	0.8300861572915381	0.5987854704914305
0.6042111171082252	0.8433032954706485	0.7934678487867162
0.7290128015273369	0.8564166237754461	0.7347426933692384
0.8207990225170833	0.9488067761590728	0.6893856851297694
0.5816225202349612	0.9511676029279525	0.6794217192930793
0.9315693311816018	0.1239075775810118	0.9088723512524457
0.9140034322349680	0.9929140085742406	0.9253907416278939
0.8980573816669096	0.8608801036689623	0.9344405449544073
0.7006566007733314	0.1320422128919231	0.8727344212743635

Structure files (CONTCAR) involved in this work:

0.6927728198777072	0.0028345972605173	0.9190631291977075
0.6981422259829433	0.8688223921477147	0.9286565268418882
0.4877943374865931	0.0439850989400330	0.7168752725433117
0.4839740989754043	0.8642268373702110	0.7182142503099008
0.3566568446630746	0.4350290005212739	0.7191423053028945
0.3139305941157919	0.4395227270423798	0.9060026567385614
0.1989778340724194	0.4382128990117953	0.0070036419845009
0.0882905874833457	0.4288512950783608	0.9005442216520079
0.1044077463552555	0.4386315287006859	0.7034096760578609
0.2286736526995709	0.4577982977027959	0.7591146725158686
0.3584457634467599	0.6735452409755526	0.7496202010093931
0.3079330012741716	0.6493346505352300	0.9271398059159738
0.1886108954284011	0.6476556866017159	0.0111956294696052
0.0817176813850479	0.6687944214242779	0.8988132156855461
0.1039644196954626	0.6572699516748481	0.7049985181050646
0.2286779801125533	0.6475829547893046	0.7683655740831822
0.3199406047971632	0.5512467144741635	0.7941436992538723
0.0815140479855618	0.5477235681802269	0.8143701522216552
0.4322967350175848	0.3728507531030413	0.5873467167144202
0.4140317181925592	0.5035490181999978	0.5676344330027318
0.3962414256110875	0.6356783340955726	0.5673617963056448
0.1990286247798593	0.3660325013260361	0.6209487665958592
0.1891428586754450	0.4956695058019358	0.5770926701301247
0.1997197906199792	0.6299149889084962	0.5745879086064483
0.9863885532784074	0.4546557030773258	0.7789868171339767
0.9832132421127961	0.6335943046508216	0.7770905080987723
0.1410098681180951	0.5681873218652082	0.2229669736350998
0.1843367391484262	0.5622520581704643	0.4083868446349807
0.2986595800126318	0.5531631157714704	0.5095444388360912
0.4064716551901614	0.5717950707402233	0.3972619069214194
0.3919604527555466	0.5570385047885316	0.1998361055312120
0.2687362375215865	0.5412991035635100	0.2604546833123343
0.1438871448269773	0.3270940296565759	0.2482219554219363
0.1925811584829533	0.3518546590933427	0.4252963762427094
0.3106516353466594	0.3535581179352223	0.5139525099533340
0.4167481408733388	0.3308294828367397	0.4003630355767505
0.3974000397302688	0.3426353067713607	0.2061287937408506
0.2725765673823322	0.3591318179417001	0.2654974941540277
0.1752952372953197	0.4504596197476592	0.2971869831609567
0.4178873754878589	0.4516536428381836	0.3171918805660535
0.0673805822192413	0.6293861434422684	0.0869930741842287
0.0894866115215030	0.4996981645371167	0.0686830183054266
0.0956436872455535	0.3667520382212540	0.0721695459394571
0.2975745607017929	0.6338729029310812	0.1230487539776246
0.3028149922360002	0.5048916965173945	0.0754658633881741
0.3038875294396101	0.3703607185553349	0.0718060907615069
0.5099036497642729	0.5459744858798293	0.2765632536103776
0.5173592565879742	0.3660359932790175	0.2826324836620832
0.4384092628572812	0.7497319516455172	0.6418638704298157
0.1933342757112684	0.7500530028503634	0.6513107683779004
0.2711035913162835	0.7507590741257339	0.0444110399208105
0.1081619425210842	0.7513126447204218	0.0497443341922846
0.0599696349328617	0.2513859824424391	0.1468509307940190

Structure files (CONTCAR) involved in this work:

0.3053579099840306 0.2518393918742830 0.1551581238239651
0.2282177096910947 0.2499029229192229 0.5418114509011811
0.3912371552574043 0.2498343781481712 0.5520178307035362
0.5626558100797663 0.2511423857060514 0.3581119555107645
0.8065378011472044 0.2520045848074332 0.3454460743023644
0.7276410281300304 0.2480844971172614 0.9511174876434623
0.8908098474928097 0.2472278938756883 0.9383328102933119
0.9390029770194821 0.7489093797312758 0.8520271666287647
0.6939999584922685 0.7504241859190242 0.8463335012245643
0.7690577283582595 0.7469883957027020 0.4470365484854548
0.6054271285517848 0.7500589476220717 0.4453622637330162
1.0122274513814009 0.5030394984296646 0.4639139791901734
0.9934846576269970 0.3394367557617690 0.5477464917625372
0.9897522072712324 0.4033833550512052 0.4231651900691902
1.0171859386771320 0.5514686529712417 0.4685174483198648
0.9991892054233106 0.3315290206534960 0.6188192914265594

Figure S1 Cu/ZSM-5

1.0000000000000000

20.0219993591000005 0.0000000000000000 0.0000000000000000

0.0000000000000000 19.8990001678000006 0.0000000000000000

0.0000000000000000 0.0000000000000000 13.3830003737999998

Si O Al Cu

94 195 2 3

Direct

0.4221100861772452 0.0570840773755619 0.6481110242077338
0.3071196902934430 0.0290892073232167 0.7970399045202718
0.2797782741081543 0.0594425004544600 0.0169994110815814
0.1202062683276934 0.0647430526995510 0.0110500400707017
0.0662120236247910 0.0285849150514717 0.8000191527669503
0.1831074944641996 0.0588521895417179 0.6658229048472236
0.4204955820390457 0.8268446087379149 0.6700313857617911
0.3054995566355753 0.8703490186226346 0.8101158233286931
0.2696889122158583 0.8292959424617674 0.0293952234739594
0.1157449763190070 0.8260221490555161 0.0179135522365579
0.0670978208747512 0.8690086486733370 0.8041462896274300
0.1840957426358592 0.8286529738143329 0.6745416556124446
0.0778571734066742 0.9416291585203581 0.1501561198757763
0.1947208709399444 0.9695883411918980 0.2966354797622718
0.2192922510525850 0.9392858891748948 0.5172276478774203
0.3790006950670999 0.9322246033348200 0.5126163582298723
0.4342062042546652 0.9688388832865089 0.3031443590992094
0.3192216790435592 0.9399573853157529 0.1657517889355890
0.0816001210207864 0.1721447833753054 0.1693152249925861
0.1965780868205045 0.1289469365615373 0.3106506860772247
0.2325092087543045 0.1699819491491929 0.5270946620613405
0.3871051390512564 0.1727663321154830 0.5105280487743349
0.4358535291462532 0.1264807364050252 0.2999720116584678
0.3171368938521961 0.1696640056446929 0.1748322518193435
0.5787004879619884 0.5584224033805409 0.3483447846405541
0.6941170517239859 0.5281391968116873 0.2046721587424993
0.7178422371419622 0.5506399710687609 0.9791114068960790
0.8753825820891211 0.5633522465232040 0.9881828228729085
0.9318477116937244 0.5292643473105098 0.1992070389836946

Structure files (CONTCAR) involved in this work:

0.8169949987032638	0.5591058811241542	0.3347495452418425
0.5805611004206876	0.3263668837504222	0.3261530104392825
0.6965447309188217	0.3704717410213723	0.1920913597975089
0.7341002062775163	0.3287846983483984	0.9761934013740509
0.8883904497507162	0.3291017528869311	0.9907874198742352
0.9365285920218550	0.3713373120104553	0.2022308880193871
0.8179157051196208	0.3301860503155872	0.3293085410993291
0.9243537258018552	0.4441129298397504	0.8520585930978231
0.8077909623042241	0.4698984389111326	0.7065502936901706
0.7800763674305079	0.4402754343620630	0.4868222041157379
0.6207488204314472	0.4329873142965345	0.4861970542866649
0.5644038545558206	0.4641763354556450	0.6968887863998044
0.6810265456359601	0.4338427954152637	0.8301375058703340
0.8012557748041625	0.6277221247685296	0.6894393933397069
0.7659175926621336	0.6677638331475625	0.4705856493042990
0.6114195039685433	0.6722515885719882	0.4854945836195745
0.5639727446949822	0.6224308966667579	0.6985147088201051
0.6797505851196993	0.6675587154174881	0.8239507049496774
0.5791011772608934	0.9413007294651620	0.3490325241332184
0.6934849457970851	0.9722849580939023	0.2024818973329741
0.7187645691318977	0.9503719160278834	0.9802245134261627
0.8775524924022472	0.9486609983024047	0.9854917355901579
0.9338746165457412	0.9691221193571993	0.1977018240786044
0.8158691436671527	0.9345474589973543	0.3255900464775281
0.5803866875200421	0.1733300482285065	0.3216226475933859
0.6974738616038276	0.1296368235064725	0.1885578540176746
0.7369837889938072	0.1671905070857098	0.9721614341930900
0.8922627410997048	0.1751762362855609	0.9776178700158175
0.9383758806432226	0.1275933153919636	0.1940252189552923
0.8195797502617761	0.1740243099343580	0.3203201203704421
0.9230412143515416	0.0645285162129342	0.8405349555040633
0.8085781391235611	0.0293989173404401	0.6931683551266727
0.7827230916175459	0.0583168647346837	0.4727053874269495
0.6230676929426940	0.0676904951030298	0.4813436484522751
0.5668422087529190	0.0345700277586744	0.6916282583847596
0.6846650669792612	0.0640041613999435	0.8204043872266860
0.9158480823591263	0.8315504312804023	0.8333559723087082
0.8060635535759082	0.8702244502501145	0.6864331506617029
0.7679327666264788	0.8287325881399890	0.4725672196887128
0.6127659776591796	0.8273451988012787	0.4905172073577005
0.5641507451089353	0.8763639947235823	0.7020968522862392
0.4208992742485003	0.4413936483488977	0.6516603992979079
0.3060575958731135	0.4705481895265557	0.7986199951502322
0.2814271510392963	0.4392521103026267	0.0201721338261110
0.1211514669940639	0.4333958260271318	0.0133280361095560
0.0678578922205816	0.4694407224360410	0.8011626914699154
0.1833323369463549	0.4407988759832583	0.6670766190777486
0.4203776349827995	0.6727986378827066	0.6707251003481143
0.3068662665465238	0.6291171771328743	0.8118851815563755
0.2689230469141451	0.6689615828407178	0.0289803759473055
0.1148901706510528	0.6722194040897698	0.0127771803722057
0.0668275175958571	0.6286325087402388	0.7984011596629720
0.1870498455891444	0.6709119657707536	0.6739967183534863

Structure files (CONTCAR) involved in this work:

0.0771923942540240	0.5576817796450547	0.1489971706764391
0.1930391606643004	0.5297180423834741	0.2978102566694720
0.2211105324971474	0.5599865787043742	0.5173271365560030
0.3797772775567920	0.5655653297973386	0.5136594881076630
0.4347807202515154	0.5303705545438359	0.3034391853282067
0.3182376758091814	0.5595770315336588	0.1687252134955411
0.0805654736820590	0.3258965648628590	0.1705955698460417
0.1962689568566742	0.3704393993028933	0.3097434010486141
0.2334567743821562	0.3300129366468569	0.5265210192461088
0.3881870186359250	0.3262339013967096	0.5127598106059256
0.4370083225747305	0.3725797767434054	0.3012468242219263
0.3182861035600323	0.3281984773162224	0.1753880109863749
0.3578301074893249	0.0665267132401143	0.7207919526564021
0.3157401792922975	0.0605211723357132	0.9082058679080611
0.1997474071926422	0.0514919975140847	0.0036987016515007
0.0880914330871963	0.0689694263302917	0.9002340861786902
0.1063345560596746	0.0573824676881523	0.7040296179636062
0.2305224892846122	0.0408159762485330	0.7607928767175559
0.3607918799640579	0.8257487843326852	0.7523353053296111
0.3073817253000218	0.8513349724341388	0.9274941635282509
0.1920547074359265	0.8535473759022357	0.0260023720978490
0.0926766140663195	0.8294650800371409	0.9023702155478397
0.1064464796628938	0.8405126266362308	0.7067093566577124
0.2311731455863910	0.8548528321606877	0.7661359820551111
0.3237439431378530	0.9492304211946059	0.7956639998523980
0.0808093734332668	0.9489596648265285	0.8167931563933524
0.4316692361021845	0.1248244361280731	0.5818356422922105
0.4141674238494827	0.9932502774120235	0.5734612405163620
0.3934030752547484	0.8609999915211166	0.5672468429916340
0.2003478237780836	0.1333708360536361	0.6240007576447779
0.1916939655106742	0.0040822994316873	0.5774511352983414
0.1997613639385441	0.8698065129720810	0.5728228895400750
0.9875730334250019	0.0410758598269374	0.7765460063837938
0.9880780364467919	0.8540327029052740	0.7906590414870428
0.1426524218098141	0.9331990395437461	0.2215090532217771
0.1847041686273258	0.9388944114947532	0.4076186990838338
0.2994705598487035	0.9462600812025580	0.5072940939913334
0.4093384871752916	0.9273735202611382	0.4007026205377692
0.3958869779897916	0.9436438574544288	0.2033609191500310
0.2708294103478963	0.9551992826452578	0.2607578955962433
0.1417991558643507	0.1725748990571182	0.2500774062061494
0.1911728422678083	0.1479637544682467	0.4279340147352386
0.3099257114540331	0.1469137635806592	0.5131054350821874
0.4149753085340804	0.1708504095527440	0.3968339339060419
0.3945531232490264	0.1531625392005730	0.2028977325226953
0.2710713721456917	0.1467805813257234	0.2695726343793610
0.1803536276122754	0.0499057546571548	0.2940491088680501
0.4190110804517865	0.0481696526187204	0.3223415885827690
0.0677403602697897	0.8722179930732308	0.0875365971634025
0.0856586019441120	0.0035498706302576	0.0721226924432047
0.1052962836269730	0.1355376491984671	0.0668014152224617
0.3061302871644584	0.8647182037480577	0.1236232104137478
0.3073632551684820	0.9950824603211624	0.0784199142390503

Structure files (CONTCAR) involved in this work:

0.2963324923459951	0.1292827158294888	0.0742940365421950
0.5128094832718353	0.9550560578903179	0.2826991058090633
0.5151015969416083	0.1349703189870519	0.2771326148245596
0.6423179735045115	0.5694606764598966	0.2742144572982816
0.6859889597484766	0.5544313317931304	0.0899878744112720
0.7977507348045216	0.5394230103052230	0.9795760772549870
0.9022138830883686	0.5679835473127587	0.1016138861875438
0.8943151205905138	0.5547069995291392	0.2995395592419017
0.7706791056031599	0.5412766247491039	0.2381325234537647
0.6405249118946679	0.3242666491331589	0.2448325386269118
0.6939853377423008	0.3561015790155100	0.0732713745540786
0.8110688765113732	0.3541847114616594	0.9858176462514525
0.9141454346521997	0.3276268622980811	0.1054749659423269
0.8954174461425408	0.3448118757926224	0.2992916966680191
0.7705685467771402	0.3535835592636796	0.2358860627808152
0.6773372298445705	0.4486123824903866	0.2131233538722736
0.9190269340932019	0.4496324046886254	0.1810806069878301
0.5652413178566835	0.6267839519001104	0.4117630373765421
0.5913489900759593	0.4965576790658671	0.4247910130121062
0.6064732646169176	0.3634760475055200	0.4268649217242655
0.8013284037032180	0.6346027278849700	0.3732661170893058
0.8033598825578020	0.5053052244206503	0.4231416898303604
0.7994007726544751	0.3712110232615072	0.4298850861654639
0.0102972979069288	0.5458550064213668	0.2150588167978353
0.0161114914444074	0.3626096447965478	0.2214092660681282
0.8590227960274029	0.4324960376345544	0.7823792847364534
0.8181334754693506	0.4414144956555004	0.5940257453892537
0.7000394004063931	0.4435034339523188	0.5035300027103943
0.5831790049741424	0.4271087042506694	0.5927635259151756
0.6055865393432051	0.4298199662564657	0.7879013872539822
0.7312947473802702	0.4538986257939266	0.7400443918539211
0.8521117600926170	0.6779004999184903	0.7419123056720198
0.8015216426277617	0.6380193655541756	0.5696149270428477
0.6877575819251948	0.6457705851605496	0.4738994770470691
0.5876016283974033	0.6639447895206075	0.6006477539209473
0.6021993798058273	0.6520357515175556	0.7972372190771461
0.7251623111505674	0.6399807973051771	0.7328577975712426
0.8217535031741975	0.5499638430365918	0.7138278316238547
0.5829144391412273	0.5435157096538172	0.6869913157174791
0.9341660201135963	0.3789532949923943	0.9238403634439365
0.9185796665928709	0.5103887773064917	0.9232239616359950
0.8894429660406118	0.6373846269708852	0.9371201255583590
0.7006520403854213	0.3615259797539991	0.8771762329989313
0.6823105607281892	0.4924355719583163	0.9155885944761616
0.6989979749452110	0.6256606059501758	0.9308853317747515
0.4858487038397895	0.4535512492710754	0.7220934289856626
0.4842391702349665	0.6313450492468996	0.7142606902093915
0.6417045408907214	0.9317209160310757	0.2729319448761197
0.6787587940830365	0.9565511169439801	0.0853715618613541
0.7980682570327542	0.9628096087539053	0.0006943084908744
0.9125285238234131	0.9345665319903594	0.0922150927117947
0.8931851585355076	0.9355970030145403	0.2896604907659877
0.7693025016340247	0.9480017629154228	0.2272323294354253

Structure files (CONTCAR) involved in this work:

0.6375404627090997	0.1744804655192075	0.2351079120478435
0.6972068186152637	0.1358891184787389	0.0676164029325551
0.8156337247524236	0.1472519824979908	0.9798625830138835
0.9247582894199555	0.1629902589115852	0.0867835570379994
0.8960886627994519	0.1652990510199628	0.2814339510196654
0.7699162083669372	0.1553461533131457	0.2279100731998028
0.6853247680429574	0.0523597406169405	0.2237324297098182
0.9168596924259937	0.0489855206819839	0.1910729187658579
0.5687862502519455	0.8738202502441991	0.4152627257719252
0.5905037149535037	0.0045261065269704	0.4230876005472317
0.6081923882270783	0.1369032602295396	0.4215119174105151
0.7990630617314846	0.8613317327814007	0.3715726530450796
0.8032668845483453	0.9930555556994488	0.4074619200584364
0.8052004343763544	0.1267942311383491	0.4163088966050675
0.0124682346897502	0.9553170913969450	0.2188499765246580
0.0176171503195399	0.1339331654308358	0.2188156356912637
0.8589644250631068	0.0691453988605451	0.7674192642424104
0.8209333941485309	0.0551540374013943	0.5795992339854988
0.7029261907940280	0.0573346664958294	0.4912484618727040
0.5886658534805181	0.0738816804416537	0.5902197818815421
0.6077436369474075	0.0675323719584394	0.7844854089435571
0.7321814007299408	0.0478732391912634	0.7249941480572232
0.8660834879624980	0.8273256264758210	0.7389649612598919
0.8107307066743832	0.8555425699964695	0.5670593354772633
0.6903162655038102	0.8517263075671473	0.4841679659074550
0.5860655252245773	0.8324278524803372	0.6040423004394634
0.6011098437122281	0.8502782410316991	0.8009467882569029
0.7349431796842615	0.8502100380211538	0.7313990722547042
0.8228505072900980	0.9497923568151685	0.7050835465457808
0.5822198155812424	0.9550701244719498	0.6788258570561868
0.9351558850464842	0.1376974084321423	0.8910064320553061
0.9118781059130409	0.0130964156842846	0.9335440905933989
0.8873220249753518	0.8836038191200902	0.9150910437193538
0.7052905897768363	0.1350155880118817	0.8714936784279970
0.6902314014835507	0.0029090005072450	0.9006279098492430
0.7100640232360148	0.8724880649467707	0.9408771942093551
0.4883131730051933	0.0469911506677097	0.7159989185314256
0.4831882967612079	0.8687197434346086	0.7145740912826628
0.3557230190712357	0.4318683893215335	0.7221775775491954
0.3157113264857394	0.4407045137332456	0.9103027051422660
0.2010489057878327	0.4453312589364247	0.0113336211368320
0.0923439756315065	0.4296816597358533	0.9007231862054884
0.1062182991618523	0.4403069509739893	0.7035169584384023
0.2292796931480402	0.4582230100357677	0.7640900423604094
0.3632009938403946	0.6736592609765504	0.7563480176492006
0.3094876321166890	0.6459233850988966	0.9299445912219398
0.1914716805393819	0.6448860037050174	0.0194692982711776
0.0900816788374519	0.6699139106150429	0.8980286384402799
0.1100364523871920	0.6554761042313613	0.7030628841654798
0.2334130541612924	0.6473307547646497	0.7679384617636420
0.3235480866330537	0.5501827601227236	0.7938002892463348
0.0824293746107739	0.5490251432895302	0.8163381284371616
0.4316722097274064	0.3729932517740521	0.5875309794281404

Structure files (CONTCAR) involved in this work:

0.4142684886354227 0.5048173680367659 0.5759816399756281
0.3920446231656876 0.6367565798627194 0.5700839244927890
0.2021656129626293 0.3672450886191296 0.6233658232774143
0.1926057252662877 0.4973932439845600 0.5814664928623940
0.2071366590227831 0.6309688125822502 0.5726316380704433
0.9891486857676414 0.4541724677120416 0.7814818107828395
0.9894703450095170 0.6424134870193761 0.7769978698000797
0.1406486289804459 0.5666133803801070 0.2233380837387322
0.1836109837831164 0.5595574787493489 0.4096471108638183
0.3008060410778252 0.5500205200685220 0.5023339697853338
0.4134933046533724 0.5706628514296560 0.4039556641293195
0.3948756118354626 0.5590511356263661 0.2072793642732185
0.2694036986037080 0.5439182559703114 0.2628714428580751
0.1411361872046250 0.3262295958733666 0.2508036749961603
0.1921795539359116 0.3520946424061144 0.4273978190600827
0.3110793811926236 0.3522747174789118 0.5119615000484103
0.4185387409022701 0.3301349014208088 0.4008133037961717
0.3955926088811255 0.3423896796096323 0.2067860652712642
0.2705588904473306 0.3528756398409799 0.2673162719723490
0.1788594581721108 0.4493285891839927 0.2933852532017651
0.4181260827298270 0.4510042242046663 0.3191059120437761
0.0675908840064269 0.6257309476936674 0.0832837732813362
0.0861092416304044 0.4946206948089127 0.0735860757542301
0.1031597501291006 0.3629601119025986 0.0680442225035677
0.3027029318024096 0.6339062022370164 0.1255371304436401
0.3091200002269255 0.5031315276023454 0.0826022943630342
0.3010637158581166 0.3688858470429505 0.0736347607431990
0.5135907856212526 0.5421097495449528 0.2804994371494114
0.5164944036084559 0.3652939207127157 0.2784359016435669
0.4411377225551460 0.7495710674832496 0.6446847623246263
0.1980047378194339 0.7501193639539947 0.6516997018701450
0.2737768839285860 0.7490872404917841 0.0442423215089036
0.1101673318949171 0.7486494765135214 0.0549485933767598
0.0618782267616418 0.2490083695241075 0.1423842220447200
0.3070661980204850 0.2490675677117868 0.1528269204853240
0.2273240728429156 0.2500622970044444 0.5446383967776530
0.3921102110591918 0.2492541912208131 0.5518508496315756
0.5607129267992310 0.2495818940721772 0.3526825883012129
0.8069923334835911 0.2512648707447605 0.3537943190001551
0.7287049942602803 0.2480301884460574 0.9683898913709392
0.8937678652103326 0.2537400599374005 0.9470716748246135
0.9199380955082767 0.7564313607734675 0.8874417079875632
0.6924351831221743 0.7433554668135605 0.8601022779432298
0.7733505810962041 0.7480695891284455 0.4632010612433376
0.6053845099429079 0.7501236931772048 0.4526974687855346
0.7991275645654209 0.6733839374312137 0.0706400961312347
0.6977335141898221 0.7707374009115381 0.1035512238211973
0.8426368811286159 0.7947741182899750 0.0660330248270098
0.9179145933952826 0.6761373187840377 0.8229438573307227
0.6824712530239907 0.8290243181844886 0.8285830631373570
0.7148672067011418 0.6984255005516176 0.0331201040566643
0.7602116644318225 0.8210851592653462 0.0419402717917671
0.8618446520546490 0.7192833847611864 -0.0003029737494619

Structure files (CONTCAR) involved in this work:**Figure S2 Zn/ZSM-5**

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1.0000000000000000
20.0219993591000005 0.0000000000000000 0.0000000000000000
0.0000000000000000 19.8990001678000006 0.0000000000000000
0.0000000000000000 0.0000000000000000 13.3830003737999998
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```
Si O Al Zn C H
94 193 2 2 1 4
```

Direct

```
0.4224458171259045 0.0598811629060307 0.6487600775535682
0.3046167748326454 0.0318778581904624 0.7915582376771724
0.2819552486557200 0.0563888791127738 0.0171417000128571
0.1221320593944171 0.0648666071429389 0.0130232371259851
0.0675160980837006 0.0321456477659723 0.8012365760452909
0.1799784441523400 0.0649574738005896 0.6642419775245969
0.4185601653453119 0.8275406411512662 0.6690178448692592
0.3007502155483834 0.8731921571451693 0.8005280902297685
0.2671279452152433 0.8305671589115775 0.0193557279183452
0.1112581016015568 0.8266095142553738 0.0117737002381517
0.0656382486123590 0.8748463423444264 0.7982339679315089
0.1788565625038530 0.8290372089928510 0.6645005784535343
0.0761378720298538 0.9416125340600914 0.1483020849880887
0.1949152048646496 0.9702836414034124 0.2902404368996940
0.2163902155991195 0.9436743951812261 0.5158337059287774
0.3766233948526079 0.9356021299453445 0.5137510205371356
0.4330801723715396 0.9681657258390288 0.3015142168359120
0.3198685778928692 0.9352296906694946 0.1642698247328411
0.0816990431461093 0.1737916850519809 0.1677616785347098
0.1989310850362713 0.1291053253458188 0.3007478077668395
0.2322260635886551 0.1699602697722824 0.5187337971893484
0.3881460918961110 0.1738867507038222 0.5092552078693942
0.4357031740492303 0.1265570819065900 0.2957420023621609
0.3199878899207178 0.1721480182974631 0.1656172034243468
0.5760670640280381 0.5553271269578772 0.3575694447656019
0.6891861916543647 0.5270555306451499 0.2010814130532594
0.7122720381103065 0.5693240402516224 0.9883372749575585
0.8727414854831466 0.5725669675867451 0.9878710498609848
0.9264378808980496 0.5320435144415896 0.1939152322449758
0.8100045332781818 0.5526450236303688 0.3377486951398581
0.5727908925282961 0.3287835857531576 0.3329887165218253
0.6941638773410119 0.3723748693016660 0.1943289379328093
0.7292931419338302 0.3271235921684124 0.9813976731095764
0.8838219659778872 0.3272653888247632 0.9974193741565429
0.9408936871006901 0.3785271365636405 0.1943421722912149
0.9185388225148685 0.4448462643945348 0.8605667630516081
0.7999453099916138 0.4736241359173832 0.7193520973676044
0.7724716081892709 0.4376932373962958 0.4931223176655095
0.6148423363819902 0.4288563306239439 0.4918776694283622
0.5680346822992703 0.4696347247910353 0.7045247515032784
0.6757293986016535 0.4477009418822746 0.8577243514257447
0.9203090999140002 0.6781820764488842 0.8329465028336429
0.7700689059793007 0.6687543343965956 0.4655593082334661
0.6147328507923930 0.6733074894344497 0.4877788609267810
0.5607868609162239 0.6278524635741860 0.6982511051011997
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Structure files (CONTCAR) involved in this work:

0.6733830835752102	0.6750142644883468	0.8249900099537868
0.5777181705202423	0.9453175291890474	0.3586725309247996
0.6983484895270280	0.9739980163004631	0.2156046356008687
0.7193256739239970	0.9383748686730584	0.9936390712946945
0.8792036596580175	0.9349779910112872	0.9952920341281981
0.9316740558718735	0.9697064869004137	0.2048274884397827
0.8224755854278527	0.9468069092770364	0.3552490263737411
0.5782704102955663	0.1736023169803147	0.3297528638988965
0.6982577525352696	0.1322792262680395	0.1942589485523172
0.7323971442163781	0.1713106374602802	0.9731974241005048
0.8872053452583657	0.1740135428356524	0.9872749091000870
0.9368528166643415	0.1272098430020989	0.1991701209664214
0.8214571879328716	0.1727077883158543	0.3312370782671934
0.9229491955380382	0.0557397540203368	0.8576473564906166
0.8025004043384527	0.0267637259404410	0.7111495598172297
0.7807631387781129	0.0662481298893312	0.4927427787920280
0.6205880393402694	0.0699333282151002	0.4904575795989672
0.5677905667181022	0.0323537054403005	0.6992668447986432
0.6785584192683700	0.0536738182411582	0.8495508424915741
0.9230975445153931	0.8304990489850681	0.8379059972681873
0.8034333636452473	0.8696809166922250	0.6966289302035449
0.7704290700478253	0.8270052967718584	0.4790769940135036
0.6153757091192844	0.8269771553140259	0.4907724457309754
0.5638403106282794	0.8752261083621349	0.6982100197223957
0.6788669051648739	0.8337629391382109	0.8328750264269473
0.4227640632979117	0.4422682642369864	0.6470802330637895
0.3046119665432059	0.4693949879372568	0.7894170681404731
0.2807962710240091	0.4455552170945865	0.0149154774213116
0.1225352171836604	0.4372388176421111	0.0148618400934026
0.0638224036706632	0.4682980680368516	0.8030842977491304
0.1778087146264582	0.4355163368735191	0.6659387100803826
0.4153413093621978	0.6736589033316065	0.6671523075308841
0.2996446083029980	0.6276962089426092	0.7998493503200805
0.2669450218734823	0.6693099853722586	0.0186680797672807
0.1113698727210419	0.6725897683344755	0.0100829914618785
0.0631757689608463	0.6273830436162697	0.7962156390199269
0.1783174373360907	0.6716350109875933	0.6643149410805904
0.0724963552556162	0.5590250277484543	0.1501285977381812
0.1920068534704455	0.5308779888887614	0.2909365848655554
0.2148576901693389	0.5560376903139641	0.5173779566645038
0.3738785092585530	0.5656963548513403	0.5147250224147086
0.4300677503960273	0.5319126972955672	0.3039312973951738
0.3184770664785219	0.5649958279210097	0.1643358756443263
0.0851720126097320	0.3270179989815176	0.1644646154738965
0.1990051621959452	0.3723388709333122	0.2999293006384818
0.2322944140355645	0.3311670672234612	0.5198650063836467
0.3873852320840783	0.3280648233284111	0.5080120878697940
0.4315004137612064	0.3742670838793813	0.2933467532701286
0.3178106000669771	0.3294711376760162	0.1609617078080348
0.3586872316479273	0.0706883427265268	0.7221041306818989
0.3156260923211747	0.0535453582550076	0.9069756878448274
0.2014879650390284	0.0494025575768546	0.0094626055476326
0.0925758619384709	0.0708677522768468	0.9010288452874633

Structure files (CONTCAR) involved in this work:

0.1033471321610477	0.0649327764302114	0.7038046550509520
0.2291352753939506	0.0524250525285765	0.7593358277503057
0.3600801328432937	0.8282325857816559	0.7529313780660019
0.3008103896627858	0.8625537766456759	0.9201312901250631
0.1885492423792883	0.8509087609789105	0.0224298744929357
0.0883283708090516	0.8324633434572419	0.8961505665947911
0.1022950858545286	0.8426626190977444	0.7006394359681423
0.2287230523504888	0.8505718513902423	0.7554637955671240
0.3152491984553834	0.9515968169702447	0.7748137975412277
0.0876282812956788	0.9530519471791763	0.8106960969460459
0.4333056967159479	0.1273064216316016	0.5820964699348750
0.4120500657339434	0.9964194209315878	0.5742944263718570
0.3924939000538714	0.8645519025039974	0.5681725192546310
0.1960747185298146	0.1380066180704134	0.6159811407602973
0.1890396204802016	0.0057251202632074	0.5823846419667618
0.1948493591893907	0.8721516183964937	0.5644434987063889
0.9875207009977629	0.0415118528137768	0.7874364396262976
0.9850871662060854	0.8701667903310124	0.7848577719678573
0.1407388749183767	0.9322118339564227	0.2202489727796078
0.1830634880242741	0.9490923759066590	0.4056571681257637
0.2969432073394174	0.9489141647257711	0.5085730031444413
0.4069868767155143	0.9312048281818832	0.4021214686432941
0.3962246046072835	0.9357317592185410	0.2047324663054439
0.2701351025888243	0.9484034207370655	0.2586054177781634
0.1408632830115195	0.1744530270223734	0.2504941085557491
0.1959218103728588	0.1394844288249146	0.4203954651316621
0.3107268100291805	0.1491251094934469	0.5165627299221072
0.4137257362399751	0.1680608933129761	0.3948637536576030
0.3969431074222527	0.1583628215595354	0.1995699977693590
0.2717962270071226	0.1525929052608674	0.2597116671371822
0.1854367070917462	0.0507754349881324	0.2733530380051761
0.4156166025329995	0.0479618133405779	0.3088595107813248
0.0652396811026250	0.8736256914877458	0.0828625169716730
0.0847095568149001	0.0046932313648043	0.0724522601037023
0.1073785812192085	0.1361441611389083	0.0674306150769652
0.3047171268341984	0.8619039886523225	0.1159916223982904
0.3107394542786679	0.9940917842883437	0.0817323231613685
0.3015188012188048	0.1276837212865800	0.0680312317306999
0.5126786866309487	0.9556977503555046	0.2879359836585351
0.5159301440345203	0.1331439478321457	0.2791390529971167
0.6397007854953145	0.5587922575345416	0.2836660557863411
0.6901332377951306	0.5763957950386853	0.1047543004512903
0.7928587055815086	0.5613481893229633	0.9764696285155381
0.8920843651445836	0.5765366136785559	0.1065593864328207
0.8870657093025471	0.5394065562180970	0.3014820065359558
0.7643231564220301	0.5267433178959706	0.2476383344420725
0.6402258884116705	0.3367511966192183	0.2682484919502599
0.6903265929261266	0.3335486403347474	0.0870933440701762
0.8065184891771651	0.3519115652035723	0.9947228158628647
0.9092360897633611	0.3265498303510910	0.1139544578421692
0.9071790275328340	0.3676268759903891	0.3060124301589155
0.7678194760881709	0.3693011628358178	0.2416436781048006
0.6698968313445874	0.4501405743726039	0.1746949215036224

Structure files (CONTCAR) involved in this work:

0.9236488220873014	0.4541753608489643	0.1577034847892236
0.5696215268274472	0.6271393846893929	0.4140443479233937
0.5849660358211608	0.4966456598774300	0.4412253087033378
0.5810121683718492	0.3625973743155697	0.4434009386756230
0.7995212172715753	0.6313095077973543	0.3659110345514947
0.7932291896643875	0.5118186208198878	0.4430212643052300
0.8202561359492080	0.3818250647988464	0.4425920678160153
0.0037452475306239	0.5525392921334245	0.2149027457100132
0.0206033289176020	0.3684377872895652	0.2053894567582901
0.8544426058641079	0.4337212298211668	0.7868818586908475
0.7889094898401581	0.4377597468600882	0.6112729189879573
0.6947863083272381	0.4248115138634390	0.4699682208696814
0.6011696876718489	0.4292504957242116	0.6108502905911948
0.6021509930404463	0.4441883262248965	0.8076017994050062
0.7284326641396106	0.4750459594239231	0.7745387147844482
0.8601024143603269	0.6811901582788806	0.7550845581863896
0.8153238616805396	0.6423587432310427	0.5611632656161873
0.6925178478873733	0.6476185611308907	0.4850274791700926
0.5857760367929785	0.6684639183555419	0.5999982566275648
0.5948683355470479	0.6615970152496899	0.7963260907915028
0.7198227978768372	0.6500754066585159	0.7337734542536936
0.8262235114816363	0.5498903701712976	0.6967088328380981
0.5816072470671187	0.5492637650118581	0.6875911385573019
0.9284666697605601	0.3785165954768601	0.9304816143289187
0.9097702484214238	0.5096359397198427	0.9334667023994356
0.8978158388875244	0.6420135871304709	0.9376712569269259
0.6945999605743154	0.3730322869353913	0.8959446121688828
0.6759188928549875	0.5011565814020784	0.9489436809795748
0.6885036204405495	0.6354913715303852	0.9291159231809374
0.4889928906416046	0.4533312855233973	0.7145309092818124
0.4800509518800169	0.6329299112378237	0.7082699748318646
0.6434946099955496	0.9401523577786222	0.2888069838710550
0.6984669096083209	0.9334534288902034	0.1104391602406807
0.7996351511279869	0.9473076757665737	0.9810329771801136
0.8984024353129598	0.9282703755898467	0.1126056411585097
0.8976537237189746	0.9484410351997141	0.3101259110267094
0.7716960617860096	0.9679033232965182	0.2660189451683337
0.6411118006069429	0.1737486972384161	0.2537969167935472
0.6960916076484622	0.1574006421336733	0.0792677958469667
0.8102169186420554	0.1480165534526989	0.9817527984004215
0.9140762020387214	0.1693711299938698	0.1011094017027006
0.8977739092368466	0.1534838645621903	0.2976355383382128
0.7712615561721989	0.1458333406135850	0.2428626259847775
0.6803364244402701	0.0526399189571976	0.1985347085827200
0.9200412902116213	0.0486700325784213	0.1805346481535750
0.5700212857264262	0.8754944076730951	0.4209219648879525
0.5819882788597113	0.0074746102869128	0.4373929357989113
0.5996626909451237	0.1396374726253313	0.4356141331363901
0.8081046197609041	0.8709798497213868	0.3945091658309394
0.8165503413153701	0.9993822423458525	0.4475091014603692
0.8047766854535467	0.1336693307559571	0.4356120120345182
0.0106405448724516	0.9533549558784244	0.2169791812764146
0.0167597512436828	0.1372131374169925	0.2160669976935807

Structure files (CONTCAR) involved in this work:

0.8570185561383923	0.0576974908352383	0.7876925443688947
0.8015599441698740	0.0718832503538138	0.6099450964451663
0.7003387784416759	0.0572392783461453	0.4809933635905494
0.5983504406418660	0.0758509755360990	0.6068205055524984
0.6035787436858797	0.0527962399621345	0.8036868645204791
0.7290860075750629	0.0283833279721861	0.7623476310761248
0.8594598304801693	0.8330579005184759	0.7637923051131494
0.8058794977235806	0.8349324636677764	0.5871499291771727
0.6929987535361661	0.8515323932259022	0.4863404387828822
0.5890195461687426	0.8290821159656048	0.6052931421892396
0.6029453970826708	0.8530832733451703	0.7993665972073600
0.7297807750043077	0.8597094338622071	0.7456813324935467
0.8206735248094290	0.9491071073502013	0.6854472762246928
0.5795105402358871	0.9534219922170806	0.6727995073982740
0.9321285377025106	0.1283005191862614	0.9124583808481717
0.9181109230924633	0.9979106301000087	0.9436025941372677
0.9027081309769400	0.8653569844282458	0.9433018415687044
0.6961501315596834	0.1295935409266988	0.8845374072309014
0.6824785968416549	0.0036181004656441	0.9453540457315981
0.6958485644088839	0.8697847387409041	0.9386931661939499
0.4888649026166263	0.0477114718195111	0.7154045614224458
0.4841392631658579	0.8646351348492942	0.7148575969184208
0.3590693981898738	0.4305646134049042	0.7204630896645554
0.3154748605288020	0.4491079851708548	0.9054946516028721
0.2007058693560637	0.4579055219204378	0.0067043197861949
0.0897247829022234	0.4327296904456475	0.9050018745134878
0.1018248078757082	0.4344414433646193	0.7082706479178071
0.2292031480454000	0.4476210827432254	0.7583418205697612
0.3581785194577805	0.6742039351882454	0.7532116370614119
0.3004349486394204	0.6367590864754433	0.9196886720780668
0.1885108534424447	0.6482029627586030	0.0224463563639503
0.0893816650053125	0.6678247707435148	0.8940466516578098
0.1014152100719059	0.6574311668622244	0.6982890012847633
0.2270635929766769	0.6500368143235846	0.7566384476586450
0.3145547516053995	0.5496957868504708	0.7713001181464634
0.0809419677240228	0.5480670893388506	0.8081320133120116
0.4338732243894441	0.3765252320867702	0.5765195193376016
0.4129968650258391	0.5075289894575405	0.5759456100763884
0.3851854862205855	0.6382747033039848	0.5672677758536366
0.1931521950568182	0.3631832413035667	0.6145975757086148
0.1847586443669371	0.4957987928528169	0.5850826805164289
0.1961854833938759	0.6287123869523015	0.5646099027887459
0.9841757492694896	0.4552004882301688	0.7909663830706322
0.9832224658154871	0.6369118758292416	0.7835278418417460
0.1350110723553399	0.5689860660042498	0.2258350597062915
0.1817632842014874	0.5507724873679507	0.4070981099998647
0.2951666302821607	0.5470247569276907	0.5100798130181019
0.4042715110229693	0.5706474276219495	0.4031136679184755
0.3942444484423504	0.5648478541780193	0.2069764728470673
0.2662939620158724	0.5536290217737871	0.2562358920199088
0.1404507147720864	0.3259576132951025	0.2528825021176999
0.1993558959826984	0.3618520884873959	0.4192729913079418
0.3104450379489094	0.3528324328553936	0.5220760040497083

Structure files (CONTCAR) involved in this work:

0.4085402021207827 0.3313626067461826 0.3910215458954198
0.3943649007830459 0.3459996992138699 0.1935930784819249
0.2709951384723581 0.3501051611221939 0.2557230421520984
0.1834577498555419 0.4503804716618518 0.2727461712180741
0.4115832190210682 0.4524608709663767 0.3122695232125494
0.0646323454404296 0.6244514580302578 0.0786145523842947
0.0824043454955330 0.4924086713011278 0.0814458418389066
0.1154528805414401 0.3633373917035811 0.0657210934835888
0.3049047819218487 0.6380658557457934 0.1148434078913638
0.3118182559188654 0.5048247960794896 0.0833647413551404
0.2964956537712595 0.3720844231787837 0.0625374165896346
0.5099913446832147 0.5415240925905422 0.2910763028428462
0.5113154716710540 0.3659236825047998 0.2751055826305375
0.4360958577233305 0.7502958248241072 0.6404575101450405
0.1887989531117995 0.7502904436668132 0.6371598742998046
0.2759399134065887 0.7498772214230343 0.0193584355367875
0.1029355715180600 0.7493727856147245 0.0483740526280272
0.0636442045558425 0.2508097795188107 0.1373671392368365
0.3095418462054909 0.2503763160170180 0.1350530140968544
0.2238075989770891 0.2506261599959885 0.5226044090608895
0.3952184459982604 0.2511759142441647 0.5461961835107942
0.5553129752685351 0.2503155407588054 0.3510339931735444
0.8156393112131113 0.2518517055591687 0.3473094872137423
0.7270179998910535 0.2499968926932823 0.9430772720186482
0.8920636707534939 0.2521305191864514 0.9522126007332403
0.9453459419607171 0.7538010447649057 0.8612394811098056
0.6851905649928014 0.7539156129655140 0.8494293465477725
0.7760560580282885 0.7485184757589778 0.4468460823468305
0.6100051592410978 0.7504570872270833 0.4494272376667325
0.9345257789171413 0.4961441199997338 0.5154811070071048
0.8219789999504314 0.3361262140795489 0.3286607504126735
0.7999803014921270 0.6360069555185035 0.6947132770923830
0.9173494666417596 0.4303201263064835 0.4238755886629733
0.8739783764424232 0.5573342237851051 0.5578430831854746
0.0547303013462752 0.4215657377229434 0.4453928870767143
0.1068981112327378 0.4271196672455062 0.4678171444943899
0.0504832853431623 0.4385420169187100 0.3675444748566434
0.0415769043880516 0.3680656992306410 0.4513233905825231
0.0249477329343364 0.4534225726444205 0.4956041011720345

Figure S2 Fe/ZSM-5

1.0000000000000000

20.0219993591000005 0.0000000000000000 0.0000000000000000

0.0000000000000000 19.8990001678000006 0.0000000000000000

0.0000000000000000 0.0000000000000000 13.3830003737999998

Si O Al Fe C H

94 193 2 2 1 4

Direct

0.4235487650649133 0.0565054356072345 0.6459751515240661

0.3063976853862824 0.0280401985454587 0.7919570041824218

0.2812013428588037 0.0613389231419744 0.0131069979123886

0.1206100719664116 0.0660547928983591 0.0092300269853825

0.0672732724649069 0.0314334379737227 0.7965556660550296

0.1823483326949196 0.0580637519708096 0.6590709292443405

Structure files (CONTCAR) involved in this work:

0.4186582930532850 0.8269574826341387 0.6650883803459096
0.3053207860195994 0.8694986883003365 0.8087174441813423
0.2680932652983389 0.8297444983770995 0.0263115245698016
0.1135677076477207 0.8266880256943226 0.0108456850026668
0.0659777743665851 0.8725326963388899 0.7971543441851061
0.1846112243577668 0.8285562286650877 0.6727778380287306
0.0793011546942173 0.9421814625389084 0.1467773944591777
0.1959490870333885 0.9699887834363535 0.2941497860834241
0.2197625739649396 0.9388654012952528 0.5136437503575002
0.3788484436475585 0.9339059209947722 0.5091643342786757
0.4347261226424473 0.9688704870174761 0.2989828733734919
0.3196500693293919 0.9422776321133677 0.1611165109037861
0.0817881297128606 0.1722009663835111 0.1687340406227233
0.1982530445644516 0.1284892756163226 0.3079645212980964
0.2351352304430112 0.1709857081991550 0.5243110692897729
0.3896810893597641 0.1729592557172309 0.5094825880327674
0.4381850524046216 0.1271951919345078 0.2978897163771565
0.3192743175090297 0.1694282228706160 0.1720668562196352
0.5784046399775581 0.5551102181731674 0.3537138230809967
0.6959743869843296 0.5277390468870170 0.2045328524015820
0.7189437459664656 0.5591619004083495 0.9870043750912824
0.8786365417839342 0.5692848260040507 0.9932085514022223
0.9350513488483843 0.5304141986587815 0.2026576982019982
0.8188323468707527 0.5567736196551623 0.3379411457187817
0.5801684403258154 0.3276543638611166 0.3377994942305370
0.6993986224971332 0.3688836849305524 0.1974541208255565
0.7320327987561567 0.3233622738986899 0.9812927142813354
0.8865083561813127 0.3291529510650946 0.9953077472764350
0.9371212944706382 0.3724447420185575 0.2055263031929760
0.8205767711132578 0.3307682741807520 0.3346431976087764
0.9231264020210906 0.4461736592383274 0.8569404375448112
0.8032534834996824 0.4694220633154426 0.7137730538235469
0.7799903356894025 0.4387324277480356 0.4894453670535300
0.6189050139597861 0.4332390688809638 0.4955074567890108
0.5664861988845789 0.4700420737133899 0.7092651625336781
0.6796325534299494 0.4362131726547248 0.8467014396605460
0.7992395939729501 0.6284855002170633 0.6918904544488332
0.7672495063906707 0.6670861559540135 0.4730269861554849
0.6115458444342277 0.6722242023096778 0.4865226082965188
0.5640631679149928 0.6288394620066816 0.7034575973611669
0.6811886264601392 0.6708189805877723 0.8272437585092108
0.5792126516587163 0.9415135123886662 0.3495331209193803
0.6953938650686498 0.9718084381403024 0.2043913899801628
0.7224851311502255 0.9410397276242651 0.9835515054185086
0.8804937770962118 0.9430797382037576 0.9862280529540893
0.9358828423180420 0.9684853232941826 0.1987482095139065
0.8189240441117831 0.9362082678487579 0.3303262756878573
0.5822145177213227 0.1737702029561246 0.3250159075652757
0.6980560792072036 0.1301793055009519 0.1895630144960304
0.7379096409999959 0.1645025315466434 0.9718277705474491
0.8927522935184463 0.1751490197844974 0.9833894484862724
0.9395723811562101 0.1270087018060176 0.1980100765987842
0.8200336935807524 0.1729628437565378 0.3224864246083812

Structure files (CONTCAR) involved in this work:

0.9238172140440808	0.0631100812468395	0.8440844666434446
0.8093575530795913	0.0299145497228973	0.6970292093950267
0.7833650937997624	0.0583446712271809	0.4764999512862714
0.6234832707167088	0.0662832550190741	0.4832513130872233
0.5676729299387250	0.0324169165105234	0.6932660473850262
0.6848312544567740	0.0553449001470135	0.8264553018452674
0.9188098773500947	0.8321783862950437	0.8257031894462782
0.8059565477154531	0.8729225104222360	0.6839555055361014
0.7691732112660851	0.8279114979414972	0.4714722114771498
0.6130135469785974	0.8260619947290190	0.4887625926267965
0.5628452816494164	0.8746071371614722	0.6990603771417426
0.4233625692409814	0.4420442673719098	0.6528075221665592
0.3062943789002781	0.4715529262044477	0.7974892968206713
0.2832791040620474	0.4389825074859642	0.0194669224983081
0.1228680552069961	0.4332458216184289	0.0156395255326716
0.0688700903857693	0.4671826658912734	0.8039480846902429
0.1825080587925569	0.4408952231560469	0.6663341151485326
0.4195482715570574	0.6735915070703969	0.6693182157235575
0.3061535730469377	0.6302374826367971	0.8115461390330075
0.2682317294691808	0.6701059796478261	0.0284073602997347
0.1138846990782993	0.6721526334978745	0.0103894505354968
0.0667036467504434	0.6250175076245109	0.7972076028618631
0.1860940098560970	0.6700945428383245	0.6736900943039841
0.0792024205848307	0.5580066027470556	0.1496257492688297
0.1955474789317355	0.5292457941434934	0.2963968622870624
0.2212961429859912	0.5590745224416939	0.5176788619142679
0.3804053550679709	0.5636007857656397	0.5135205098398244
0.4349108472439513	0.5303135029851244	0.3016835876097374
0.3200475351934722	0.5594132091622591	0.1658162721367532
0.0814457260810877	0.3259352702781629	0.1732526440963778
0.1975438937566693	0.3705048829966434	0.3107284299642866
0.2360668553805655	0.3305243322813273	0.5283016908312244
0.3908258216652605	0.3267972584568445	0.5156810037793178
0.4382066519547796	0.3723335322839237	0.3016599269722642
0.3195876381014254	0.3278829835833162	0.1757020904038472
0.3580385554599826	0.0647800775255798	0.7163833646922105
0.3127473914719368	0.0623606318258553	0.9014583742557265
0.2006047071653057	0.0545766798811113	0.0079503405717957
0.0916852259494555	0.0705068281510241	0.8965507280878624
0.1060923779351357	0.0604134006597821	0.6995195761604720
0.2302575086911854	0.0370836024778369	0.7521464768839833
0.3597477656957890	0.8254678388820629	0.7484101877751627
0.3087615563340871	0.8492199878848521	0.9256783353221900
0.1904785602586461	0.8530874237301854	0.0140426937989194
0.0858223500633198	0.8314031430619792	0.8973736897942527
0.1067428205591338	0.8424214454043832	0.7021589377421097
0.2305528698761377	0.8538269583164773	0.7663356977302214
0.3237969063205214	0.9484095144800969	0.7955801162231185
0.0824564899836307	0.9516812078366627	0.8114382878355790
0.4337465769016554	0.1247571233549190	0.5811531758594974
0.4168752676256038	0.9933010778035528	0.5697318418476272
0.3912552708925782	0.8620913167663717	0.5632749745960987
0.2020428484709066	0.1320961942167166	0.6183329188799258

Structure files (CONTCAR) involved in this work:

0.1869794068074932	0.0030270242164744	0.5699362937373659
0.2036722028315508	0.8692788295031508	0.5717629207861371
0.9883420931496459	0.0445549034005650	0.7763660181223471
0.9864009110268437	0.8624365368757552	0.7771499253754104
0.1454173222389658	0.9343593836131106	0.2157371830230229
0.1877762371341680	0.9341150776609926	0.4022918182581728
0.2996813395302973	0.9510116109571658	0.5067709496422438
0.4080376996897854	0.9285085468092582	0.3966141414717367
0.3964995084855735	0.9430391341552725	0.1991581822313401
0.2724045411279284	0.9612680774030653	0.2559407538274990
0.1446584468938703	0.1716558526461919	0.2446595713257124
0.1943896321462088	0.1527183297567666	0.4231506807955274
0.3123864225292738	0.1474543517859288	0.5107305517024879
0.4175917476626881	0.1706082409984320	0.3958937660504164
0.3969890209885726	0.1555611966811135	0.2017263859396873
0.2728791951800292	0.1415396788690790	0.2635353022463179
0.1784736520559117	0.0495724670231292	0.3002969759099869
0.4207110567737358	0.0485608355378103	0.3165723060336169
0.0682548383135465	0.8727734902940044	0.0845808740885827
0.0857435484015429	0.0038446771790889	0.0678806986003658
0.1020580738294932	0.1362024725406225	0.0641549441759491
0.3015295776606810	0.8676221126900151	0.1209864093360654
0.3106530290616444	0.9965344198821122	0.0717745223900365
0.3015089138626594	0.1308446213633138	0.0685973779495205
0.5135370783573140	0.9539293698810729	0.2809564661153032
0.5177321700970691	0.1356143169944715	0.2771529512647508
0.6448763059098209	0.5601465551859369	0.2847983817006922
0.6865340031594882	0.5656934094966160	0.0977446010784866
0.7994616958098731	0.5531424270124010	0.9950921362199929
0.9080669649309391	0.5715230302033976	0.1056095841234225
0.8963533102635525	0.5553656617947988	0.3023511933942208
0.7724513765509813	0.5379965879620592	0.2418923779812762
0.6458588496099186	0.3313982279335825	0.2679171164297661
0.6948720215712640	0.3356418673674654	0.0873902685822465
0.8083147462286828	0.3516193688068329	0.9890920968312821
0.9118050337801561	0.3285298798850389	0.1104413007332470
0.8980291474603317	0.3466192223021317	0.3050529932896377
0.7739349082526242	0.3587436975514025	0.2435311737367833
0.6810196700479215	0.4481554623459629	0.1912279769515234
0.9211251620109965	0.4510500686125870	0.1833258883313374
0.5669575547022717	0.6256230314273802	0.4124688932833165
0.5845371846879105	0.4950699218455436	0.4353880908245955
0.5964713377921806	0.3625700928985939	0.4448881002084160
0.8012241876308489	0.6319767942115609	0.3761462122185442
0.8079902590678688	0.5022512367278391	0.4262963383011281
0.8024170600232190	0.3681519583784986	0.4387755686974523
0.0138981092751405	0.5456486276332922	0.2192830089723401
0.0168162951987959	0.3629494343535627	0.2225001669858079
0.8587974540180432	0.4344286991273979	0.7853547762595043
0.8116722987381259	0.4415926037018332	0.6007743603800427
0.6991656516619482	0.4427874543233452	0.4925847349560658
0.5928888064601808	0.4320091040174985	0.6096631487243633
0.6031641941687444	0.4395282546885944	0.8073958215985286

Structure files (CONTCAR) involved in this work:

0.7288706294834101	0.4496791002965312	0.7523337235666746
0.8524038571289042	0.6754720148672622	0.7457910044788429
0.8032527502349239	0.6372568997439332	0.5717288814625250
0.6885833405031412	0.6472245533208032	0.4785639367646535
0.5860384788168737	0.6656530187639396	0.6007948848444572
0.6025830480344943	0.6644020071829247	0.7977603485111935
0.7235581520860049	0.6483902510177378	0.7295126233989807
0.8130916666193354	0.5500565505606175	0.7204266541880613
0.5835817767861383	0.5497272751189254	0.6994834413034828
0.9310021001725021	0.3815717299569322	0.9305544026518189
0.9162455620891229	0.5139385378081192	0.9248185615005851
0.8926034954780643	0.6439841472362319	0.9450891280932266
0.6928095406312373	0.3622835837448998	0.8928774862302009
0.6904165048686683	0.4926144172324727	0.9329569983714007
0.6993866574857182	0.6268071316549713	0.9259157981981316
0.4870986170328959	0.4568014145588139	0.7244304618862966
0.4841360428067051	0.6366051042552259	0.7187149162731336
0.6435857532315794	0.9323106141159894	0.2765506357756883
0.6839230891135321	0.9477864599918813	0.0896708371836902
0.8012749360108716	0.9575705476409135	-0.0027886256033456
0.9137010955811631	0.9320424113511688	0.0949989235352751
0.8960005043595659	0.9362210467305400	0.2925582253568150
0.7718376169008867	0.9539633496224108	0.2345959216988629
0.6405548228942726	0.1761900739181088	0.2404092146852067
0.6964869460428351	0.1398209632074010	0.0695298074860609
0.8165899283115915	0.1460240386075240	0.9851323841886657
0.9244781699349114	0.1654996601266060	0.0936422143376320
0.8971687618313043	0.1614973376960557	0.2881000171789960
0.7715369786257814	0.1527696611521571	0.2292743152591766
0.6828490271266604	0.0521190032460965	0.2176740684828437
0.9191667892089879	0.0482354763680994	0.1893007438293173
0.5692769022025213	0.8735684384468028	0.4148346341774554
0.5877683035685998	0.0047060123738383	0.4247567795921997
0.6091882956982897	0.1361353008122149	0.4246424672887184
0.8000841898736096	0.8619745625366430	0.3713268683946691
0.8099130999754398	0.9928096285571505	0.4165097616718254
0.8028083512638948	0.1274176856515107	0.4192842545014727
0.0149078580116488	0.9552229914194643	0.2179829943505358
0.0189983728527550	0.1339732021180217	0.2218313038397033
0.8583511960965293	0.0696785985566148	0.7735692765583074
0.8190705361387245	0.0599567524155613	0.5853838921919744
0.7031087529508789	0.0525339369705408	0.4890328741670010
0.5919260874473559	0.0729623703679303	0.5940827392644216
0.6080044618678581	0.0608159899284041	0.7898817519612287
0.7319324878902844	0.0404607094922301	0.7300559595099275
0.8621797730554167	0.8276434020484759	0.7410076993396707
0.8114385868558932	0.8563107836355655	0.5655917045590945
0.6909974595016668	0.8489816070553128	0.4826260101832358
0.5863981602631215	0.8304989386903917	0.6024012621194926
0.5991343451990121	0.8478680301444331	0.7985846596245557
0.7327410595194782	0.8573052324189805	0.7257837543332766
0.8284155226037446	0.9508512534808700	0.7023943241855762
0.5816547093243002	0.9529823447993424	0.6763562510259260

Structure files (CONTCAR) involved in this work:

0.9359767668859018	0.1343116026460438	0.9005961772211079
0.9154727684835740	0.0054655409805126	0.9295306394148583
0.8931722589891992	0.8742491212818283	0.9231808354409163
0.7072110180619897	0.1259734564602689	0.8761007814529544
0.6899199893084536	0.9933067949143849	0.9051837319059055
0.7136476914487276	0.8643135336882842	0.9401175702756575
0.4890410566504411	0.0461935251500091	0.7154294201593908
0.4819538591158672	0.8676784012994716	0.7100691321217939
0.3569158685429724	0.4340945226182457	0.7211160335449548
0.3147217277496065	0.4389265884363877	0.9077361886006196
0.2027307563032039	0.4456785506251700	0.0152834527699515
0.0948515290992685	0.4275095002393062	0.9027215801770530
0.1058407260707894	0.4374711932820428	0.7052487360875828
0.2296854180961865	0.4609224715081139	0.7608896638953198
0.3610173872878289	0.6747780886575070	0.7527904127722730
0.3094970499683120	0.6493218586288865	0.9289015280531744
0.1909020001326942	0.6461347001477648	0.0163347811643195
0.0875297700688230	0.6680689446519571	0.8965312529214194
0.1090454535449599	0.6537427571582485	0.7020120946225921
0.2320711861933752	0.6468637091414411	0.7683376711362515
0.3239796718815748	0.5512518096949326	0.7968560509402620
0.0859697638046308	0.5464884263336433	0.8171121005573811
0.4347880302223833	0.3722571605049038	0.5919581247999885
0.4174864870230596	0.5032064053110662	0.5729567096284310
0.3938541167430982	0.6344914818252524	0.5698572046887538
0.2032360271088757	0.3674808767402361	0.6241416520005058
0.1886731469262547	0.4970120679935564	0.5789573833377781
0.2075178754046261	0.6302493018618379	0.5727695164483619
0.9894314228485098	0.4538194331226315	0.7886503727683186
0.9886622300288207	0.6339898339553902	0.7755437166515111
0.1441689967773521	0.5668151912095419	0.2210383243622836
0.1872949749772951	0.5607245625288891	0.4074749333039629
0.3012250890631116	0.5469212823975372	0.5084566006360385
0.4111146847781342	0.5695002256899552	0.4019817522204990
0.3966818463703001	0.5606656986327369	0.2048799236295440
0.2720302409252010	0.5408271539567441	0.2599246801992325
0.1415615991277993	0.3256575502751275	0.2544482296355452
0.1955783013535939	0.3524406610705861	0.4284993039167931
0.3138035246887529	0.3531389126567155	0.5163051563311207
0.4200843759291352	0.3320649285069803	0.4033240809306280
0.3970629157536522	0.3396365616135053	0.2086565126688321
0.2714682911923580	0.3537718621504002	0.2663843631198489
0.1791072329015693	0.4492347767982255	0.2944146094587471
0.4178768423477750	0.4508234473507804	0.3141314651196609
0.0684091325487209	0.6262958128760715	0.0845853323781390
0.0868355734357708	0.4952648077686210	0.0730259280495627
0.1052651662345842	0.3632496811967980	0.0716001453363758
0.3015905986078616	0.6335111634389606	0.1241301485842715
0.3128860554495720	0.5036356415772487	0.0782955719424422
0.3041148787496596	0.3691826514131917	0.0737554649123506
0.5142958532903854	0.5413928724978847	0.2825282468154267
0.5180739263630019	0.3649068774062351	0.2812989931804595
0.4385613794341168	0.7499279106832942	0.6381330498131479

Structure files (CONTCAR) involved in this work:

0.1963852001044603	0.7494848715414048	0.6512839363983605
0.2721923886851950	0.7500569976479271	0.0471878349253771
0.1080657728383030	0.7494767274427140	0.0485567643285551
0.0620792086734797	0.2493809664030295	0.1440811798993295
0.3062983098787181	0.2488898006276006	0.1538884600630275
0.2306865714165131	0.2505258096811230	0.5467650185794914
0.3951050181134568	0.2491590936728023	0.5517463216197123
0.5618420785409660	0.2495315020592487	0.3572918467540422
0.8087182580082468	0.2510834837449885	0.3520751127576356
0.7302848592723276	0.2443894208781758	0.9539363629545152
0.8949019839284635	0.2537044597756291	0.9512665013087955
0.9300029898466046	0.7564680825476534	0.8727674810913751
0.6992871241581300	0.7480610410559575	0.8631151166035033
0.7770362334192741	0.7472870703582190	0.4634395738950334
0.6042756692694633	0.7493085191769732	0.4500757466695785
0.8131236549393875	0.7667487757825059	0.0860913478166109
0.9199112378126523	0.6725985682120393	0.8232952408471668
0.6819478818949331	0.8331662228260284	0.8227269986269594
0.8725025452374128	0.7397813294512877	0.9947753125689786
0.7534425675666944	0.7719004941069808	0.9862313455223236
0.6957448823409760	0.7358397402466483	0.2290765656190451
0.6748456169707451	0.6967807817733381	0.2775109883758105
0.6821171851957314	0.7234348754880471	0.1515750433501379
0.6747128711481628	0.7848766024051281	0.2491688203245119
0.7502295695673694	0.7371554296693820	0.2357326494315615

Figure S2 Ga/ZSM-5

1.0000000000000000

20.0219993591000005 0.0000000000000000 0.0000000000000000

0.0000000000000000 19.8990001678000006 0.0000000000000000

0.0000000000000000 0.0000000000000000 13.3830003737999998

Ai O Al Ga H C

94 192 2 1 5 1

Direct

0.4216439610252512	0.0586670742349957	0.6502046827899562
0.3054918834103816	0.0298275430686049	0.7966910898782539
0.2809511484514134	0.0573921486753836	0.0189489139410436
0.1211284713211747	0.0636350700409118	0.0129168341459107
0.0661990718819203	0.0296614091883775	0.8005017265680764
0.1815797721106326	0.0605915197140168	0.6666381039847807
0.4205807727903511	0.8273898707478421	0.6736577681587742
0.3032160664388731	0.8708303773655647	0.8095277911347686
0.2667625269711001	0.8301006816110054	0.0279393855551539
0.1119933283972025	0.8270683590400665	0.0176470748662660
0.0633562581042486	0.8709017803150118	0.8029041914817359
0.1810991638697977	0.8271694663011122	0.6752989354283626
0.0768234727186215	0.9420258504563914	0.1531121586917094
0.1942491509859962	0.9702011299315061	0.2980340517444895
0.2179936334195422	0.9389612411855823	0.5202898597897249
0.3784344624713057	0.9332081734653034	0.5157942932593979
0.4338767768557897	0.9677263076984024	0.3041617756400457
0.3186784395993016	0.9381619775640935	0.1680564218581307
0.0810569594102655	0.1734679276082041	0.1668726560899160
0.1960821165181086	0.1297393941225542	0.3081352186811255

Structure files (CONTCAR) involved in this work:

0.2322106593621192	0.1703284548729870	0.5251208053440168
0.3870154930518744	0.1732422616161090	0.5107645484371358
0.4369328647424832	0.1262827979027058	0.2995336806528217
0.3180993511537151	0.1694391053341554	0.1733218764426675
0.5796757766860893	0.5572874537418057	0.3472506807116681
0.6917992216807126	0.5321901606780685	0.1900115464516649
0.7144030895598862	0.5650955602067745	0.9741818173761001
0.8723720020100492	0.5601543825162694	0.9741119963632616
0.9312644802541480	0.5292329089679301	0.1876419159670908
0.8152212267811987	0.5610406103610001	0.3200870407415184
0.5771306086622328	0.3286921741865861	0.3273783295746313
0.7034273136231121	0.3753570041975973	0.2082372874426573
0.7357404289741667	0.3292246113583281	0.9874708645775889
0.8875409508311446	0.3267585504072656	0.9752772056387056
0.9362931466691320	0.3712704911762763	0.1920025996151123
0.9252938586686311	0.4378022758926829	0.8347643981554415
0.7812099403071835	0.4412448804462987	0.4728578693074957
0.6206542361852524	0.4326232136290722	0.4863914141967308
0.5674869151504364	0.4675629780759428	0.7017148650992318
0.6737757056834598	0.4362865811946636	0.8493286644866299
0.9177743223550804	0.6729620172873284	0.8258415491276982
0.8007080620093168	0.6356873596333927	0.6924555762359159
0.7657504900947919	0.6654873359614807	0.4727794046129202
0.6109578487872623	0.6710880664431779	0.4855794390264064
0.5644540348108052	0.6259989167150417	0.7025295360203595
0.6821937966021401	0.6807899553435626	0.8229997875033165
0.5779459520727099	0.9428875364904750	0.3573713209961141
0.6956599782123327	0.9717903361982539	0.2127235709874721
0.7205423803370260	0.9443039122929899	0.9905665788521194
0.8800199408338722	0.9346098794925750	0.9934272784591764
0.9325978925885389	0.9701855555440256	0.2045341696622787
0.8194280177603599	0.9392023103307938	0.3466921219460875
0.5806856894698483	0.1739804271061424	0.3275435288201144
0.6974274273712140	0.1297289962241461	0.1918043271309266
0.7330898225529537	0.1709918390744593	0.9729224334104482
0.8879627052823738	0.1726640066718519	0.9855051151183130
0.9359450320086307	0.1287016927203326	0.1990432885104282
0.8185872603688901	0.1692915935027707	0.3299708813222990
0.9234368518648145	0.0551442908737158	0.8544856593493648
0.8046969019770666	0.0271990376918665	0.7099656869491693
0.7811875080849507	0.0575292397085523	0.4894504190704392
0.6208721717785604	0.0684499038132174	0.4888757082994439
0.5668203678166835	0.0339285486328929	0.6979883378152271
0.6803467388233174	0.0592754288300475	0.8424036596040061
0.9185148988968036	0.8257087436384101	0.8373818257837079
0.8038328789137840	0.8690116816447102	0.6933911122012368
0.7687402234094549	0.8258678161461643	0.4767993450390979
0.6139899259318546	0.8262289754573485	0.4928151052100923
0.5638533513714702	0.8770665008664787	0.6998544696655873
0.6805486880240860	0.8367478526149001	0.8303104977405550
0.4207842718580743	0.4420589288622704	0.6455405847425483
0.3090510142216564	0.4682655940008367	0.7972013864214522
0.2833917836872396	0.4402779347855860	0.0181508399675503

Structure files (CONTCAR) involved in this work:

0.1259663496356789	0.4348218815970657	0.0091621007431092
0.0727136207171042	0.4717441847600104	0.8008594072085564
0.1869797739105338	0.4425675911067928	0.6630806885424475
0.4222944219902084	0.6732299241493854	0.6715468655194786
0.3038524269002981	0.6267383414847449	0.8038957825804255
0.2667040748693893	0.6696975022225277	0.0224630195581074
0.1122797922839679	0.6737397402150338	0.0128230750023106
0.0642487494948984	0.6291589076573399	0.8025227225478921
0.1807065771446595	0.6690532696571149	0.6696904876109894
0.0762330261134577	0.5557232808536547	0.1439195454245663
0.1938822921773298	0.5281045420780878	0.2907789633686009
0.2200044109724336	0.5630486005601066	0.5107542978114499
0.3801344061515436	0.5697713285173353	0.5098237968190679
0.4350512712358675	0.5305919187927595	0.3004715604515319
0.3206313270114753	0.5601629904169567	0.1635305676056940
0.0830769020543423	0.3271384524981962	0.1616794420474303
0.1951552803379172	0.3686174228830898	0.3074997974588554
0.2320311691594117	0.3303968211895970	0.5250975100912045
0.3865266217476095	0.3272614840983160	0.5085731167746984
0.4334309034862009	0.3730814802160681	0.2958368707804682
0.3157060990396081	0.3270569288692497	0.1716024070215440
0.3573032017758546	0.0677648225752515	0.7227417987831845
0.3157546115520914	0.0573592354138167	0.9094667073666967
0.2007214206002980	0.0495098830906918	0.0086986025732748
0.0907765441298851	0.0676676245990612	0.9011655898457001
0.1046374582839241	0.0606663176127026	0.7042253677392130
0.2291894203816083	0.0454149429701996	0.7625470720666934
0.3605132365104143	0.8266082341553874	0.7551102639645397
0.3053132321162671	0.8549562646902383	0.9279672667356348
0.1889510851074727	0.8534273788589973	0.0217416096562645
0.0851533736098166	0.8317264777705287	0.9039263788421056
0.1035779575018372	0.8383114976406262	0.7086855460124878
0.2295285216806166	0.8518131733241171	0.7662828618979197
0.3194435114978003	0.9495339658189319	0.7893252480928555
0.0823940186831459	0.9499205351369818	0.8117423989511181
0.4312877227028173	0.1268895619981973	0.5850372615699313
0.4129377636593543	0.9952475966487960	0.5750309263828415
0.3954567777836582	0.8626022267523230	0.5708380611915327
0.1989140405106420	0.1340110354224875	0.6211697117183219
0.1906654453951763	0.0032163242279465	0.5820551523449027
0.1967539505207573	0.8690261679389955	0.5739553038950018
0.9871062229688748	0.0425834296187220	0.7817890270231423
0.9833568909741768	0.8620112502382331	0.7868288977150916
0.1418971449728796	0.9330736458295310	0.2241207791675012
0.1845242552173560	0.9407645379092267	0.4099500667665384
0.2984398459207638	0.9444856476932194	0.5123788945678868
0.4080507674915976	0.9289521017255609	0.4036285628711432
0.3953840198905750	0.9386116011892384	0.2066269257901184
0.2704053448573770	0.9552516018523121	0.2625664813838199
0.1407845791480485	0.1735070876827186	0.2488377011618704
0.1914099663233436	0.1487177659374656	0.4255156368388073
0.3097980590604696	0.1472672013252922	0.5130719993626641
0.4157464372933388	0.1688667127562679	0.3980043552679461

Structure files (CONTCAR) involved in this work:

0.3955589621142965	0.1553562891095077	0.2039609717464563
0.2707057788427941	0.1472383516060459	0.2669810295118152
0.1798984032231147	0.0505170255169180	0.2928251878369303
0.4187978022508503	0.0476241964821612	0.3169310381689466
0.0660797907387857	0.8726165037205296	0.0909270124662000
0.0853852481684144	0.0032779972930371	0.0741001271091858
0.1057284563889064	0.1349071375108324	0.0665804052706468
0.3018425786186422	0.8639243046007411	0.1247074198858640
0.3098038425324103	0.9939768852066329	0.0810158053307313
0.2990671072838668	0.1276634401645909	0.0734847704411701
0.5128592517234181	0.9536544361838220	0.2868554119519900
0.5165217405299262	0.1349628618733908	0.2794867390591566
0.6429399101140497	0.5651457395760406	0.2731716013068547
0.6791288191602913	0.5692710417674055	0.0836429314857027
0.7932138442758758	0.5476971216945840	0.9893110443893345
0.9103286633788810	0.5623691815819641	0.0809968854544827
0.8918454223984026	0.5633666733228528	0.2813214232705093
0.7684682007134790	0.5470290520773086	0.2238535254138872
0.6390425685830877	0.3346222324470349	0.2510208761968025
0.7258389554122130	0.3363911514710882	0.1068383878098139
0.8114173604693581	0.3543707946808922	0.9592124999803943
0.9115187628819125	0.3342423985376018	0.0895619724559941
0.9039846114249682	0.3373247172726694	0.2886179603046977
0.7635726404504696	0.3766163222830214	0.2879324825964540
0.6792345876445464	0.4518373191688650	0.1808375224260625
0.9144739705516959	0.4499697720924441	0.1828119490785299
0.5673008130593510	0.6277266455746807	0.4059243007754145
0.5926739409958360	0.4988774537464801	0.4301494555512311
0.5936464661839528	0.3648481883196009	0.4338522188780838
0.7979033537814451	0.6317163967463391	0.3735664825111953
0.8059436446873814	0.5010826091471566	0.4021551729864866
0.8278071350736785	0.3723672930032146	0.4634116350671478
0.0098270062568551	0.5432890425387970	0.2106469537749517
0.0177271803011677	0.3684578581437058	0.1975262391897323
0.8716104594460512	0.4269007052143373	0.7415107401553364
0.8114602096625294	0.4577175360252291	0.5874236329373149
0.7021627973251116	0.4330351535135630	0.4812383444937505
0.5971923580046703	0.4322762595269007	0.6015302557432491
0.5994419470813136	0.4323387834298758	0.7998336290447392
0.7295644407770796	0.4341771893659589	0.7625830336778389
0.8638424646679534	0.6781927426429313	0.7357991833489239
0.8054324709990855	0.6380117689131922	0.5707231687963986
0.6876575795124172	0.6435482014554705	0.4831039438762236
0.5810350928116441	0.6624087043926561	0.5970190249694199
0.6057660934445167	0.6617889236968577	0.7924533225757465
0.7302189959449252	0.6708840941668700	0.7254057505097000
0.8040954710512795	0.5603602530616394	0.7358165063158766
0.5855896447679109	0.5472833079026608	0.6970501285871559
0.9350094722452559	0.3696659236556076	0.8991450607071612
0.9002267134422269	0.4982994547861385	0.9056859499868098
0.8872473560418510	0.6312421932628111	0.9196220054741924
0.6817117988612826	0.3735533919347985	0.9263957186916993
0.6780462399298154	0.5066847890123296	0.9107637269592863

Structure files (CONTCAR) involved in this work:

0.7069745500576055	0.6365211789326068	0.9175379739569710
0.4874058736168664	0.4576948288626610	0.7093821767613722
0.4847643844513639	0.6342066193167660	0.7241332018805197
0.6432779669832016	0.9347834561195059	0.2867920713911674
0.6912817282253025	0.9374386240432582	0.1030318261677948
0.8011634065636286	0.9530853559883060	0.9913150984679439
0.9060518601210605	0.9285682199230356	0.1076557273391510
0.8954822095494014	0.9442188902660728	0.3053396180171892
0.7709247733578254	0.9622210692551512	0.2554133142956008
0.6412656993708665	0.1747924989948259	0.2474981727118491
0.6949213512375113	0.1482622381783593	0.0741109416698584
0.8108039013704740	0.1472015883275690	0.9806803046498379
0.9143929093991314	0.1704170949875267	0.0996703333482094
0.8962703129143909	0.1581429703143434	0.2949682974225847
0.7712876545371303	0.1441844921567805	0.2367955383826068
0.6775397121480680	0.0511413306428750	0.2073459281121151
0.9184968562941676	0.0494787740671851	0.1841088045827416
0.5687478956574588	0.8743277061970971	0.4220680878839564
0.5834369053116006	0.0062964292357460	0.4335095791922340
0.6045648096985790	0.1380334529122924	0.4306249224465099
0.8036099457805650	0.8624487883368009	0.3815067087950761
0.8099625768767125	0.9877904020037579	0.4430764054386491
0.8057960107619283	0.1217528150682112	0.4268679703260827
0.0117592505586764	0.9561675747163447	0.2219830460971180
0.0160136664243570	0.1375152102590823	0.2162782504426139
0.8566311833198943	0.0620282193064215	0.7869427175505785
0.8097516851006558	0.0646535478208987	0.6027157849844658
0.7002542991964668	0.0533935788060445	0.4898088946466495
0.5933586198763269	0.0767322726387874	0.6023479211900128
0.6045737159219677	0.0568513812578876	0.7997640382547244
0.7291209195286605	0.0347393610729356	0.7523547152154157
0.8576524541196364	0.8268181923342770	0.7578665330863072
0.8086899731229877	0.8444973340761618	0.5784623100728408
0.6915127273127515	0.8508130967599039	0.4873041127361851
0.5874438355750832	0.8297383680892888	0.6073297256693987
0.6039875756841177	0.8553261711597542	0.8003309499628390
0.7287789825588669	0.8559780337514258	0.7361926257128335
0.8228979405662012	0.9480812777101556	0.7003914419195851
0.5801669343736450	0.9549314382228274	0.6732716539796080
0.9340225223241670	0.1249894929911340	0.9152762702916308
0.9198021078935924	0.9937083863946923	0.9344351268127710
0.8954302794035056	0.8630402337303136	0.9397523941278969
0.6981800112392740	0.1354208289632293	0.8768210814951294
0.6871694047508049	0.0098400346190334	0.9384488765667570
0.7017764599493044	0.8766879877409521	0.9303129531545206
0.4879067357576193	0.0475100116198593	0.7177126252776407
0.4843203961064554	0.8674964823433384	0.7200111616907442
0.3593082899071126	0.4291455509984787	0.7223305491304989
0.3179614735873945	0.4378535010930271	0.9085730230073958
0.2041051728762814	0.4560155990581703	0.0081732854791338
0.0986545228342710	0.4280128800092394	0.8952794822487767
0.1095903795643951	0.4497673179858594	0.6979127163946487
0.2323813538501828	0.4561639185645910	0.7615237239771530

Structure files (CONTCAR) involved in this work:

0.3586554621462090	0.6719816319160861	0.7463591355125542
0.3040927465679677	0.6484134469210394	0.9200489673496320
0.1889057249269126	0.6464283385456843	0.0158930132791098
0.0858093323509938	0.6739182186211216	0.8982987443563754
0.1037180932705207	0.6561829617662011	0.7042477334914786
0.2299904225712195	0.6389459168731523	0.7559927107490817
0.3251694153277175	0.5482726526092038	0.7935238544692708
0.0837299605924811	0.5510343846413149	0.8240327853627448
0.4325824510492337	0.3747194276312591	0.5791790542536797
0.4046655163507034	0.5045196685424100	0.5719053872281180
0.4024500967274485	0.6380940203804121	0.5662708013034836
0.1986587618882995	0.3670555137741106	0.6212549667188452
0.2028003140392350	0.4965492094127483	0.5758931969094315
0.1927686851974467	0.6307408538637701	0.5642789043374370
0.9944513260128331	0.4563463096786631	0.7793774706497526
0.9844980781135249	0.6355442979527609	0.7829747265798711
0.1404882975660006	0.5639087349496638	0.2168868225044786
0.1831624129370137	0.5566910147178101	0.4031503986586585
0.2999182742238409	0.5676775104579339	0.4965041250531340
0.4149770199264997	0.5708150702643895	0.4012047917524257
0.3963188136936485	0.5635248409272325	0.2060261813798844
0.2697369939507095	0.5444148742038737	0.2555042381073044
0.1376223630614524	0.3258999650932330	0.2515308093851747
0.1907646097015180	0.3526796976946877	0.4259967304368091
0.3095307293821203	0.3538378408792210	0.5136608871804287
0.4125188277539868	0.3302726945630559	0.3942293976422580
0.3928909753126925	0.3440328256085739	0.1997772026268575
0.2689349394410609	0.3479021930766027	0.2666515843457057
0.1810876608582769	0.4476715944984261	0.2868806893072820
0.4147106348175190	0.4518001227565674	0.3131898133966438
0.0663177927252001	0.6249118885748183	0.0810557431460611
0.0843383107678689	0.4932505092338848	0.0664459234747481
0.1157370161086207	0.3626075519053371	0.0632456111149882
0.3026831235393793	0.6325212888072119	0.1154023852566920
0.3174364773513524	0.5008305784932889	0.0806606579203978
0.2942196659144820	0.3683044930839322	0.0721761647925829
0.5146070949725211	0.5385234682612074	0.2807357079800996
0.5127540204410024	0.3645881774016685	0.2752547535290970
0.4418691478986502	0.7506646394575293	0.6484517824189240
0.1944589973411761	0.7483122956360878	0.6521531229667445
0.2722529133358414	0.7496220573455414	0.0399375708872166
0.1077725281173907	0.7497249640522280	0.0557516130639819
0.0636673187120780	0.2501620148215803	0.1346188519570698
0.3068814212360608	0.2480454877452970	0.1471152104158490
0.2268633620637288	0.2504417587338722	0.5427495238983108
0.3914193926763312	0.2505707039301031	0.5486918164534519
0.5601761052532667	0.2509253512326113	0.3525123093197418
0.8039800112014438	0.2453713178614001	0.3606121140166978
0.7274186089513959	0.2511709861298840	0.9555855635393419
0.8932249631585901	0.2486417233996711	0.9422742122983258
0.9363549110748449	0.7480918903830286	0.8643428577336743
0.6861367739045361	0.7581455667598518	0.8583994440711940
0.7723064690828436	0.7457098389322854	0.4591680305925386

Structure files (CONTCAR) involved in this work:

0.6075015636568361 0.7494597057492804 0.4532986138959242
0.8262757319151188 0.3277414256195993 0.3427117472928815
0.7970682696663455 0.4761683332421532 0.7174984300689441
0.8800300397394448 0.3897708884591015 0.5961545685243042
0.9336166758987449 0.3345569708654452 0.6013414625269530
0.9941175540061804 0.5206307577969498 0.5995031717540009
0.0085958912889912 0.4382480033200579 0.5506350302217264
0.9311855377077383 0.4845791687469035 0.5219035918186492
0.0073628075166629 0.5084860496017034 0.4672030445462941
0.9856664197006042 0.4873019710182829 0.5356293128448492

Figure S2 Mn/ZSM-5

1.0000000000000000

20.0219993591000005 0.0000000000000000 0.0000000000000000
0.0000000000000000 19.8990001678000006 0.0000000000000000
0.0000000000000000 0.0000000000000000 13.3830003737999998

Si O Al C Mo H
94 192 2 3 4 4

Direct

0.4239043626053421 0.0579908216867701 0.6527901709167947
0.3062793369456823 0.0298234317947015 0.7976920852222276
0.2814952308730211 0.0586405987569553 0.0207545826430933
0.1212920290990496 0.0659585698346991 0.0173621558799643
0.0667298634628135 0.0313164104414076 0.8063049202972341
0.1809426750203568 0.0627466827394343 0.6700048988923948
0.4179149000880785 0.8276931544266470 0.6705881427805367
0.3050042041125872 0.8706082864341645 0.8115708695724132
0.2702808409733078 0.8310844586852539 0.0299682634281093
0.1160140210155828 0.8266509603295590 0.0168136047550307
0.0689731240008349 0.8737761007602780 0.8047315191034101
0.1847626292582735 0.8296754011307593 0.6748231857409323
0.0789939132473668 0.9405725997879381 0.1531143836937449
0.1947164635772783 0.9693195388009116 0.2988093140878752
0.2191543141929883 0.9433683193362395 0.5212893102494620
0.3777922283362129 0.9355997052927212 0.5156594882996456
0.4349171447065507 0.9691262207694700 0.3057460221880995
0.3193586540087646 0.9388342220816938 0.1708208990352017
0.0798211236263849 0.1729517417365386 0.1749711617772883
0.1970008275309307 0.1279067066499949 0.3086653672346301
0.2329354421631129 0.1686091206170659 0.5260032789931759
0.3876374865955475 0.1729069040065340 0.5159252205565763
0.4368829132587753 0.1275056456738249 0.3040013833806589
0.3194424462836958 0.1706540856798906 0.1744110473514423
0.5771749304805047 0.5583513564733253 0.3537559163196136
0.6908034791700202 0.5264280441057989 0.2061766625221813
0.7141497781419320 0.5578475753147243 0.9843837645199481
0.8732202366694651 0.5679501560762522 0.9850474361556072
0.9322444848416503 0.5351114713439431 0.1926114705291338
0.8159494494116639 0.5582099929271873 0.3310875289493148
0.5815847951424030 0.3258941313302438 0.3338742263606496
0.6946589121310482 0.3697435827735719 0.1945393101874356
0.7319578905413159 0.3296255749853644 0.9779344514072719
0.8870020815747691 0.3275558729345229 0.9884005089237793
0.9356679402291639 0.3770138280285267 0.1977840326687180

Structure files (CONTCAR) involved in this work:

0.8183979831082098 0.3328585791551657 0.3264910502627785
0.9201469700619850 0.4430972707708909 0.8512219197978329
0.8036319016805377 0.4675581489196047 0.7055787700912901
0.7803622030107019 0.4415838067844576 0.4838569604837298
0.6209289377453994 0.4357134604967676 0.4902121253822953
0.5652799431412487 0.4680151086125030 0.7015996103517275
0.6804298472196874 0.4356245129659622 0.8356100777551524
0.9205986604616866 0.6734516049507693 0.8292000106996513
0.7640629239615880 0.6696662664310193 0.4670599544842887
0.6112449216912669 0.6724112028965153 0.4914067511351917
0.5603108392066943 0.6266198242278896 0.7032271598935786
0.6747099205459840 0.6740132626594012 0.8349184611027275
0.5792015157507708 0.9422085972483187 0.3543228177062830
0.6939832216144940 0.9756203049346764 0.2078110335194606
0.7168971229547760 0.9422875875746929 0.9857024704212288
0.8763737077393483 0.9318995578385108 0.9881684491561310
0.9344732673533969 0.9664484002655707 0.1984334298738955
0.8178626170304796 0.9411144620299977 0.3325080038337053
0.5815961831577262 0.1739004602975327 0.3327911171622697
0.6960446080586133 0.1327224244063700 0.1939592587331531
0.7328578269306136 0.1686023243127503 0.9775127280292223
0.8878381462678434 0.1723421294191565 0.9886932885182954
0.9363134909883236 0.1253083660490815 0.2015640392797882
0.8180707208371086 0.1741748592202829 0.3241200646945754
0.9196204454843093 0.0576787941840113 0.8502241452298103
0.8062551390945318 0.0348707466139187 0.6981832082721134
0.7820777042346200 0.0619321251881575 0.4789884530667946
0.6233498721224754 0.0651518354678017 0.4894326155036411
0.5688666125975421 0.0319790592937020 0.7001337935607435
0.6854663287017938 0.0632546783074801 0.8315752428494052
0.9230757073569132 0.8268339316167530 0.8301589970045475
0.7654971126880404 0.8277198494624151 0.4704414584183554
0.6129896690490130 0.8267542426678801 0.4923494011062345
0.5621123527832640 0.8745281711534424 0.7012544017708241
0.6733471498330356 0.8290877959784130 0.8385963672514745
0.4213210556562708 0.4426374969705114 0.6490424045647804
0.3033380391382232 0.4693360508871839 0.7943504936011616
0.2806917461785250 0.4390269975388688 0.0170308141138917
0.1200699860065514 0.4329472918642654 0.0131058301611356
0.0664439794201729 0.4694312466021270 0.7989654135188436
0.1797600712704071 0.4366902286100545 0.6643801549074450
0.4176446289590084 0.6736397276570066 0.6667825205838325
0.3005177899791435 0.6291949826373400 0.8050079635357953
0.2717238681278841 0.6704463649558894 0.0253955433684626
0.1179531272918576 0.6722773501883084 0.0128273589889568
0.0673446922825865 0.6268012771165322 0.8023208133769113
0.1809980840622010 0.6720894581887910 0.6715623115314812
0.0777588899171797 0.5585854975846707 0.1489732484061039
0.1948246638623104 0.5317412026293242 0.2942652460114816
0.2175316146589668 0.5582216042331288 0.5184719400277050
0.3781749381085786 0.5662985490997798 0.5116977162144029
0.4337575150856318 0.5287877336879966 0.3017202750944191
0.3198228578396972 0.5603056108488053 0.1636084689169911

Structure files (CONTCAR) involved in this work:

0.0786127040542862 0.3273832744933796 0.1695848344830212
0.1973259809720440 0.3721507010740030 0.3048948900041175
0.2323670936175675 0.3296555879673112 0.5217908699829974
0.3871895872131889 0.3263623372308181 0.5130527561964709
0.4374146011907854 0.3707955916667530 0.3019619120401660
0.3199546396676478 0.3284708964608043 0.1723939847974821
0.3594612727496949 0.0671936975650855 0.7254002263025922
0.3163763620244756 0.0556961518580049 0.9114365711764412
0.2010535880247720 0.0540873057172486 0.0102421746631243
0.0893864626932526 0.0708497743919123 0.9067323667025654
0.1045353631375802 0.0634282949175569 0.7101401332635383
0.2302942863270614 0.0470758867663773 0.7637574250134025
0.3612428979863841 0.8254442904108622 0.7573637838694343
0.3084314016278268 0.8572112652098760 0.9305073645099302
0.1923106449094051 0.8541175006143162 0.0246455877015828
0.0913132725323294 0.8309201077524953 0.9021116514841798
0.1077072761669564 0.8425157519480549 0.7080846305755223
0.2315660839082719 0.8484480785089168 0.7701136402071849
0.3185662675180927 0.9492695523124907 0.7878425187276962
0.0880361924390178 0.9524516099146687 0.8183157144082471
0.4334521293492078 0.1263896348362345 0.5878433965536531
0.4152360582646851 0.9948246798955718 0.5770266164043274
0.3877366859561605 0.8636586689421148 0.5710961005000023
0.1979437731723818 0.1362016089423459 0.6239632018381079
0.1884219810078965 0.0048303047126566 0.5855069259201603
0.2045055389862203 0.8719778300766902 0.5761411520952794
0.9871592601544196 0.0391619499552614 0.7883786393227731
0.9895535858758235 0.8652359888371686 0.7887284967182407
0.1429283646493652 0.9301119388744165 0.2259858058556473
0.1834396555110944 0.9433619689227571 0.4123721732747718
0.2989149027497919 0.9538473609608759 0.5087901925157685
0.4095136830128616 0.9293709272192744 0.4048036153302715
0.3961946469335266 0.9414582489880291 0.2075854940301829
0.2711401414783216 0.9529624358557919 0.2664768620996809
0.1399177697836619 0.1735307120432558 0.2563697849940544
0.1945767581156078 0.1406801680757671 0.4277889345075891
0.3108596132962337 0.1458916509364467 0.5203916803440448
0.4144512569222363 0.1698098462893406 0.4019895846182562
0.3964082568816887 0.1566540918090629 0.2076352625760783
0.2705108026467216 0.1478870585491517 0.2660181816425473
0.1806803695833466 0.0493525905747081 0.2861430506482968
0.4191457103687125 0.0487207694357874 0.3208841407820024
0.0687058372378267 0.8717822503941778 0.0888791178714090
0.0876108411689059 0.0035169884013935 0.0772979702990381
0.1049589249935283 0.1362316148865359 0.0733649698570236
0.3050756816149783 0.8641242119120592 0.1272254037120268
0.3071777872042980 0.9947459436181494 0.0848956797018257
0.3023725746945899 0.1287879706635373 0.0736726581490061
0.5135703412026809 0.9551873667140292 0.2857472101329416
0.5165158313717506 0.1362915710229418 0.2854686756708137
0.6427157555419603 0.5666104256891999 0.2834209735859586
0.6789534113039464 0.5540871627470317 0.0939324465190673
0.7945093425327064 0.5545969638840428 0.9994929550145095

Structure files (CONTCAR) involved in this work:

0.9088464920668293	0.5764122186515610	0.0935583186449126
0.8922472806104054	0.5609055001197258	0.2906277553368131
0.7686360918735587	0.5365872810012049	0.2375908699655047
0.6413550734392593	0.3225336553812231	0.2522408578964139
0.6917604600115236	0.3548187932516701	0.0761861197209826
0.8098119550125782	0.3536300841851128	0.9839353210688676
0.9137929815651352	0.3313676713326508	0.1027711558355517
0.8947681331382188	0.3528692465348446	0.2965091695908029
0.7701494992230451	0.3543262963986690	0.2335842056244526
0.6729141872282649	0.4470067496112724	0.2157097465614136
0.9195803099639462	0.4553234549040339	0.1734413305675886
0.5660758625720957	0.6277226732630290	0.4155599368195458
0.5834851745881555	0.4967281597350816	0.4326000169985691
0.6063292148234056	0.3652941876811114	0.4332648038292495
0.7945622014275882	0.6324021319991268	0.3694480661791097
0.8110763957472094	0.5046965742372616	0.4220225917100363
0.7963289947035511	0.3713245811113539	0.4275630294049866
0.0108103599403690	0.5492385867170172	0.2150902427947482
0.0152364513180596	0.3667915154393799	0.2185388222907761
0.8576117925320841	0.4296014215492100	0.7776140282991242
0.8148613260506984	0.4388077430807610	0.5928300366581618
0.7001500033852429	0.4517817384685731	0.4928964445257239
0.5908848206372321	0.4290606095523579	0.6020264160940078
0.6030977138879009	0.4385820141296931	0.7992598144424106
0.7280173086221975	0.4468791666765848	0.7391206437715112
0.8723522462351674	0.6722217933304541	0.7305662944690575
0.8097045621029373	0.6527369686471364	0.5646457137783022
0.6879986990209535	0.6444663361246680	0.4896810724131178
0.5815536787191904	0.6679179300964693	0.6034920819202643
0.5978546845854116	0.6570067410012119	0.8001832875005354
0.7255583878991141	0.6615704763009812	0.7437814913321718
0.8132836058473336	0.5469399729460442	0.7133760595325751
0.5794854917767441	0.5479171122813611	0.6880026972697491
0.9327574727050485	0.3750225195498207	0.9166812425731370
0.9079480526038575	0.5057049675428956	0.9269295393528824
0.8835285636929721	0.6375908470591179	0.9226740725768587
0.6954984094939283	0.3615839456157387	0.8812130079002468
0.6918481889691476	0.4925333865308539	0.9204562145009635
0.6921695838863354	0.6270348153082270	0.9313928027882642
0.4859870953990061	0.4545082075345983	0.7193129911994054
0.4796718962405904	0.6343463302139483	0.7190845177686771
0.6442210989725988	0.9351203036694925	0.2823488356353608
0.6804483831683623	0.9547032484115439	0.0929427822773814
0.7967468502801982	0.9363310819819000	0.0042346089708996
0.9132723650973702	0.9285228524881747	0.0961670091239168
0.8947734358996524	0.9339958696350947	0.2933686179363186
0.7712323816488433	0.9586561802852182	0.2366104085781966
0.6391067313038774	0.1778442919341630	0.2474806823817900
0.6916078282138951	0.1412900074850125	0.0740261534022828
0.8108583884214589	0.1456428593976815	0.9864922308589300
0.9165347472898340	0.1670645155510992	0.1018584149453678
0.8949256372318340	0.1548517716587866	0.2963295569524610
0.7705166715919815	0.1560135538118749	0.2288164704899318

Structure files (CONTCAR) involved in this work:

0.6813417438557066	0.0553584601945906	0.2256629197637610
0.9185659734857121	0.0460889015701896	0.1874659834830653
0.5693779840836818	0.8727291737291070	0.4163099814494589
0.5853183520473109	0.0039291261763387	0.4330758445206028
0.6090551637822581	0.1351904120307411	0.4312184874451837
0.7969851894238096	0.8683696331422187	0.3766740224758419
0.8141476686144551	-0.0005369459914996	0.4165298979645681
0.7941592465455370	0.1326332879883575	0.4216181215843117
0.0130805427849428	0.9525435041775330	0.2215615809781794
0.0158916661090483	0.1338221435563840	0.2228281569299153
0.8592088048378164	0.0717651580864206	0.7730445369783423
0.8181975137148498	0.0661104268315944	0.5867861721928053
0.7025536358048216	0.0485353047157954	0.4909794970596715
0.5942150255311939	0.0728220108606284	0.6018376001847633
0.6073877418764553	0.0576621552044710	0.7996371344259126
0.7304043209356157	0.0550176139529117	0.7316609610604310
0.8701438062110588	0.8293249560654302	0.7393545872390860
0.8105103437807374	0.8420629231855860	0.5704813044149853
0.6900127997711213	0.8539987721195814	0.4927723444400549
0.5838144353461584	0.8302467947763064	0.6046846807929511
0.5968512442366311	0.8454972003961216	0.8014795756452867
0.7247178505248840	0.8459577840947052	0.7498530679540266
0.8158045739918299	0.9554065483699201	0.7010048869285358
0.5826565763842252	0.9524134392731811	0.6816325240245453
0.9328122563622183	0.1257756350768311	0.9150703670070400
0.9033178982350863	0.9963651535150588	0.9265294609716321
0.8949086398350354	0.8626705951961529	0.9304011628961093
0.6986060448617951	0.1372469754031432	0.8786624653386956
0.7032986774299561	0.0061787356697640	0.9137133123550251
0.6878461412348533	0.8737044512998184	0.9386705843179542
0.4899952366940834	0.0462400163904152	0.7201605354448639
0.4813922772550189	0.8690659669923404	0.7137318309481199
0.3556262167483534	0.4335437064118063	0.7190672238738242
0.3141858175671591	0.4410487690092880	0.9066152108993735
0.2001656421661244	0.4423735997476089	0.0090656942351151
0.0904909569558262	0.4329953346842599	0.9008221793858876
0.1027849766774337	0.4357263054399086	0.7026580435712465
0.2272603415541853	0.4528752208074583	0.7600395716901228
0.3533834591359636	0.6728711225485332	0.7413693390347234
0.3072894568731827	0.6487526296481420	0.9214635641634785
0.1942530370010429	0.6453165133131783	0.0232518656705566
0.0969532463109808	0.6688320199184271	0.8953775214508264
0.0989272198387885	0.6638976680309585	0.6987890468949719
0.2242773775237438	0.6468818419513352	0.7667060892289747
0.3152923341659872	0.5500853849682308	0.7888940993761125
0.0896349242004422	0.5487582285298575	0.8030216372626987
0.4318784680804106	0.3742981206692292	0.5844972058268161
0.4136827002319783	0.5056493741219705	0.5726361185203382
0.3961283995727709	0.6380781157029253	0.5622540015571691
0.1976993341077007	0.3634723797983126	0.6190075689802038
0.1886002379783881	0.4945376355641237	0.5797608287886321
0.1949068142127722	0.6281392192818996	0.5725801658820721
0.9865961685046664	0.4606736882374617	0.7854781979434954

Structure files (CONTCAR) involved in this work:

0.9872433865676422	0.6304453234838951	0.7991771592839964
0.1411415029464325	0.5693924997650027	0.2228948279755179
0.1848851137708040	0.5582899554818577	0.4078533043674709
0.2979603247904938	0.5539742668113065	0.5134215115019245
0.4051724235304681	0.5691994580756248	0.3980485115483143
0.3962014820547117	0.5540777898797321	0.2012950769551857
0.2702785210979211	0.5496550720290567	0.2588135592129329
0.1405530676969268	0.3293042707424286	0.2475459098274627
0.1930979736208889	0.3554574709580270	0.4229648281840317
0.3101103317661610	0.3529351631917148	0.5143628724742469
0.4151983261211081	0.3279759577373689	0.3996296278098406
0.3970152845829570	0.3423458005935486	0.2051525216962851
0.2712092046982106	0.3524945179344069	0.2634778156114571
0.1825882372864300	0.4513472733060281	0.2862121447985969
0.4193353235410792	0.4493318233083110	0.3200801843707466
0.0691977316663815	0.6251328655418799	0.0790521046921941
0.0873059805380310	0.4940120012622320	0.0765205828293754
0.1005912112449054	0.3616744186945209	0.0641836551999627
0.3098247145515790	0.6351944372697634	0.1180008514353824
0.3057042600074872	0.5044616590237871	0.0782810844834050
0.3032917818170591	0.3698181916784273	0.0709648541664895
0.5123176036301553	0.5442842706491856	0.2840497128802851
0.5170494881277884	0.3625306488706359	0.2831447241293805
0.4377032281567165	0.7509042326662645	0.6426513847690973
0.1931061801363011	0.7503720433599731	0.6457646452129989
0.2757588105344060	0.7505916375984842	0.0399939061286793
0.1112801603250919	0.7488621087285312	0.0526300310596581
0.0596841012562106	0.2496157024206739	0.1474503419631037
0.3083541841307983	0.2494847664296974	0.1491699764456427
0.2264999922736853	0.2492526481035215	0.5328351223471453
0.3912585928248510	0.2500120768034104	0.5549679052299109
0.5618720549268161	0.2497952390734324	0.3659662349277220
0.8126029149480476	0.2533146021712708	0.3492227596907143
0.7280660494754250	0.2491086713680085	0.9697539177747997
0.8925301521994805	0.2499493095028396	0.9515156141965945
0.9411869970028104	0.7494044589543998	0.8604713588233703
0.6771959248164739	0.7511526837841075	0.8741584983955915
0.7641007204161390	0.7491459055643348	0.4406171189457787
0.6087498894267681	0.7497485571243928	0.4535129404856808
0.7970660457059393	0.6300420745979854	0.6919675279425376
0.7980720290431391	0.8713543395170698	0.6965797262180929
0.0201571645558093	0.8089782815864266	0.5251832402366743
0.9831331046069047	0.6876048778618618	0.4551476705566873
0.1712127317946437	0.7396544569773175	0.3829039263933648
0.9607972774182264	0.7770343399537499	0.4184628994160787
0.0312956623452549	0.7198669506677354	0.5756860439268485
0.9138516598444441	0.8047033028895441	0.5722326195862670
0.9171218518156993	0.6988411717822803	0.5875508209145214
0.2106534934970695	0.7558722344237315	0.4343175786450256
0.1902991910994666	0.7009603336437950	0.3320553403011948
0.1295612162919551	0.7182013954626602	0.4260015175216251
0.1528369168755726	0.7829880349549763	0.3403614068609523

Figure S2 La/ZSM-5

Structure files (CONTCAR) involved in this work:

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1.0000000000000000
20.0219993591000005 0.0000000000000000 0.0000000000000000
0.0000000000000000 19.8990001678000006 0.0000000000000000
0.0000000000000000 0.0000000000000000 13.3830003737999998
Si Al O La H C
95 1 194 1 6 1
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Direct

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0.4249398106946196 0.0580314549853991 0.6431455580444219
0.3059554006383049 0.0313789770846840 0.7893201902214797
0.2803403044674703 0.0675207310593345 0.0091073453161968
0.1196225766024898 0.0696636333076413 0.0066303671092649
0.0675679026955313 0.0328244816528758 0.7947525444480421
0.1810635251184026 0.0588434685543271 0.6528591757109660
0.4201952741973120 0.8278718029390677 0.6662824730336032
0.3044110761021189 0.8731091041561289 0.8083611637943211
0.2670614707304279 0.8335793307637180 0.0260933816516279
0.1130195466444606 0.8311296992196514 0.0108541324603977
0.0639191376938328 0.8751241099108914 0.7977018459165477
0.1828195150548117 0.8316529022179758 0.6743074688846911
0.0776814662910646 0.9473351787787782 0.1458875712488080
0.1962378244042997 0.9749428950995724 0.2946947892140339
0.2199263766011834 0.9381749557975654 0.5126046138432958
0.3800284310225297 0.9346015355015944 0.5090808103872241
0.4327757960491038 0.9725330049635548 0.2988176801156217
0.3194621331625927 0.9497223989620415 0.1558169207104785
0.0798732406259768 0.1748525078876736 0.1660498714380551
0.1973384688529918 0.1320434981028304 0.3089640091719596
0.2351499959980753 0.1755592717615284 0.5242362813443152
0.3889430229655352 0.1751536636659782 0.5093415049914027
0.4367483703258560 0.1303601962614886 0.2980731524791093
0.3180368510748189 0.1715719824648074 0.1713749083042231
0.5750943156626200 0.5572379072691680 0.3479994399452330
0.6950436706744360 0.5270353143078883 0.2023539669035677
0.7184684004188580 0.5639151394663184 0.9852832877282639
0.8785871390363537 0.5682016066545608 0.9831268403251817
0.9322895391326588 0.5340291152319397 0.1912176655103716
0.8198822566935000 0.5551637005139051 0.3357873953849410
0.5842115122498394 0.3296120997336401 0.3302449362598298
0.6982538424757940 0.3699634684221285 0.1843050772084275
0.7344920125135935 0.3279250017525194 0.9677323287006171
0.8886289857184329 0.3250176702689088 0.9849759694675627
0.8135301088427033 0.3339718483102073 0.3298072455024376
0.9228563630835664 0.4431124478209426 0.8501848710499316
0.8045370166108875 0.4745861876868985 0.7056414265972558
0.7754202415787469 0.4426011496691818 0.4841619351080010
0.6185423983136594 0.4392218333382570 0.4871417327874146
0.5677175706359718 0.4718833956115266 0.6996242865748270
0.6805440205020192 0.4456791750056192 0.8430393643206365
0.9206002557959738 0.6745583849639805 0.8230053624176130
0.8055680655833078 0.6320552178644805 0.6835054771566919
0.7646148491681284 0.6703792568476973 0.4656966620637469
0.6103231185734171 0.6742288547601620 0.4818685179665739
0.5643370224381845 0.6295449651020065 0.6964974857496412
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Structure files (CONTCAR) involved in this work:

0.6840553655315523 0.6721879251633781 0.8224726770091287
0.5772335590504495 0.9452337582973195 0.3519454559819682
0.6976205206994608 0.9731229945411874 0.2078475678960873
0.7210730446836090 0.9363775679200135 0.9868923777853803
0.8816389892529189 0.9337992592547495 0.9883835195734826
0.9326362796609375 0.9724374795364538 0.2016323935983644
0.8218733130879914 0.9455232006242552 0.3466297312273731
0.5807632719789230 0.1755239911097567 0.3304819593098310
0.6973135757506259 0.1318159375401433 0.1876029312266178
0.7339858845769117 0.1709940894219623 0.9694941488097726
0.8882764365635504 0.1731267453995382 0.9812809703637823
0.8181678547534045 0.1751973958212109 0.3232577355552191
0.9230756795436247 0.0550549531345284 0.8481056500391667
0.8031387674275340 0.0270858143185325 0.7010540096660173
0.7819407225606431 0.0663677259252368 0.4834059271720351
0.6218873666943600 0.0681367007485918 0.4864275663653675
0.5695913662037145 0.0306661492873778 0.6978433276770052
0.6812822450743010 0.0537436539789892 0.8422165051630646
0.9215253233479703 0.8288834152553035 0.8315839568051897
0.8027438173224629 0.8700639382248528 0.6883424471549833
0.7666522124060982 0.8269816527632616 0.4727103303353981
0.6121716204902536 0.8276580571798803 0.4856336293664308
0.5641953538795242 0.8724603411280855 0.6981902088892481
0.6822291735849789 0.8307757529059493 0.8268061520359695
0.4230980709540000 0.4456288278838049 0.6500378507007846
0.3056515911091558 0.4749126760997683 0.8000073240342030
0.2808887100006944 0.4359664536919743 0.0175108419716852
0.1193107096442226 0.4352059967412783 0.0143370510536027
0.0677926845887007 0.4692995360244832 0.8005410764355974
0.1833470614332004 0.4468173810170919 0.6633658086573619
0.4210075280475370 0.6731970137620953 0.6666490664475830
0.3047680491636628 0.6330765472090800 0.8124206143521364
0.2675198901337965 0.6762679913990262 0.0268565237278989
0.1134661702357070 0.6767319006896125 0.0101050898128417
0.0648604213180457 0.6280069915641466 0.7981272513030602
0.1841835616934699 0.6728174072906308 0.6754707413582107
0.0784824511470630 0.5622255630570766 0.1469691853513104
0.1943725973269867 0.5323627008139082 0.2964526513896044
0.2204166338957765 0.5656166701475557 0.5167814283609127
0.3807890802726656 0.5659064354333363 0.5081583085468819
0.4323531515288573 0.5313793344654063 0.2947006840861309
0.3165335305225562 0.5596850158285943 0.1586444770064730
0.0778738423177630 0.3295768593663598 0.1774403441100613
0.1989189005012115 0.3734443169427665 0.3098535798097686
0.2379306403387574 0.3333173913657857 0.5266888541043125
0.3920466292527550 0.3287179068774768 0.5155075501993275
0.4411767453451543 0.3735762810370102 0.3023398805037092
0.3216215822189948 0.3299762943631158 0.1784946004666292
0.9363555953401207 0.1308505609788371 0.1969612454042904
0.9324828824036101 0.3737246250825626 0.1977156583147410
0.3597356472750022 0.0654396244946724 0.7143131301714343
0.3086636244516951 0.0705386590871816 0.8956256382926396
0.1997934504723444 0.0587398349109342 0.0100459496179904

Structure files (CONTCAR) involved in this work:

0.0937218673248489 0.0738076255083584 0.8922590183634259
0.1052502451950486 0.0606052261366243 0.6955726632738066
0.2311499924896526 0.0384369971607150 0.7434866170874945
0.3580757799175955 0.8305157840554023 0.7438977582031363
0.3075455826281827 0.8469096434921976 0.9228235930617052
0.1899677040975343 0.8580718994948056 0.0116036628982591
0.0837217844556188 0.8345791549898366 0.8983942323680931
0.1047617392840274 0.8435392343965843 0.7035905742737193
0.2294931984261105 0.8616068896524712 0.7638594704884453
0.3237823441109797 0.9523224192778024 0.8035685894183676
0.0838383086351289 0.9536141309389857 0.8112033758860139
0.4343466559766723 0.1268063196980465 0.5790539339276685
0.4181861186631374 0.9956425419124295 0.5655950330702114
0.3996825576654570 0.8639583535445657 0.5617406532360616
0.1980658764226929 0.1336851434376883 0.6117894846824614
0.1858022241720022 0.0041051491649405 0.5631591071791151
0.1989968815310664 0.8695265508111210 0.5697134402337325
0.9881664651704319 0.0443421241793485 0.7774395399421261
0.9841801061212367 0.8671557292003523 0.7780280459222900
0.1431758183022274 0.9430730245381967 0.2168233949145777
0.1939180843782823 0.9322966219988450 0.3980238460629089
0.3003258396010600 0.9478933002357680 0.5168061019637310
0.4033322446348443 0.9305867917220380 0.3933710723851511
0.3957127596453845 0.9493802390445175 0.1966593957362764
0.2708961938130320 0.9713055049473588 0.2478097850218065
0.1425169551760201 0.1708980870535646 0.2423328587820824
0.1957078296290905 0.1659109100430728 0.4191858555983054
0.3116317994174774 0.1491344622864356 0.5126306936070458
0.4147737173909835 0.1746699898197089 0.3946644118123003
0.3956170611105823 0.1566054142610716 0.2005358482097092
0.2712164190061887 0.1402419984672924 0.2597848916232488
0.1778551397599795 0.0531081819293502 0.3170709184210911
0.4197784298923993 0.0520039242922103 0.3200353856703871
0.0687581048266711 0.8767151305663590 0.0864827084932927
0.0840357073001518 0.0074296862029343 0.0641531072406081
0.0991530792463289 0.1396763505913814 0.0604972317063615
0.3011183073536903 0.8749833053998526 0.1168184853743975
0.3133216576568005 1.0030971480454591 0.0646370176074623
0.3007645189785457 0.1371543105428110 0.0645133183474059
0.5117228659282941 0.9573846355206013 0.2829234342365403
0.5161857412273309 0.1399978897566287 0.2781533178181737
0.6427231062087826 0.5587080915577157 0.2818359513492614
0.6912333731791562 0.5701826153882019 0.0993757091810696
0.7987738121584037 0.5536283440588993 0.9832635147893122
0.9068942270634700 0.5784602005997124 0.0953306869196097
0.8950656050435097 0.5608486950317002 0.2925463381225961
0.7702572260403009 0.5305110016850979 0.2468732657979923
0.6452318951239308 0.3282810869185677 0.2512864878298868
0.6951433077706265 0.3400971131356086 0.0722067889880357
0.8113751093902816 0.3521279028384952 0.9790313975536595
0.9147350765956501 0.3230498123275757 0.0976972719580353
0.8921741041369998 0.3522253427726626 0.3127912230535705
0.7728541703492817 0.3602849293212935 0.2311019034080848

Structure files (CONTCAR) involved in this work:

0.6766181870558992	0.4486623182157930	0.1825211727149000
0.9178638947320882	0.4565079398661370	0.1702404296095249
0.5665666920681331	0.6283689516545259	0.4061471264801377
0.5753036395924904	0.4968903927649356	0.4303929682706088
0.6073257511233944	0.3673731474107607	0.4322995826357848
0.7971818129279202	0.6289166811865082	0.3742485556749437
0.8176891696189809	0.5011768996971558	0.4277351573777699
0.7842591286715315	0.3704033318082478	0.4294362085964122
0.0116781754041043	0.5480448181248435	0.2107815691497090
0.0156217032340728	0.3590643673031140	0.2422238384101278
0.8587671296608850	0.4367980661361632	0.7757974817855342
0.8025010345986604	0.4361757773595652	0.5983541559337625
0.6964942980209726	0.4623028165494274	0.4838903218658383
0.5930436601819677	0.4309706115438481	0.6014268992755986
0.6051756961929005	0.4441685057344653	0.7985519328575206
0.7306608835370242	0.4707712891017803	0.7549565338335135
0.8620669813422960	0.6764464470882975	0.7393054302542721
0.8054527895227171	0.6546491229626632	0.5675495827569945
0.6872190828323396	0.6477338524764086	0.4816835511439839
0.5810973551190607	0.6700240909129372	0.5944533916118387
0.6066451894365460	0.6609432618960375	0.7890181042477133
0.7323622096488782	0.6452575624930161	0.7328792916094887
0.8253535535384996	0.5529837488007597	0.6923437581778428
0.5838671333953461	0.5510616451898706	0.6819983607926923
0.9325575035926387	0.3737864111038291	0.9120512064458995
0.9153553456854091	0.5058501811859134	0.9271816179967967
0.8937381133524189	0.6373932018370219	0.9228681399947773
0.6989277895998295	0.3703236989672193	0.8790218057819436
0.6835216930413245	0.4980448882031627	0.9359586240643596
0.6985348863053372	0.6320854729836902	0.9257012188406105
0.4882571619638049	0.4607456117344588	0.7181633773710941
0.4849414297695715	0.6374250585270564	0.7201445608957104
0.6425237111074887	0.9393534757807774	0.2809814239822324
0.6969993066471724	0.9330346667433427	0.1023684062244483
0.8016090908857084	0.9443642395224361	0.9788352608907680
0.9041993972500576	0.9327832877125521	0.1043917045912535
0.8971973609995987	0.9437106557142894	0.3019057718553280
0.7713426555435553	0.9664283518874314	0.2568495089263154
0.6422618934047691	0.1723795077879128	0.2522034766662124
0.6937773350556569	0.1580578436204145	0.0732430984176087
0.8110900962229023	0.1467033265408491	0.9840838260913453
0.9188156418717174	0.1684356553500630	0.0931357632024757
0.8959518092196243	0.1657557484477657	0.2893054214151288
0.7713607934807272	0.1460230131030856	0.2334434958206098
0.6802609771555673	0.0520610115377425	0.1916471768347604
0.9163488253564880	0.0520272873293841	0.1888129693433388
0.5675531525234049	0.8757848733386773	0.4141360428519336
0.5833782300482732	0.0065774202568961	0.4315955403706528
0.6002894808822350	0.1385727182518436	0.4347411460687268
0.8045283244072142	0.8713882899368963	0.3888903920841345
0.8182384215240279	1.0008058019324579	0.4357242898399135
0.8044949465698943	0.1346677554540300	0.4266000703693203
0.0123538123938616	0.9600794659819530	0.2147967717912281

Structure files (CONTCAR) involved in this work:

0.0161158520034867	0.1382210453900321	0.2189072249518110
0.8570118510866405	0.0576479815146503	0.7787046890325615
0.8043130388772607	0.0721325876722132	0.5997913756251800
0.7016320924170077	0.0563670184092701	0.4742447940428663
0.6005381651423456	0.0714484161886117	0.6031085343295253
0.6051370240737231	0.0545833885360386	0.8007523453370826
0.7292815823539744	0.0301101569874831	0.7507005126628736
0.8576596205447153	0.8336088883872699	0.7580155846948409
0.8040102802588398	0.8339320238255942	0.5799329404601534
0.6896701106343760	0.8528726444017178	0.4831584395862211
0.5851394436675873	0.8296718929166488	0.5997496677280978
0.6046528267740996	0.8437000032981365	0.7948105205520613
0.7291373649843291	0.8619638901284463	0.7385736031668720
0.8208642681959407	0.9492242298667715	0.6754345391089857
0.5820387524039993	0.9509237333341253	0.6791308132787567
0.9314936246289163	0.1257114053160172	0.9067665701683456
0.9191127071382864	0.9945522315550799	0.9296389817940941
0.9037229155795676	0.8626118266907851	0.9390707915221296
0.7001457302934847	0.1286750060378162	0.8794028286354304
0.6867108341450152	0.0014987245592433	0.9349898452638021
0.6976577401825276	0.8673639121766439	0.9327163511892868
0.4905917762502752	0.0466784687799625	0.7117086856922195
0.4843935044217247	0.8642788804331646	0.7179998756595205
0.3572898013561580	0.4426645280377096	0.7203591024174258
0.3107122870226983	0.4342598440706839	0.9046965953710382
0.2001478119779617	0.4330632686178815	0.0175096698896537
0.0938104541622533	0.4301756346972681	0.8997776770380309
0.1068551679322463	0.4401915947897068	0.7026376932087436
0.2299311294195539	0.4680244391672244	0.7574868551647873
0.3586177788621159	0.6716136636802804	0.7433747629970460
0.3087712195072207	0.6642615682483785	0.9239206907949074
0.1908377948636395	0.6510410346136253	0.0111395772680523
0.0844385616096091	0.6703864777304294	0.8975610564068938
0.1063746054509603	0.6581142452933739	0.7033296823878247
0.2301426243272653	0.6438777728163095	0.7665699267405445
0.3230767417947694	0.5536975788248945	0.8164649164034775
0.0830965439013280	0.5491691353645285	0.8135866258505693
0.4327251824431110	0.3729635326401303	0.5967232074554716
0.4164225318750312	0.5027403727061288	0.5636587971012802
0.4015296685072567	0.6355085259256373	0.5630178892601461
0.2060658850904222	0.3742559982034363	0.6196503105289387
0.1869181960885271	0.5029921182068169	0.5760457148836408
0.2031293701939770	0.6363735715598927	0.5708069878289104
0.9890210389486659	0.4554255856710523	0.7818616343652939
0.9854595001814295	0.6362895701750303	0.7762987731154012
0.1414833186002538	0.5684242926735603	0.2228661115534116
0.1888629061182450	0.5673982366367566	0.4053710347586261
0.3006309246014829	0.5546768674547152	0.5130517744245189
0.4057075429925326	0.5709315055129163	0.3933492326035016
0.3936093930794362	0.5571692851634639	0.1954840534276631
0.2698588729363725	0.5422917189267585	0.2546469082041240
0.1443922563984489	0.3299178009934107	0.2482556231279792
0.1946921822722776	0.3494113337869941	0.4261644132779037

Structure files (CONTCAR) involved in this work:

0.3150176224728877	0.3555857304692311	0.5085345901021782
0.4260991670612919	0.3349587363478143	0.4065928560409811
0.3990927018939996	0.3377235035162374	0.2129588339185423
0.2736065755219814	0.3602844474165298	0.2665757477848114
0.1785835025549928	0.4521725280580032	0.3027669186649786
0.4188472122883780	0.4515920092782717	0.3113899903671368
0.0693786274397569	0.6326226450084232	0.0872326611193828
0.0923629212432829	0.5041560078140239	0.0641594411291849
0.0898746542243478	0.3715525365523412	0.0753369642213493
0.3011851417423090	0.6346422644690329	0.1176756619597854
0.3045520281946785	0.5054511539079943	0.0700364049524316
0.3100069101899146	0.3705652478398158	0.0750962019832482
0.5109888979769528	0.5466325964988035	0.2754516483318575
0.5206189557668889	0.3677269069105867	0.2789144928159969
0.4382802975598021	0.7505876868423432	0.6401128703568829
0.1973006200845863	0.7523268461178440	0.6597129907854137
0.2702759443824592	0.7550021874890152	0.0564808522838405
0.1093625400699490	0.7539236698419378	0.0479221093340997
0.0630622326264447	0.2527105412776274	0.1440673482805762
0.3043667583755186	0.2514493715522885	0.1602611944249556
0.2331333070576969	0.2543069913307989	0.5548185519407255
0.3940266213860320	0.2511466823768037	0.5521755731788369
0.5638304469558884	0.2530045464453167	0.3578295154452815
0.8026284958715544	0.2536919897989557	0.3440356627990089
0.7297643306002921	0.2492327101796490	0.9377584713676894
0.8921920608136751	0.2490605748615963	0.9385558124391027
0.9404967532534303	0.7510539064757817	0.8519486150233134
0.6971818817651007	0.7514487061718944	0.8418395544248333
0.7689779123230606	0.7493475008283048	0.4371206202551317
0.6059671951242471	0.7514531403092327	0.4438458101107205
0.0121271229360419	0.4718839709799278	0.4445963720056892
0.9188573865697969	0.3440267580807569	0.5472329741721188
0.9896633507356408	0.3690407382780445	0.4369931239628315
0.0112328226548212	0.5206462704575585	0.4454300113953823
0.8817341832581410	0.3479233404352640	0.5934472848024193
0.0864272820178630	0.3276523736704496	0.5805882440351469
0.0152797758858239	0.2718293335262663	0.5924890444739465
0.0849626309698270	0.2491428946487823	0.5115018878511538
0.0947051675894735	0.2507640192319648	0.6435000841968505
0.0694732252883862	0.2749799103043505	0.5803734445728618

Figure S2 Cu/ZSM-5

1.0000000000000000

20.0219993591000005 0.0000000000000000 0.0000000000000000

0.0000000000000000 19.8990001678000006 0.0000000000000000

0.0000000000000000 0.0000000000000000 13.3830003737999998

Si O Al Cu C H

94 195 2 3 1 4

Direct

0.4212825525090770 0.0561317673341371 0.6441535022839826

0.3042374174461980 0.0283765289033295 0.7917563228785008

0.2786933387903653 0.0630838068549574 0.0116858689888918

0.1182760299265263 0.0646011255251488 0.0074709835631245

0.0643114847598788 0.0266245535785336 0.7947034164895784

Structure files (CONTCAR) involved in this work:

0.1798874715544327	0.0548420301088441	0.6558805461599840
0.4183667748115866	0.8274317133416973	0.6659187652223937
0.3041324568391875	0.8703620557748152	0.8093741807518687
0.2680086433822045	0.8294799148624432	0.0280475701534355
0.1138477619312872	0.8265853405996476	0.0133152352378266
0.0641807141732265	0.8657025426823416	0.7969947199259324
0.1850363670084617	0.8283380138617645	0.6727808314804270
0.0763083295815577	0.9424342738426417	0.1469620399496526
0.1945558972410758	0.9707264862560985	0.2930449570841332
0.2193403552968188	0.9363067443610763	0.5113607521676109
0.3787831483597830	0.9321895819988737	0.5085996744603972
0.4334836949185563	0.9703053948580231	0.2994871127931017
0.3194236296462333	0.9450844353016131	0.1579127570922000
0.0802960169864970	0.1717455861613974	0.1640191352661650
0.1958109472281493	0.1289736950082124	0.3079565845000272
0.2308908516173626	0.1714817834884581	0.5245124087202925
0.3856144450597556	0.1730017428969747	0.5076550101830906
0.4352265476728817	0.1277879026603301	0.2974802654689234
0.3164232397153666	0.1693775261173596	0.1726100999565463
0.5771577831144817	0.5584466858275945	0.3510427214327298
0.6955222355926548	0.5282215847982916	0.2127111557685670
0.7166386789287209	0.5507181407796911	0.9831944246014573
0.8741220062359747	0.5644947837595732	0.9897178396433481
0.9305735983869140	0.5300343054622025	0.2016141274342301
0.8197408217403044	0.5597641783461418	0.3442183492117371
0.5809679671101692	0.3264823789426395	0.3287366329971061
0.6979179586840257	0.3709748212983808	0.1966988909266195
0.7341586050336174	0.3293740940912764	0.9799224057936327
0.8882085922852742	0.3303295041910306	0.9945916706315348
0.9367571047205351	0.3715348188532485	0.2064977499559728
0.8191753635825675	0.3307338034958789	0.3338168502824547
0.9251445904981573	0.4449292154766465	0.8566457218319620
0.8068701636898152	0.4690491866240108	0.7134923689185528
0.7812533258446129	0.4404771659682638	0.4915993150399562
0.6210429514656548	0.4336977895932477	0.4876951522076589
0.5647566924924047	0.4649472987188416	0.6989856332820252
0.6788223722699941	0.4341546675650710	0.8375550714465665
0.7993105838577105	0.6264584621470222	0.6966562153981722
0.7649016787948858	0.6692266462915823	0.4761692205015344
0.6099953828831601	0.6730132352375872	0.4867143647117093
0.5636682482248679	0.6232834239604198	0.7002482915280467
0.6770942661042628	0.6676084841021434	0.8316789772312305
0.5789074095639776	0.9416368694649261	0.3463007088113537
0.6949728710299540	0.9734582924324033	0.2036670415679680
0.7187364799595503	0.9505206990595768	0.9776998183885252
0.8790966172683321	0.9484200280161773	0.9852713322675847
0.9324105997217569	0.9694111894210956	0.2008483431613990
0.8160587920868534	0.9353067280568281	0.3300013953970650
0.5801094500130030	0.1736981723694870	0.3219897187257060
0.6981103944558419	0.1304594193648299	0.1908416502967734
0.7369450050883187	0.1677940843676479	0.9740634525878360
0.8921333800326634	0.1761359543012392	0.9798436148112254
0.9380346001818859	0.1280433018913653	0.1968983562749870

Structure files (CONTCAR) involved in this work:

0.8200982745158939	0.1749017204800377	0.3232566321303356
0.9225563817751345	0.0663346750438480	0.8436783475406002
0.8073680157790835	0.0323421584194911	0.6972242018190061
0.7830309527716244	0.0594244790457128	0.4759207855232692
0.6230712025486658	0.0671938050166854	0.4813160895750069
0.5656471695058600	0.0352396780477993	0.6924337455242737
0.6828762958395181	0.0661802821243393	0.8220834085155772
0.9156640978330958	0.8307337131738906	0.8321151446173618
0.8019534838608211	0.8737841183284345	0.6905280433059471
0.7663094457774505	0.8302167618780327	0.4771023391706373
0.6100090843746848	0.8278689516684371	0.4893736488525469
0.5605054041645019	0.8768724152321462	0.7015821380828683
0.4209435621583755	0.4424197903617286	0.6490931759772811
0.3043321723316928	0.4717978207341661	0.7954269124771732
0.2810123593638795	0.4368944294564330	0.0164262959419532
0.1207658072057781	0.4334797814515730	0.0119032746381189
0.0689631817679116	0.4703749752394540	0.7998819917002162
0.1813040853997414	0.4451142230781717	0.6586930137854655
0.4199104998693486	0.6730561750649182	0.6677399083271575
0.3067087563203963	0.6294374933677791	0.8121502829368905
0.2682785156332340	0.6711489360752670	0.0291859655948419
0.1145396255882794	0.6732363047820191	0.0102414546675691
0.0671750891544424	0.6294181644338649	0.7962891252995281
0.1876415322491378	0.6700815198078682	0.6723375660968491
0.0758894853333901	0.5576054971099786	0.1443606950633240
0.1932660740829760	0.5284760983514418	0.2923675934888625
0.2204692759667151	0.5624226286115314	0.5112949810250067
0.3795706620649226	0.5657206057709687	0.5110970534161644
0.4340018458631396	0.5298886214410039	0.3005308317682890
0.3193854965102028	0.5561947764493945	0.1601088095101613
0.0801465118335384	0.3259447489532916	0.1684027767193287
0.1958097189938633	0.3701448356212301	0.3091212211614180
0.2329726686347244	0.3293728262100195	0.5263340154190053
0.3877961087584037	0.3260744476843980	0.5118526199067464
0.4374870152129912	0.3719666066716819	0.3003229383729084
0.3180586965215466	0.3287494972218404	0.1754955858535878
0.3557236951254443	0.0638071528563152	0.7146233315650019
0.3080506534122206	0.0666948813465740	0.8987473894186460
0.1982951095620571	0.0527940817631779	0.0104832003678919
0.0917285733065061	0.0652774822486344	0.8934330174082787
0.1037299222762509	0.0538850102511734	0.6970100683030408
0.2287232541748422	0.0346206045449120	0.7482920885940035
0.3573078858942199	0.8268371805404474	0.7457832392035377
0.3066233045447005	0.8447179216290197	0.9240320106346852
0.1905157180615712	0.8536963828111681	0.0189846230534993
0.0890259577234523	0.8292899850235006	0.8985141182548120
0.1067426910105825	0.8386314032218160	0.7017124269963808
0.2293349434484798	0.8591319792286821	0.7643333778365385
0.3236132607440022	0.9495269491879541	0.8040963626663753
0.0737560570238588	0.9461946996991369	0.8091466224909911
0.4298440324438780	0.1237913994524655	0.5774620404838838
0.4162442906464676	0.9918297957920309	0.5695911623858454
0.3930263808668524	0.8600934626413785	0.5609514510457060

Structure files (CONTCAR) involved in this work:

0.1972007420920626	0.1296137751401788	0.6153005514415181
0.1858484190269534	0.0008730864931712	0.5656151417207096
0.2015468407213548	0.8669402669618488	0.5689308002670235
0.9858882356964231	0.0435100321970002	0.7765776057858808
0.9867833099244215	0.8450659867531815	0.7777595334889170
0.1423444483407595	0.9361378022935729	0.2162456028629709
0.1894929168160913	0.9313929613441807	0.3988916373567264
0.2993996449936097	0.9481357470438785	0.5083048370107192
0.4069750637048730	0.9279662226333327	0.3953321775566295
0.3956476895737606	0.9464095622172548	0.1984717337293656
0.2701195118895929	0.9644872503934182	0.2500621399750924
0.1436671795671415	0.1699968501734515	0.2389040504907251
0.1907163263189656	0.1576649607934952	0.4209915755222876
0.3081637983842631	0.1479436201651990	0.5096819120519173
0.4132599102926158	0.1723048592540339	0.3937123014808258
0.3942238099631402	0.1536594948778812	0.1996248852287805
0.2709679284070960	0.1403161117578536	0.2642938105422866
0.1763691775861423	0.0497825681200993	0.3065966632091184
0.4188856588224286	0.0494794212670605	0.3206493140214299
0.0669254259990352	0.8730030857397481	0.0842523932155725
0.0820123763593442	0.0044026948358662	0.0685322856936297
0.0988661743848127	0.1361190537789213	0.0582558230845556
0.3036779907173748	0.8698106486979237	0.1184136607574302
0.3118884141224990	0.9988512259756492	0.0674416502030476
0.2969949071706723	0.1329271622048511	0.0680286535706976
0.5124164156421244	0.9567227422795344	0.2808984487710596
0.5145748785317378	0.1368190329790758	0.2756276566641850
0.6417624732890101	0.5696377413948439	0.2786268705933058
0.6912004862986829	0.5566003585357185	0.0981661404549787
0.7965086951429220	0.5413453132887156	0.9731447879117521
0.8962298866168695	0.5663239088492933	0.1054746022727176
0.8959100704029556	0.5569755278907751	0.3034607471780972
0.7709362228412006	0.5402663369615759	0.2510883928037370
0.6423627972937811	0.3244504739722629	0.2497627340221619
0.6953120946694599	0.3565713503634302	0.0780970791502540
0.8110011622947256	0.3557546228836190	0.9864598680828790
0.9122430135997699	0.3285422317234654	0.1101018074430964
0.8970138638952772	0.3442158400777355	0.3044547609660445
0.7721781540497309	0.3554507619226848	0.2405798126342097
0.6775565736423832	0.4490038485552237	0.2168119049062787
0.9187234708412552	0.4499314246022429	0.1879765362478097
0.5633239578466666	0.6263988520449643	0.4152431152017426
0.5883409762712569	0.4961873837568464	0.4273540466168572
0.6055732932709386	0.3638055462175912	0.4300428421405197
0.8035717944062808	0.6351207496160598	0.3824058788862062
0.8104350168589050	0.5056995784373952	0.4337031607595508
0.8008676747206023	0.3715749645965222	0.4345286281055497
0.0091970898878201	0.5476129639447942	0.2114075800832959
0.0166628110262757	0.3624964241650171	0.2223253492313833
0.8595255732244875	0.4322860462926408	0.7878208493509424
0.8142451473537534	0.4378784610046514	0.6021437985166544
0.7005899482170940	0.4465379844534866	0.4983458104863583
0.5871843859835516	0.4273233795775707	0.5969316036866353

Structure files (CONTCAR) involved in this work:

0.6039594201527559	0.4316435823868955	0.7929114412407967
0.7306260102981199	0.4555405602648452	0.7503584852186993
0.8512701324181690	0.6766596238469239	0.7465076858149209
0.7956962421762274	0.6385143247260094	0.5776158089355796
0.6865323355559524	0.6482601296031555	0.4712360713097983
0.5892713284592294	0.6648288099654249	0.6033085346615150
0.6000013349727116	0.6525880444977824	0.8005300060326321
0.7246311137121250	0.6360980190982688	0.7458332218473528
0.8222814772290524	0.5488369809228075	0.7160769882263234
0.5826719337854599	0.5443555309224833	0.6885873542171079
0.9352392985353262	0.3804081332635210	0.9298173315796893
0.9189595919418858	0.5118208413294781	0.9264125013155574
0.8915795648079720	0.6386024210586436	0.9417883297232230
0.6980527004250345	0.3610182302907108	0.8821515465324976
0.6791058610847653	0.4906611830370655	0.9264802511907717
0.6915562974667065	0.6251891367461969	0.9398757859692700
0.4857474366365725	0.4537570235876959	0.7200694370634955
0.4836561408761935	0.6320725829153834	0.7125205073462271
0.6412760343909504	0.9318602855459516	0.2696197120495070
0.6828306121806081	0.9576179566274996	0.0860750288311877
0.7987409569001888	0.9586608352936468	-0.0122591695727503
0.9074352544717667	0.9359575873510025	0.0966712474201502
0.8935608735202140	0.9353926191987364	0.2944694198629856
0.7702720105905883	0.9495665303720852	0.2311288571802973
0.6377623871418410	0.1753010747651047	0.2361611959639422
0.6983404521279163	0.1357878153908824	0.0699507969033865
0.8156200431190840	0.1475735468173510	0.9786815701214056
0.9229916033313863	0.1628791571506221	0.0897091171448093
0.8967186223663660	0.1668403663165423	0.2844311698829268
0.7703507201428401	0.1562384073002265	0.2308423754672072
0.6857954906060049	0.0531993733582640	0.2261200431121007
0.9161915390845555	0.0495439959315667	0.1969139752308870
0.5679316214787932	0.8735278149304488	0.4106560556674834
0.5922721895865487	0.0035125537553528	0.4220673955766072
0.6071757993152616	0.1360062776147425	0.4211556321260956
0.7972356645838610	0.8626465691799258	0.3759101961889273
0.8039845246290601	0.9938941645930228	0.4118288415913290
0.8060911914883238	0.1274829058054834	0.4190411549658914
0.0114198231609945	0.9547000875087150	0.2172868198371315
0.0177110041922975	0.1343026869622152	0.2187450044400247
0.8575916853579009	0.0717037692943578	0.7721275941045080
0.8207120823486108	0.0567601945249191	0.5832476918715815
0.7030482926064834	0.0587603894080261	0.4928278532846375
0.5878781044874777	0.0726006435989925	0.5896363629917781
0.6061420703724169	0.0695146341421064	0.7847831460003918
0.7308457172498356	0.0516739372762828	0.7267090707078845
0.8594586947975047	0.8297618162419850	0.7463679492803733
0.8080511315499304	0.8596566679189304	0.5710259768759605
0.6879646259266965	0.8510083135390822	0.4861680907795064
0.5812103098803234	0.8349248703302287	0.6012546722331819
0.5958868545113446	0.8466756895493156	0.7989753669684443
0.7294688846652606	0.8546919910095381	0.7311878812641636
0.8204065753921430	0.9526565264635674	0.7110329521571270

Structure files (CONTCAR) involved in this work:

0.5811262574738820	0.9555255098832189	0.6837488216586567
0.9362170034127095	0.1394303173396910	0.8938167908222884
0.9122126576222159	0.0154221639167194	0.9376416145088782
0.9014070457119003	0.8854738253574655	0.9176762171120642
0.7028721959481360	0.1371033247430329	0.8741876740550752
0.6887584050712452	0.0047133666434939	0.9015802953253627
0.7008156401688388	0.8736831395041310	0.9403577328561560
0.4867994387619337	0.0481404451916146	0.7142614549497445
0.4792742244474514	0.8709913893835517	0.7124984649494102
0.3549555244877363	0.4351282113538242	0.7182938739310019
0.3076128064157077	0.4332817445970212	0.9020979627790260
0.2005425778489177	0.4458553249143078	0.0205230448989300
0.0980538621313264	0.4298343596890630	0.8961437862845972
0.1049716040156266	0.4432083855295602	0.6989828750119340
0.2288502485294332	0.4672125849194487	0.7517863872456555
0.3616976468517550	0.6725454170415132	0.7515029088383933
0.3082455889680461	0.6550751267419287	0.9266967878792516
0.1911921121961184	0.6463065706928973	0.0180823708614815
0.0910388729931625	0.6713799152773766	0.8949175493364894
0.1101207031582077	0.6558643858238317	0.7003154558017417
0.2331562642215244	0.6412238248320568	0.7639293265099796
0.3259143409204415	0.5501122759657495	0.8072465438301061
0.0827320248990645	0.5499955974740198	0.8158316440026298
0.4309112432745357	0.3731673904200004	0.5866961763718523
0.4160221184341901	0.5053127425987527	0.5719071853851517
0.3930947398630335	0.6372517408641796	0.5659453132207516
0.2013713597779596	0.3709190397055615	0.6189198037894710
0.1865263183060639	0.4993381480346034	0.5686692323583377
0.2061450270462562	0.6329218740317549	0.5678724921199049
0.9898855970060619	0.4542836374198987	0.7858179212779193
0.9896172348534514	0.6428947127249950	0.7760120012512212
0.1404511165761311	0.5639015012393980	0.2170262719421907
0.1886992364946405	0.5660394397982300	0.3997640571615532
0.3004175923891220	0.5493900457212003	0.5057249716685985
0.4100905612598150	0.5705995987042397	0.3993266923857504
0.3952010775535229	0.5570008992407959	0.2023937501279471
0.2690343689807460	0.5356752122825550	0.2503321317156307
0.1425290255077845	0.3265016045269671	0.2454671588840684
0.1921699315196212	0.3457183778510749	0.4243572366640752
0.3105295795927993	0.3516245346009938	0.5102970025176966
0.4186855060539676	0.3301605091590469	0.4002758104791678
0.3958403481095411	0.3414341398195043	0.2062190962395432
0.2707830542106248	0.3577165590470398	0.2651975669870301
0.1754643171218221	0.4490270667027822	0.3019484332422587
0.4186192595824196	0.4504512876553310	0.3170955409127739
0.0671948330949250	0.6261634988862483	0.0796921056876051
0.0824073374256991	0.4946265143564329	0.0679366706643753
0.1003011367992693	0.3630536879665996	0.0646803534467853
0.3028337077450724	0.6312736680347794	0.1208849133418406
0.3145335591058266	0.5020505357579869	0.0695718466121015
0.3021843447662149	0.3674110497662701	0.0713660297348586
0.5130436673580877	0.5430096330153700	0.2807060705627772
0.5172033218860244	0.3646777598256344	0.2785405674818594

Structure files (CONTCAR) involved in this work:

0.4403442194925138	0.7501492313143295	0.6432678309220012
0.2017481261464789	0.7495590881804389	0.6566514654250891
0.2719785430348975	0.7503745651391248	0.0545986190488210
0.1088645193664444	0.7495775783802531	0.0522950484553711
0.0609453627571186	0.2491862512502602	0.1405940486801041
0.3044012446966548	0.2493621867486794	0.1585995494275110
0.2270623730258086	0.2503584206595098	0.5534839267049557
0.3917701993638908	0.2490264380118939	0.5508207064231990
0.5610720975079045	0.2497240889948536	0.3550635447727816
0.8069026655807222	0.2519104143241924	0.3572730974070330
0.7295057877408516	0.2486782225348813	0.9730523178757197
0.8938604428144495	0.2549888551823161	0.9509860335585008
0.9176687798237647	0.7561142603773380	0.8870990051859616
0.6901639085528987	0.7442882807657649	0.8614162974868681
0.7741669383623254	0.7494859951146755	0.4706162682342885
0.6015335735832393	0.7504488967896957	0.4530938214639897
0.7975245184467412	0.6719618244363809	0.0654564744108777
0.7010927170486954	0.7555168234517895	0.1393063456168963
0.8124541354109571	0.8000864565023050	0.0134278251462754
0.9184610494556789	0.6753316942116414	0.8251551748113264
0.6780524725313328	0.8286939868795662	0.8266507249154373
0.7078097974348172	0.6852699285051053	0.0600857529715444
0.7255071048320418	0.8125980586660092	0.0449670758735192
0.8509161374491621	0.7214887394132115	0.9875429366182881
0.8724122247613085	0.7525894209996653	0.2405642359092360
0.8869164739018380	0.7044641627645001	0.2070988380349696
0.8926106610047652	0.7943335127097292	0.1963786201147831
0.8177954083000002	0.7558235714911290	0.2412141337886085
0.8914561903123422	0.7554219232954057	0.3171879505126763

Figure S3 Zn/ZSM-5

1.0000000000000000

20.0219993591000005 0.0000000000000000 0.0000000000000000

0.0000000000000000 19.8990001678000006 0.0000000000000000

0.0000000000000000 0.0000000000000000 13.3830003737999998

Si O Al Zn C H

94 193 2 2 1 4

Direct

0.4218186602566483 0.0599765837453815 0.6483216376438793

0.3045098407176811 0.0316041740610530 0.7921584561884162

0.2816092984760112 0.0571455974861769 0.0168266121053747

0.1216984391702727 0.0641716913584923 0.0118705092302155

0.0672759849947027 0.0309570096465680 0.8004621133454539

0.1800169218185337 0.0641266608096812 0.6642833501239035

0.4184374587658655 0.8273684480357085 0.6692939635693143

0.3009863083629723 0.8728496697282359 0.8022135701270008

0.2669233467132521 0.8305941574840643 0.0211194616427317

0.1111550922781760 0.8263008756285022 0.0140138964539082

0.0656763473284197 0.8737352614645392 0.7998728938205825

0.1793098979072175 0.8287963753029006 0.6664870174770315

0.0756779556501185 0.9416012217208649 0.1486680320217622

0.1941868545115464 0.9701904163859744 0.2911830586290219

0.2166685091549052 0.9429608047653113 0.5161636441790397

0.3769358102533380 0.9352825943117258 0.5135453095368279

Structure files (CONTCAR) involved in this work:

0.4329991178338163	0.9689019501462639	0.3015596570070841
0.3194176544011040	0.9362324373030165	0.1644409726474330
0.0805924211563433	0.1738916081595001	0.1666709525874735
0.1972239736037142	0.1292316106065660	0.3015660516686485
0.2310972049594215	0.1697302544582064	0.5194813184215701
0.3864156939523221	0.1737950099437527	0.5092510138574652
0.4348494698593821	0.1273408848832860	0.2962900129375161
0.3185846957233144	0.1723749127638062	0.1667348161229552
0.5775054869824235	0.5558362808398902	0.3551589514070135
0.6911218250733041	0.5277425559219380	0.2026261228410793
0.7152637914808595	0.5679648479290031	0.9863039535253645
0.8748207243440888	0.5695023050687067	0.9876644864214245
0.9255958490100445	0.5280814540849544	0.1953800001737369
0.8130970988530976	0.5537017592508607	0.3420558319186247
0.5736937386479580	0.3292234684695057	0.3322678050835507
0.6954018629928083	0.3732302177040723	0.1954664897737745
0.7320337497964845	0.3278198782466991	0.9787958033421839
0.8865167833262791	0.3257904953715387	0.9839894256445418
0.9395919155537096	0.3720966238526420	0.1892518752525577
0.9209712795037864	0.4452250566750044	0.8561945226029670
0.7994560887795126	0.4742686285729383	0.7184515131385206
0.7808474276271752	0.4376737119114161	0.4926884329654861
0.6231252179621396	0.4295115542031593	0.4883235995026947
0.5710176053348196	0.4695047983509038	0.6996680134699363
0.6753566705362396	0.4468819320329809	0.8566854813309591
0.9213544886983107	0.6770413091000772	0.8356354123596391
0.7678688795994902	0.6708248433034623	0.4661653745958485
0.6132051670007631	0.6734149445160735	0.4879650155909489
0.5600955692308818	0.6276268371290011	0.6980754685845524
0.6705992221457083	0.6752393691490776	0.8285363088181121
0.5773510470922627	0.9453802558236336	0.3580102451233241
0.6977043803580567	0.9745773163324694	0.2152141818725288
0.7190827825450290	0.9396184633735993	0.9932687828405018
0.8788043207021171	0.9351726102652790	0.9947298252829985
0.9309624684484120	0.9720127370943801	0.2048836966980963
0.8218097916451123	0.9464455600094366	0.3538329034752411
0.5779993249182674	0.1743050878164580	0.3294894057139346
0.6971036145968965	0.1325863711972431	0.1933842661315454
0.7324198053139656	0.1712418054636936	0.9720997530485758
0.8869683624513046	0.1731058670000284	0.9828050218831722
0.9348057476178442	0.1305216205759447	0.1982077189324407
0.8185937154930053	0.1739849686883239	0.3324468001221187
0.9230758235828611	0.0541405820479787	0.8553990042734587
0.8015905936935550	0.0253872656063438	0.7109090401282960
0.7807603091714806	0.0644548175899406	0.4924459397453928
0.6205280023947116	0.0697257217052320	0.4899182910581839
0.5671670812516012	0.0329086634601614	0.6986380666519084
0.6778755696293043	0.0543874259690564	0.8489200746386955
0.9225232738689781	0.8295793410396886	0.8385135821483093
0.8029947902268353	0.8674516558663958	0.6958626773551614
0.7686578657006451	0.8280014982266246	0.4774150341091632
0.6139999220284754	0.8273027908041843	0.4901722906820191
0.5631334641605286	0.8758122704436307	0.6978884643308433

Structure files (CONTCAR) involved in this work:

0.6779208875358781	0.8332893140743564	0.8338394781662317
0.4238659644089639	0.4421574461298270	0.6428769399770962
0.3061703830504964	0.4694088962808916	0.7879163130125788
0.2809345147670015	0.4447605819096888	0.0123996967293529
0.1232255170498668	0.4363565598105967	0.0113589389916410
0.0649817808283197	0.4703922961277769	0.8016932038051318
0.1783091286449881	0.4368720509450779	0.6629135417033618
0.4149918784418186	0.6735814814512818	0.6666490740492806
0.3003516084628786	0.6278220618041612	0.8009125550726794
0.2669899113344767	0.6692913126362211	0.0201209629563153
0.1115432012183080	0.6725580306404322	0.0108520251502908
0.0642427870172900	0.6289255028754605	0.7967639861081734
0.1793711922732299	0.6715677779494493	0.6647243466133342
0.0722451694863741	0.5574638064994009	0.1473549094645404
0.1913492818421323	0.5307320277931619	0.2893616838464447
0.2148191505590205	0.5568631394361940	0.5149590767110931
0.3736255175518775	0.5662551700498145	0.5133016233418496
0.4295745558483913	0.5307180673215377	0.3046792241071903
0.3188730862732854	0.5634627566507028	0.1625602451098000
0.0849987082296918	0.3270080567421788	0.1599532432759562
0.1966052709038106	0.3719090422694398	0.3004756578295972
0.2299879583960079	0.3309683634622007	0.5194518418344745
0.3844751064897247	0.3274640711350486	0.5064369970640649
0.4301789464154296	0.3736879345253175	0.2947124580024558
0.3164077159589819	0.3300762904082334	0.1627285407597893
0.3579571664824635	0.0702637466167305	0.7215194727740466
0.3156895482387854	0.0547412277873973	0.9068830085230333
0.2012626574472204	0.0499265376801638	0.0078128327857451
0.0916800226160384	0.0703313556889413	0.9000703967495776
0.1032820750422190	0.0633800889279629	0.7030384461925753
0.2287817686101385	0.0509287727814671	0.7595984152403938
0.3596293741900451	0.8278230629361752	0.7527263530365785
0.3013236591215753	0.8614828742063839	0.9216390643803084
0.1883653201089810	0.8512253365577028	0.0235581346492809
0.0880962253870437	0.8319188266132612	0.8983887815779291
0.1024893750657490	0.8411909569658853	0.7025481187169774
0.2285617691726173	0.8508184051007665	0.7578633763109278
0.3159446061728164	0.9512570690501755	0.7773853775245783
0.0876092472845998	0.9519890639242102	0.8113041797533274
0.4321146020274012	0.1275377631137700	0.5818284967877676
0.4121025163509053	0.9962414875487968	0.5741448034491472
0.3929292036480282	0.8642386788918760	0.5680188588373355
0.1957519494518774	0.1375488800435646	0.6171838506476195
0.1896272081484709	0.0057416981102189	0.5813154312342310
0.1950550438240086	0.8720412192899635	0.5665658674740024
0.9873537311612972	0.0397016309633749	0.7847209368775545
0.9851177567675391	0.8687992820132250	0.7864625569368208
0.1399786804752313	0.9321462117063585	0.2212437591473068
0.1831369863959344	0.9472296109172234	0.4060661567407880
0.2971930874395328	0.9480567003914523	0.5084397989230436
0.4073735942975323	0.9311884775901015	0.4019067720930530
0.3958233670106160	0.9370588870564417	0.2046809043681839
0.2696550539631429	0.9498133261174326	0.2585385686613546

Structure files (CONTCAR) involved in this work:

0.1394460955361430	0.1741780554441120	0.2500176031474624
0.1938812073887313	0.1406342292156954	0.4210351561304472
0.3093492802715541	0.1479148823938138	0.5154178963602367
0.4128258488969966	0.1688700878352223	0.3952840826809507
0.3956156315000006	0.1584852370538544	0.2001653109429149
0.2703721156092989	0.1518822514218439	0.2603428901802701
0.1836066738785718	0.0506282064530785	0.2761149282790505
0.4155390732127460	0.0486036369565232	0.3102302743024584
0.0645781236979975	0.8726035375263207	0.0854820677875953
0.0854559137126386	0.0028405786883421	0.0701023306672490
0.1060699796027055	0.1345437516217022	0.0676995213224644
0.3044074781303030	0.8625146145902418	0.1173703566537765
0.3102805731638358	0.9945440832624410	0.0810346480649984
0.3006297446832598	0.1283615012419493	0.0683919244602601
0.5125843916924504	0.9566873437797291	0.2870220744420689
0.5148959954988175	0.1348545684794319	0.2793392389525499
0.6374342375782934	0.5639736110809069	0.2750150332209497
0.6997109951564953	0.5748315630607382	0.1047986531413591
0.7953271577959719	0.5607243653543683	0.9661763986725247
0.8895843421005816	0.5715948704900892	0.1074540105362182
0.8890132493051138	0.5427478677172514	0.3032006067714854
0.7626716548771711	0.5250071934024606	0.2603193407900411
0.6379010865812508	0.3357555867645203	0.2606208918241031
0.6973646008826714	0.3359421903118729	0.0871275397670258
0.8096795226750679	0.3529297563865658	0.9824664587636813
0.9142831134712743	0.3254706925697300	0.0973073384370846
0.9066939021821049	0.3465127656761557	0.2918464260010016
0.7662600656753753	0.3707984774371159	0.2505754232202060
0.6707000893073605	0.4511202277882319	0.1765847909812564
0.9181230901200224	0.4496966803994274	0.1658825836087792
0.5684325864387588	0.6264318821266426	0.4147561589750800
0.5947736472144668	0.4974027224054451	0.4362097384115650
0.5875468638110100	0.3638971873278439	0.4409831203917242
0.8007928499194880	0.6321038253752705	0.3703781796937402
0.8020219611379591	0.5144300852886965	0.4515291392611996
0.8330564138083207	0.3856724142781776	0.4404987851012505
0.0034439662758264	0.5487432277882379	0.2107447222316908
0.0205405186023230	0.3694334431401881	0.1966662186291091
0.8556178150090602	0.4373829743482563	0.7852224581841126
0.7940649779108018	0.4356901828357856	0.6115078832880901
0.7035930926323931	0.4237686405967768	0.4661279199827925
0.6091056487150728	0.4315664983211111	0.6075176871198827
0.6021003655236651	0.4447425739195945	0.8054617001458239
0.7277029226353839	0.4729489953729851	0.7719038081027857
0.8594540517354503	0.6791831613296379	0.7606526688285631
0.8125062738847937	0.6484823029704098	0.5650315255763557
0.6910120354084444	0.6473553893362687	0.4842893676218954
0.5852081364327083	0.6694707126417319	0.6008624756974250
0.5926556389268843	0.6603451642966907	0.7982086236025134
0.7172583213359297	0.6532925899646131	0.7359015834429519
0.8212946035972749	0.5517706016004262	0.6947069519577485
0.5823050409240421	0.5496592884961565	0.6848217493555255
0.9322789539352071	0.3746887336772463	0.9145878051214592

Structure files (CONTCAR) involved in this work:

0.9131181950967002	0.5058647386032125	0.9366883685156998
0.9028777244923100	0.6388210117430314	0.9402818022322694
0.6932108844651045	0.3721826111250962	0.8952532060568097
0.6772415198803190	0.5003736755394982	0.9480328155119269
0.6876118596961776	0.6341066887429904	0.9305581789132602
0.4924074796234832	0.4509901146912464	0.7053749898396064
0.4792494703980573	0.6316553984889992	0.7068803177283673
0.6433737065337953	0.9399319956454435	0.2886166496020173
0.6980078047862334	0.9341254853298098	0.1099132287039890
0.7993870648007139	0.9487388434257886	0.9810848467086836
0.8985686348327384	0.9304691171881582	0.1119268974944029
0.8971162448080181	0.9482726683728177	0.3093223204542853
0.7713311029321344	0.9691341150555185	0.2650438358348640
0.6396382452454167	0.1745394948854937	0.2514346433616750
0.6960014286184747	0.1569002306195466	0.0779654213977395
0.8099440282467809	0.1468152807523525	0.9794499298899700
0.9138761186415008	0.1700285416244785	0.0967246015980411
0.8953027826377079	0.1610267731885139	0.2937250544222017
0.7697018260424997	0.1459842382013266	0.2430829964199506
0.6786737916664245	0.0530007706556361	0.1986401336907508
0.9175973453192833	0.0512813528994460	0.1847161788801675
0.5687194205638556	0.8752352716758792	0.4193767585760934
0.5818716513546174	0.0070116450689972	0.4375645752285059
0.6000412705040590	0.1391264819065865	0.4341212931258400
0.8064260020929012	0.8704387083647908	0.3914168166113622
0.8155744741274727	0.9966852878706500	0.4487044469731487
0.8066193029500208	0.1303203875860955	0.4340825007624148
0.0101313784634200	0.9560657066226121	0.2161409118585522
0.0148413742170222	0.1392302992505304	0.2156629484181867
0.8566196620428321	0.0559026682160253	0.7867567335897472
0.8014666919774877	0.0702593070053967	0.6096204251846162
0.7002144916294322	0.0568178362076045	0.4808452052820564
0.5980036667811430	0.0761875577155906	0.6061507846032246
0.6028864256010847	0.0531403259797149	0.8031849529504276
0.7281914961216986	0.0283417584974987	0.7619305369648399
0.8603647151866622	0.8312732077880829	0.7612866603343652
0.8052041259261169	0.8344484270194951	0.5849941528983407
0.6914283162729631	0.8527272406027084	0.4864424363408482
0.5876218209577320	0.8295528158168167	0.6046630463451793
0.6028143115061486	0.8540951847939092	0.7986573473508005
0.7299281910405967	0.8544226185070223	0.7453022091272685
0.8184581171215906	0.9472513468906342	0.6866374303100489
0.5785147469548891	0.9539263921889660	0.6719898266235281
0.9323980251909678	0.1264835454727569	0.9100762691367709
0.9190062104478064	0.9964513266255096	0.9414655857227107
0.9003918197286763	0.8646832633507558	0.9430585815217817
0.6953757612329626	0.1305206205257405	0.8829539565058370
0.6820732416116519	0.0048441644165426	0.9453288745947509
0.6960350490029039	0.8712280524930461	0.9375260157690003
0.4883347145849325	0.0484716769180628	0.7149825328666917
0.4836119705939685	0.8648061160536983	0.7158373979366939
0.3614122298795809	0.4317068233407944	0.7190152133545431
0.3158694249768946	0.4459330866454645	0.9029408662929536

Structure files (CONTCAR) involved in this work:

0.2011043707531951 0.4578384889368218 0.0015685050493440
0.0889993885275402 0.4320979483128504 0.9020263083206154
0.1023184062282889 0.4376695218985012 0.7056391190325055
0.2306433932450879 0.4500300509394778 0.7537038801156586
0.3580823764387691 0.6747730451758422 0.7530452235264855
0.3008019331766902 0.6381175237573208 0.9204240963988759
0.1886098743510412 0.6477373254829236 0.0228180633372049
0.0897235960369764 0.6698766871079599 0.8943326044257272
0.1021274972057319 0.6581043494882806 0.6980219117278654
0.2274242345058645 0.6485330283663939 0.7569758131183802
0.3168972541122242 0.5499432636927931 0.7741988017987302
0.0828291423026071 0.5498317924715002 0.8101388265898498
0.4322072670747757 0.3761997553580145 0.5722928386379478
0.4137362275258539 0.5080593661173903 0.5730804851300626
0.3843030768784301 0.6386545148660381 0.5667392332600848
0.1921587035651980 0.3633188050205881 0.6151132550996071
0.1835634468734124 0.4956161029183337 0.5794362445739788
0.1964433691952130 0.6289119267568078 0.5645847075136601
0.9850834822331586 0.4601334754088921 0.7846681960806616
0.9842208277560101 0.6378257905022783 0.7820178792890495
0.1346196586748652 0.5684284447378327 0.2232254128583785
0.1821455576828632 0.5543077520608416 0.4043063787533218
0.2950532441116829 0.5469117104091742 0.5096232252073497
0.4031570834207204 0.5720559775789780 0.4012436375236976
0.3946416239638570 0.5620826206758873 0.2057099142530420
0.2661645683214400 0.5506890936981156 0.2532751158875946
0.1396439628245589 0.3256970360325973 0.2494572373296502
0.1947236749470354 0.3598747298329605 0.4195611770257798
0.3079674385132397 0.3537823856047562 0.5193090781394338
0.4059334255879450 0.3289098871918811 0.3896092350954072
0.3933619898037381 0.3468454648248286 0.1937844090830536
0.2697277799347467 0.3511993111061898 0.2575711966414523
0.1809346593481967 0.4502432494564476 0.2756142348085194
0.4100765461136652 0.4516611993748329 0.3161476294245634
0.0641534987619643 0.6235905141252334 0.0770065009393116
0.0834804621257648 0.4917316799083293 0.0776108932289850
0.1174807057170814 0.3623857876035130 0.0616166223945148
0.3053351582184634 0.6373709260143677 0.1155469510854955
0.3121679687375871 0.5050490354117259 0.0787547009239230
0.2953350686312900 0.3721652582339101 0.0635930280393539
0.5098537291870588 0.5385238077136032 0.2943314874362575
0.5102431637435603 0.3662122628472657 0.2791185514930352
0.4365278667118879 0.7501571388211840 0.6408092267139197
0.1906304780640080 0.7502461149307036 0.6388876225331351
0.2754128687688334 0.7498802064542173 0.0228274342443901
0.1036110449720729 0.7489968353097415 0.0509004302401811
0.0642516008032180 0.2505090677648371 0.1330124452714375
0.3080039143100259 0.2508337313407547 0.1377147001110473
0.2234574297970077 0.2503589328837319 0.5252353741487225
0.3915786616538409 0.2510713879295228 0.5470741217285828
0.5563845013818121 0.2510718556081720 0.3535910438469450
0.8054767753062899 0.2513376112671971 0.3570910028214710
0.7279448089713243 0.2501630141831065 0.9434060146602169

Structure files (CONTCAR) involved in this work:

0.8912171165514711 0.2497175399505546 0.9411287309305891
0.9446542942207847 0.7530966761505460 0.8639990761412213
0.6809211976768170 0.7538043613677935 0.8562033357216564
0.7725641727755230 0.7498156463828363 0.4435023904423459
0.6089385061520503 0.7505349074113767 0.4492863927741545
0.9334971210530315 0.5039386392555419 0.5248393094479682
0.8237671825279063 0.3333886877647955 0.3289490571204537
0.7971583348734788 0.6385684489944946 0.6986392469811271
0.9341740958252901 0.4077383253579222 0.4479199917056516
0.8685856961657006 0.5654376911534420 0.5599431518263702
0.0310960073217315 0.3994238833644052 0.4405413216831837
0.0550111121261877 0.4194549668659359 0.5080730688172163
1.0464023566869469 0.4302006084970610 0.3761801975624048
0.0474563881091878 0.3475443033702754 0.4281182639840929
0.9750439333322276 0.5050999817500402 0.5625922766920897

Figure S3 Fe/ZSM-5

1.0000000000000000

20.0219993591000005 0.0000000000000000 0.0000000000000000

0.0000000000000000 19.8990001678000006 0.0000000000000000

0.0000000000000000 0.0000000000000000 13.3830003737999998

Si O Al Fe C H

94 193 2 2 1 4

Direct

0.4237099829211577 0.0562430535919277 0.6452374954247700

0.3061061236940126 0.0279807846678354 0.7913730511605871

0.2810683940454748 0.0623220918310336 0.0120783237600889

0.1203688899883202 0.0662690784581039 0.0084613788552226

0.0675749041816884 0.0311143759260949 0.7956724881149263

0.1822628147593572 0.0570916975557993 0.6567124837310468

0.4195558302189115 0.8270897104531205 0.6649351926267673

0.3051991737418678 0.8694708063626692 0.8085222660316571

0.2684011230992461 0.8294269457081661 0.0265144979246085

0.1140091317537313 0.8266599276900261 0.0114749450812513

0.0655057499258391 0.8721464166290495 0.7983738599167862

0.1838892854476529 0.8286467390151729 0.6729974668197151

0.0793102178074361 0.9425821139506553 0.1461574705158330

0.1964588921093541 0.9703408273123307 0.2933596981621303

0.2197216021945695 0.9377536266219842 0.5125683436620854

0.3792632734682607 0.9335453376174860 0.5085460499183009

0.4347868955657374 0.9691842448180019 0.2983384884623939

0.3201752705695975 0.9434268123551409 0.1590680902936930

0.0817528313796849 0.1721199765403136 0.1680758664414995

0.1984762521261108 0.1285019847247211 0.3078682446436584

0.2352034073122431 0.1714241862395970 0.5241153455752008

0.3898487247802623 0.1730976091114663 0.5092859029964713

0.4383434052736969 0.1274933459955778 0.2977028017287012

0.3193293249445084 0.1693943484097453 0.1720358319323335

0.5781929130287836 0.5551518196549604 0.3537677551544345

0.6958714009017477 0.5273072506902924 0.2042420166049018

0.7184012822448461 0.5582309285614528 0.9872050232998389

0.8776589590954994 0.5688758789013784 0.9933835591960550

0.9347902869092333 0.5303749577346369 0.2025601162119177

0.8186684216695597 0.5562933383184637 0.3383847393686809

Structure files (CONTCAR) involved in this work:

0.5800704488800884	0.3279761986708533	0.3381663417207098
0.6995408168452245	0.3687211542942070	0.1973229362460523
0.7320750432646745	0.3229435299695640	0.9816882330387847
0.8863347947817291	0.3290891320466990	0.9954526608312377
0.9373492412460667	0.3723858840256961	0.2055112281683113
0.8207314533912177	0.3309941185048152	0.3347396898974617
0.9232538457938806	0.4464309796628178	0.8573807010444443
0.8027996502299263	0.4701103829777351	0.7146065228831801
0.7796859225803513	0.4387490492315095	0.4899541216361041
0.6185375930283689	0.4335293829372973	0.4958131035872229
0.5667849803338807	0.4704935333507209	0.7099039491430745
0.6790323466711756	0.4358457917203005	0.8486541631661840
0.7993450652153258	0.6295016323199144	0.6913103652210664
0.7669379017143270	0.6670083033885782	0.4719960763659867
0.6118575714559004	0.6721942785938451	0.4856563305571190
0.5646137277876482	0.6293270217876736	0.7033907734939689
0.6817356835969857	0.6714429469463430	0.8276565134293150
0.5795479730031657	0.9413410868132942	0.3484345161819949
0.6955481458486085	0.9718180466235934	0.2028762301978115
0.7233441626867266	0.9424634878165563	0.9819924216127809
0.8801643885354858	0.9442806371744469	0.9861816253143227
0.9359236374791503	0.9686355469605957	0.1986775079477146
0.8189495188511010	0.9364862100224303	0.3298361226359052
0.5824644513427083	0.1739851826101976	0.3246069025610321
0.6980917058169085	0.1303075296883864	0.1886357920229828
0.7382611631345103	0.1644211255291975	0.9710274839428198
0.8927729474652547	0.1748548259638039	0.9830704662814042
0.9397269015825211	0.1271306388056239	0.1979671156454376
0.8199973481536668	0.1731605736946763	0.3220390599517006
0.9243127537852689	0.0629685443506059	0.8435064233285320
0.8094015166544671	0.0291819080356859	0.6963820673765712
0.7835942021343677	0.0584038270772440	0.4763028332570614
0.6237280320195592	0.0661730769702526	0.4823386512438522
0.5678658494707762	0.0322646790690839	0.6925153667969844
0.6847950658019002	0.0560352725093324	0.8256205329006281
0.9175466287534362	0.8316719384601063	0.8285057203386347
0.8066891062592658	0.8717242653920129	0.6822695526170608
0.7692768822693407	0.8279077796658393	0.4703608810288218
0.6136838036619269	0.8263590695558105	0.4884798723613212
0.5638053764505819	0.8742403643237177	0.6994305124071072
0.4236127983003504	0.4424471494831910	0.6523953195304221
0.3061704692004846	0.4719611868740489	0.7970550661227113
0.2833022941339852	0.4383847090206553	0.0187760191218329
0.1228684391107553	0.4333527463537935	0.0156902607869235
0.0691228902162713	0.4676982674065566	0.8040735852993990
0.1822863013850238	0.4421292153850995	0.6646865315138136
0.4199411987814601	0.6735670106123143	0.6692047396958065
0.3063910269451312	0.6304605910271940	0.8120564694455362
0.2683330652560845	0.6704203026377018	0.0290333962067573
0.1141394392794031	0.6724553527506847	0.0107857871201854
0.0663202230343293	0.6256674057123149	0.7982186295458740
0.1858995993118179	0.6699240178262547	0.6741916564175533
0.0789592809049596	0.5580106352405320	0.1491643279102215

Structure files (CONTCAR) involved in this work:

0.1955743805392870	0.5289734599660444	0.2956246755022200
0.2212815022403494	0.5598866966269174	0.5167047846957205
0.3805186899592434	0.5638461253654250	0.5132657607040807
0.4347457169880543	0.5301729230273688	0.3014851831888506
0.3203864692238015	0.5583041233379097	0.1642629621854649
0.0815738830824694	0.3259588988869728	0.1731361587137215
0.1974503199010875	0.3706008626645815	0.3110572236381006
0.2362641502991512	0.3305004730876865	0.5288375221075723
0.3911102726226995	0.3267883027418603	0.5158653287762482
0.4381887193146642	0.3722606751603518	0.3016996237061474
0.3194528771983077	0.3281153789974845	0.1759183815489883
0.3581664567003818	0.0639775274126817	0.7156780888626993
0.3110746366747252	0.0644415654720771	0.8995324546517146
0.2004164011230808	0.0550532817032513	0.0095129471051305
0.0926751796938080	0.0705499103627395	0.8950740673743343
0.1061842629738444	0.0591509704785461	0.6978569854995430
0.2304299665980488	0.0356455517372145	0.7491787518732761
0.3595873006469606	0.8264478597354388	0.7465661999783347
0.3085265780788428	0.8465846286486339	0.9244577765803862
0.1908923981324098	0.8531627214747816	0.0147153822224507
0.0867839098393692	0.8311018542073876	0.8978970295878030
0.1059813967866997	0.8421497641116941	0.7028545627319679
0.2303934336451384	0.8551797990186929	0.7651660936744148
0.3239019802626582	0.9486147728486860	0.7994285882317087
0.0820448314459497	0.9513936615540588	0.8117767123959957
0.4337630558026749	0.1246741467939513	0.5807805677502570
0.4171574672149831	0.9933771029591010	0.5683411982785239
0.3935569575305417	0.8619741585339068	0.5621333470029304
0.2017611151728200	0.1312970650798134	0.6166202180382238
0.1865429158997459	0.0025951808882477	0.5667988232913207
0.2019670288688874	0.8686441065710346	0.5708807847520280
0.9887856199822663	0.0450961750148780	0.7753148502050612
0.9857743509860248	0.8619241814543308	0.7813140563874800
0.1456178947208887	0.9354567511586426	0.2147490603111213
0.1894649194158458	0.9324661617835489	0.4002071718225500
0.2998235175005932	0.9493694797134358	0.5085780076866451
0.4072575039902224	0.9286012671146336	0.3952506114084152
0.3968610920317103	0.9442104331920936	0.1977985294800131
0.2725884061880625	0.9631115411025417	0.2531852025567066
0.1452220939286730	0.1709468029500427	0.2427911853676967
0.1947680965727382	0.1549292151248603	0.4219778263264902
0.3124590966749793	0.1478592584706978	0.5104209086879048
0.4176838517509124	0.1709484716585670	0.3956281865823044
0.3971181620946723	0.1556412581441486	0.2014260343352708
0.2731748805548530	0.1401934331251821	0.2628476804470468
0.1783337833546643	0.0495793268526958	0.3035510399302492
0.4212574651419876	0.0488567973128786	0.3168429044796806
0.0684454646506124	0.8728696061039227	0.0847349930405141
0.0851823727341963	0.0040270845965381	0.0667107720668235
0.1009511028663818	0.1364199476307281	0.0628127912401252
0.3024742867062850	0.8685892839980489	0.1194548017912632
0.3116059301024603	0.9972176804090506	0.0688845699305835
0.3018008456504810	0.1316704604668711	0.0677737009324247

Structure files (CONTCAR) involved in this work:

0.5135292513046882	0.9536789840497278	0.2805920725590875
0.5178546490270531	0.1360896990449386	0.2767328793541375
0.6448182432718247	0.5592176234335580	0.2849356186790064
0.6870813431546101	0.5671438566559801	0.0986937414310169
0.7988426452380116	0.5508650755204786	0.9952637853473036
0.9067933876579747	0.5717533359013077	0.1062717318359944
0.8961966624351928	0.5550202977575812	0.3027222845897786
0.7723004678402871	0.5370613165679267	0.2425236212028987
0.6461364135449200	0.3323558895648395	0.2692116105278821
0.6950124995702337	0.3338112461495966	0.0883249141036357
0.8081531622028586	0.3518328863767138	0.9898784579780382
0.9120814882666706	0.3284605499282257	0.1104198671173603
0.8981866753702188	0.3465708674831783	0.3049976745455333
0.7741046707443966	0.3593771707203743	0.2438292670536239
0.6811384366423550	0.4479402574640307	0.1881586226597833
0.9212834165649989	0.4509777342907490	0.1831818488069173
0.5669532599587235	0.6262258237473949	0.4111313664312968
0.5839590898817103	0.4956929280963960	0.4365192597785888
0.5953548820659792	0.3629558106211143	0.4455815792483423
0.8008442264099178	0.6321884551367379	0.3743477646525351
0.8078804790257078	0.5029492279149120	0.4282203727187493
0.8029575094736678	0.3686121272646749	0.4388797816817496
0.0135467603324630	0.5461535986639456	0.2189005308084342
0.0170417421217965	0.3629636369539684	0.2227692601316521
0.8589839726071499	0.4355471236298357	0.7854361778368031
0.8101507491944339	0.4411650533350093	0.6019641401927964
0.6988575173346604	0.4425453996949009	0.4908752953857776
0.5937322635323001	0.4324756000165124	0.6105491858897313
0.6028778976208132	0.4393941818187469	0.8080998085157344
0.7289096925391850	0.4507554055210348	0.7555903384769183
0.8531488998558059	0.6757424303026929	0.7447715603055363
0.8035255363224093	0.6385164025067180	0.5708316882741332
0.6886136645608401	0.6461178929337195	0.4777913578391931
0.5860056072233487	0.6654901930737066	0.5997358544775395
0.6031376420808136	0.6655920806419617	0.7969103078845008
0.7239180071367136	0.6501040296252368	0.7288573557026555
0.8124461961824618	0.5507347365182461	0.7188676584482925
0.5842208118026782	0.5501177457198602	0.7005353278687141
0.9306904986844180	0.3813811447525102	0.9302945966849075
0.9166390608889786	0.5139876285133432	0.9258053639976822
0.8894733102672362	0.6437779781832508	0.9456508381868403
0.6922160263003703	0.3615659907886803	0.8936265756409971
0.6886630608701061	0.4907210967326040	0.9372819404761192
0.6990047636173710	0.6241996640770524	0.9230660819983003
0.4873037814358290	0.4573507830331855	0.7240792772718353
0.4845907221306084	0.6367345848355188	0.7187143031022044
0.6437344733049941	0.9321848510244943	0.2749722981200296
0.6847056300117471	0.9464591878566929	0.0887021474390348
0.8015171804615429	0.9619580212591855	0.9973967082970111
0.9133516566743791	0.9324152765311752	0.0949472174796646
0.8960983398481829	0.9358743005522047	0.2923384514208536
0.7719950222502455	0.9544797446765474	0.2341483153055777
0.6407396807625220	0.1763193175450647	0.2399032696498569

Structure files (CONTCAR) involved in this work:

0.6964087363500776	0.1402895512882159	0.0686383117608007
0.8167627454827929	0.1453621769986042	0.9851837767925281
0.9249178379727641	0.1649505488363292	0.0930013808792027
0.8971839065686429	0.1621425915299564	0.2874951561501541
0.7715191101582730	0.1527312557259614	0.2288612349843858
0.6827183475110529	0.0520972995799999	0.2156382963992347
0.9190936611310849	0.0483854097863172	0.1903581401185434
0.5699289022228081	0.8733796576605423	0.4138536752943560
0.5883239913661252	0.0046508829152129	0.4233799700567438
0.6095083755834120	0.1361327051016560	0.4239998457632008
0.7996883292800356	0.8617695833319429	0.3693632787272429
0.8100941027372547	0.9925571881552373	0.4167459776430315
0.8031129588628334	0.1272940124297487	0.4186820104691210
0.0149572116551904	0.9553340481429387	0.2176650230302956
0.0191334714630834	0.1340919756388924	0.2220187590060007
0.8584618709534432	0.0683747375002818	0.7735271522671413
0.8191647306893532	0.0601771397306088	0.5852128829962787
0.7033572960929908	0.0526052762129338	0.4885456016686645
0.5917737594351283	0.0725489906933217	0.5928876730214203
0.6081228332273566	0.0618237189538160	0.7884035887465044
0.7320755671347450	0.0397690702649952	0.7299020936958432
0.8627623382901225	0.8273239425042285	0.7408415657430302
0.8131878753472834	0.8545806564361644	0.5637908625393661
0.6915491278505491	0.8500808023220976	0.4831157886406002
0.5862793238007424	0.8304570928473706	0.6016353839954077
0.6010568772271226	0.8475277070213580	0.7980829113679462
0.7331779785646978	0.8552659828921381	0.7220723479890016
0.8281435294054393	0.9500757757710279	0.6998471881894300
0.5821310433828079	0.9528050658405763	0.6765889107371961
0.9358169646685490	0.1345007081534684	0.8995207247550552
0.9173022395428596	0.0053267390433871	0.9292637574649446
0.8898592166170624	0.8748313311623260	0.9237580557712041
0.7076256033977739	0.1267949286500407	0.8744836269173424
0.6888920901439017	0.9951222861173294	0.9061291560387907
0.7174551919255181	0.8665949006477784	0.9357725936620558
0.4891653380725188	0.0458560557310264	0.7147181408562442
0.4828767454441601	0.8670983137163958	0.7115013730720977
0.3570139558096727	0.4349436951296060	0.7205449712233170
0.3129726782026367	0.4371030280194269	0.9060371305282651
0.2027324746276763	0.4461335056040972	0.0176871785445696
0.0960962376994350	0.4276795064874117	0.9020690984929295
0.1058585859176119	0.4387709119544097	0.7046537943325266
0.2298234394004317	0.4634283559391343	0.7582003088448930
0.3610795438221814	0.6745605948844658	0.7521906705610300
0.3095618969998485	0.6514738123784324	0.9286878170071700
0.1911003381889599	0.6462724847708418	0.0166920657050693
0.0882713800224824	0.6688515737023273	0.8967998294963759
0.1088217750230117	0.6535249840273304	0.7024744915418517
0.2322648101860073	0.6458475035257345	0.7679598188228074
0.3249093521876784	0.5513632483468779	0.8005060105624563
0.0853364305394223	0.5470375810565296	0.8182017786765460
0.4349764542135157	0.3724164001728001	0.5920805571991306
0.4179117784645464	0.5032956116681863	0.5719833160644376

Structure files (CONTCAR) involved in this work:

0.3945019147484151	0.6346514508574006	0.5694399543697868
0.2032917722390045	0.3684693574038316	0.6237086167248870
0.1876019474951357	0.4974057281063106	0.5759517271371559
0.2070015597396077	0.6307180528299409	0.5724881177974159
0.9897315462017723	0.4537519389995375	0.7893938556200282
0.9882393631501418	0.6353414947135325	0.7783197464939695
0.1440986137849359	0.5663803859217302	0.2202706540139512
0.1886549867010580	0.5624302568606802	0.4056320908370059
0.3012720555012841	0.5473246831295313	0.5095316905938035
0.4105837928875409	0.5697047678760909	0.4012961703650063
0.3967854475088362	0.5601385162379138	0.2042456596549851
0.2719332683147370	0.5383746537841878	0.2572306529843368
0.1419706230218788	0.3255895145240034	0.2538665187331234
0.1959512799868411	0.3513167875297443	0.4283697982668937
0.3140184229438943	0.3529553558461153	0.5165718688176916
0.4202920683828477	0.3319886005877284	0.4034305569709915
0.3969984961474067	0.3396490947347168	0.2086997459480424
0.2714874705025129	0.3554238346186058	0.2658448207775851
0.1778355433776793	0.4492451596196044	0.2970297971657035
0.4178106487823913	0.4506934015440388	0.3144296941902640
0.0683760166164545	0.6263770827019415	0.0843077832177920
0.0860413981275069	0.4951323849215573	0.0726129103645990
0.1049663947980389	0.3632349328531688	0.0712146580536617
0.3016725673120909	0.6325518687444724	0.1236403204934594
0.3145632559163695	0.5031233397607799	0.0755444408149736
0.3042414895799325	0.3686163992161168	0.0731387298334460
0.5141596410323723	0.5412411233782365	0.2825763364456306
0.5180629806667147	0.3648898771796532	0.2809865807843295
0.4389732137980292	0.7499115453702019	0.6383294803940840
0.1962585370827509	0.7494645740617097	0.6530131109022147
0.2721484486634661	0.7500932393121240	0.0507008242896545
0.1084213163342746	0.7495917189599742	0.0497485672893293
0.0621177243586153	0.2494074843142510	0.1442288604362564
0.3057874287127347	0.2489857230799759	0.1559245686319978
0.2308495082480048	0.2506704198096048	0.5491309152096826
0.3955703326217696	0.2491757916118242	0.5519331341508268
0.5622516851240650	0.2497139711163410	0.3572196202420206
0.8084454855925917	0.2512870839630055	0.3517649782820615
0.7313629987517202	0.2442866764722036	0.9530832820837297
0.8945503438590994	0.2535525350734095	0.9516600315919116
0.9277356124030564	0.7565903763009544	0.8770234121533765
0.6999077455684616	0.7479224703797599	0.8657149012214527
0.7755399056835882	0.7472286826339829	0.4588452954263907
0.6065409033728497	0.7494925950202901	0.4490173101617654
0.8123830569364392	0.7761624229607308	0.0993304275984838
0.9189227888375590	0.6735678623259088	0.8256832613874103
0.6841171534078976	0.8324638946486115	0.8220090295441859
0.8671056872210983	0.7384211709067243	0.9988151768809276
0.7482720552550283	0.7730272879198899	0.9949127480830409
0.6771674110788597	0.7534615776626121	0.0925141386049328
0.6305309239241004	0.7542332120708087	0.0491843084974410
0.6783136661086818	0.7941903694824882	0.1481673487962775
0.6853209994157190	0.7038559774990945	0.1265657883625737

Structure files (CONTCAR) involved in this work:

0.8030927476483890 0.7531963113984459 0.1623845227021578

Figure S3 Ga/ZSM-5

1.0000000000000000

20.0219993591000005 0.0000000000000000 0.0000000000000000

0.0000000000000000 19.8990001678000006 0.0000000000000000

0.0000000000000000 0.0000000000000000 13.3830003737999998

Si O Al Ga H C

94 192 2 1 5 1

Direct

0.4216212035856611 0.0584469494234572 0.6500332543469400

0.3050277053059343 0.0294673743362070 0.7958225349237723

0.2807623109693781 0.0570904467633419 0.0184879231793704

0.1207365767478460 0.0632610419700768 0.0127236279895623

0.0661603102828918 0.0290867200070559 0.7999153911826430

0.1809707713340458 0.0602132587271357 0.6652756655958616

0.4205273774754312 0.8272627650256664 0.6735267502852170

0.3030350079154732 0.8705045004521051 0.8092667790379515

0.2668509897097804 0.8296818640676655 0.0277461667954791

0.1119870447803155 0.8269476297210292 0.0174353310646653

0.0632576427288355 0.8704569615078834 0.8024030522125222

0.1810017921262363 0.8266317048714165 0.6751656457966173

0.0765518957730406 0.9418201542217580 0.1530615806763055

0.1942615570908398 0.9700196139716464 0.2976241161467255

0.2176545145515547 0.9384978624501910 0.5199649507655653

0.3781872172586346 0.9330428042097485 0.5158974495733870

0.4334571635063585 0.9677930198275936 0.3040851591070702

0.3187481321680717 0.9381138608617864 0.1672671069792485

0.0810029949110970 0.1734322961483403 0.1660002021549753

0.1961175551651132 0.1295368442724669 0.3075091716939712

0.2317744169435574 0.1704422020383395 0.5245818716804650

0.3867057890297003 0.1730809371531737 0.5106101187065052

0.4370714725770355 0.1263790569696547 0.2993808741626008

0.3182635534937890 0.1689798527737418 0.1728905437862168

0.5826678419312959 0.5549553155601055 0.3484974127210457

0.6931572442093866 0.5316509684324994 0.1884214604811261

0.7171084554683805 0.5651870660252015 0.9733616022031575

0.8747047631581418 0.5643812138789638 0.9830599259421150

0.9307940475941721 0.5312093928527230 0.1924689234748590

0.8144907603822398 0.5585651231811020 0.3268546242110962

0.5757869793052228 0.3291341991351276 0.3272371458567473

0.6985648752743085 0.3757177489954434 0.1976975071235151

0.7339313188453378 0.3272422197363658 0.9814194651650789

0.8862783355733560 0.3262957757868989 0.9778650487570655

0.9364229356180870 0.3731610624010629 0.1894588886795763

0.9297004434382283 0.4427000830041337 0.8515628358605665

0.7846069677132622 0.4405697403917083 0.4841374765421436

0.6254098009179514 0.4296371837899891 0.4873253409479510

0.5686959530713159 0.4677286523516674 0.6995802242206016

0.6736228932116728 0.4373305789404896 0.8489261464479679

0.9186428571682015 0.6726775872809282 0.8268356467041310

0.8015036477333451 0.6357218951655349 0.6902146311027885

0.7659931566214752 0.6664806778543086 0.4714132540717454

0.6110661507936732 0.6709528670221636 0.4854184521030311

Structure files (CONTCAR) involved in this work:

0.5646828770323437	0.6259929253800839	0.7013365154873779
0.6833425973084920	0.6802287615889968	0.8206947133629952
0.5773415318833832	0.9428057259962049	0.3585111730482052
0.6947701632402637	0.9713217343216116	0.2132504384256456
0.7206351304177454	0.9420603541743335	0.9919719628347102
0.8802743534546074	0.9338820154768955	0.9935771865595109
0.9323629081976683	0.9697657329563016	0.2046605807823030
0.8190918350726522	0.9413640571594069	0.3483566916842161
0.5808518107040491	0.1738253676509048	0.3277333800650902
0.6963563795467854	0.1279960991907569	0.1901485972798925
0.7331930221587564	0.1699820977064089	0.9712868335125346
0.8879020523103459	0.1724571971422375	0.9854054853526043
0.9359990547849132	0.1283246160017584	0.1987971689218549
0.8171673112574076	0.1672355201063394	0.3271166264461550
0.9233719359234648	0.0546932329089861	0.8550994763046391
0.8044905191529321	0.0264523633110973	0.7106639828300549
0.7809879228760050	0.0595661272428529	0.4907462374721177
0.6207075119657406	0.0685182934030561	0.4893387125284748
0.5668672692624628	0.0330882953024408	0.6980615688682432
0.6800243259860820	0.0561971327297861	0.8439999966542860
0.9189205878827628	0.8257074992152568	0.8368887800281841
0.8037339180635481	0.8690550787885613	0.6936197052463239
0.7679657825406376	0.8262312225298603	0.4769033881941872
0.6130943284012391	0.8255872343642641	0.4931666747384770
0.5635636628528695	0.8765182747632522	0.6999153754192371
0.6803176769824794	0.8363982041397471	0.8304878161560019
0.4211198381098679	0.4416602520641938	0.6446645070500441
0.3096902698809830	0.4680324530859425	0.7966927565048642
0.2849376472842502	0.4407488106159858	0.0196926977441118
0.1283420235103584	0.4359361956459173	0.0123745718604566
0.0764614894980074	0.4730617708485709	0.8047354211038561
0.1868070948362295	0.4431518677179964	0.6618746363323396
0.4227817754901115	0.6731825197078866	0.6719658397017972
0.3039201760352463	0.6263415376241737	0.8029675478901037
0.2672424247303173	0.6693443350126244	0.0224863579641376
0.1128186209382681	0.6740282670082897	0.0134158838925519
0.0654072778600292	0.6295141263867171	0.8041601291016574
0.1804488981709182	0.6685963236681803	0.6688094248802794
0.0761014338519495	0.5560302244191982	0.1441226218870263
0.1950172107602106	0.5281431410917958	0.2887407324951403
0.2199932283303038	0.5632858095403680	0.5094942756498416
0.3801571321274187	0.5700509017829591	0.5104237137758169
0.4356917871346844	0.5294295700794324	0.3025870105504581
0.3234776739934925	0.5597162082516594	0.1629440750357497
0.0835877931496043	0.3270571443523458	0.1613266067809989
0.1950084520171042	0.3686999157766893	0.3071786490310265
0.2309560039865343	0.3304570957132922	0.5256502670872402
0.3852213968773704	0.3268875585865160	0.5088129034415113
0.4311956883791661	0.3728756084877561	0.2965574400952898
0.3153128672128231	0.3264490330098075	0.1706477197869930
0.3572284862553093	0.0674269730320580	0.7224799748252930
0.3145957066534066	0.0574623394041542	0.9084487978110700
0.2004117122783758	0.0493453090472566	0.0102175493052704

Structure files (CONTCAR) involved in this work:

0.0912613637514516	0.0668567439809124	0.9005024264268011
0.1041671301420389	0.0603802750647465	0.7034799231992016
0.2288843021727972	0.0446273295651805	0.7606847604592130
0.3601148575067780	0.8262941711554024	0.7543257806146748
0.3054424198352008	0.8542625699357564	0.9276246283883386
0.1890608218628193	0.8531022154829848	0.0207503089955403
0.0846194699402166	0.8316001878889540	0.9039758371011979
0.1034604973979450	0.8372674150523388	0.7086563742603736
0.2292677384920487	0.8516932520170485	0.7661148210708491
0.3193626855968320	0.9492163214728824	0.7894568275824300
0.0826430645607037	0.9494020576188167	0.8106145218533898
0.4309773753501585	0.1266767180617479	0.5847874783664004
0.4129939118732758	0.9950001017017936	0.5748765000011758
0.3957586334089589	0.8623770550953208	0.5703891910190123
0.1984073709916766	0.1336794397849742	0.6201234494870731
0.1895615637736837	0.0030233804131756	0.5802685926595592
0.1962859804621092	0.8687174382658017	0.5738970366982420
0.9869368219398704	0.0419417168736050	0.7822989967354873
0.9832427230531209	0.8623372880116673	0.7854776191698016
0.1418559509582916	0.9330905447237527	0.2236211696040150
0.1850466678289495	0.9396243067836393	0.4090389579835709
0.2981694005284295	0.9443008123610875	0.5137839404875115
0.4070302840257269	0.9291294919390986	0.4032689193967847
0.3953794688969098	0.9386322341487247	0.2062219494176806
0.2703984527392150	0.9558057722565638	0.2614475354777563
0.1412098973346825	0.1731178060901908	0.2470994908731730
0.1912149596074302	0.1494636433383291	0.4244711158365358
0.3093935319306237	0.1473882514258270	0.5125151605797585
0.4158447874519995	0.1688234467354447	0.3980129079201469
0.3958086557464256	0.1556205127599856	0.2038211460009366
0.2708980965584494	0.1463660096983545	0.2663946467605792
0.1795060888105500	0.0502832507300430	0.2937142107278410
0.4186922333472126	0.0477696854239351	0.3165358029614937
0.0660964629152221	0.8725638596875605	0.0906075499281555
0.0846145840470143	0.0032790699232078	0.0742987242604279
0.1045229403986224	0.1346849925979273	0.0653837973568205
0.3017357986222682	0.8637858765506605	0.1244979193099950
0.3101750301383697	0.9935173022131041	0.0796076596135645
0.2996278891357691	0.1271618431562307	0.0730061052672430
0.5124767673156075	0.9536197710296759	0.2875993733733438
0.5167134998861207	0.1349564018279370	0.2793332765977709
0.6429221293809838	0.5647813725021180	0.2695153646345040
0.6856558521717087	0.5734058549752944	0.0848934623919784
0.7959455674106639	0.5460514629076771	0.9844458398335911
0.9042115875253104	0.5727677020587399	0.0953944183331880
0.8923263318513972	0.5565484211222280	0.2930552626959246
0.7692034760507976	0.5397338529791894	0.2305973448861021
0.6358200982337845	0.3368995160617829	0.2481931829444186
0.7181163390036787	0.3322794261080627	0.0994830229452090
0.8102694158877770	0.3537806959380232	0.9600133064140871
0.9071536605507803	0.3315936064196910	0.0941759899518420
0.9035550375622652	0.3424125579180727	0.2891124685399880
0.7616409608872067	0.3776303752424622	0.2714900531900262

Structure files (CONTCAR) involved in this work:

0.6763048588482906	0.4526144547102747	0.1693120477189481
0.9167063955377789	0.4519759693714890	0.1741807015938526
0.5688175738063935	0.6253796298463182	0.4066083129883895
0.6033830740645045	0.4979598796934739	0.4303017162339838
0.5939472866887204	0.3642735104947118	0.4337434164237153
0.7964469801458082	0.6318995555840613	0.3712214972641367
0.8032559798575142	0.5041254666860910	0.4167379080295951
0.8310005897815609	0.3738214962171862	0.4426123181323576
0.0097650503113896	0.5452457057840547	0.2120494022443062
0.0174459766911496	0.3681332515023411	0.1948613337097203
0.8746759132753593	0.4363365139764936	0.7613863645516905
0.8162412084577485	0.4468858342765901	0.5950468225203984
0.7070585116869890	0.4218838295853434	0.4842081207627899
0.6006416800576232	0.4313314365684086	0.6017628262792322
0.5990307733279538	0.4348923140796646	0.8002795563302594
0.7291749379127607	0.4364013923794617	0.7626739787305304
0.8648822969182692	0.6765839881988174	0.7365683854683385
0.8072063884592837	0.6403958042140193	0.5686049586787807
0.6880995102395600	0.6445194252904382	0.4846846986945270
0.5802550689960868	0.6636718462162248	0.5964930673673217
0.6069414038614679	0.6602604272026218	0.7914071703357749
0.7312511154623959	0.6717989305013650	0.7228253369674120
0.8029249889438588	0.5599501167663119	0.7303177325413494
0.5857725860474995	0.5475059775922464	0.6922935658453613
0.9365037965182827	0.3716259250433179	0.9098138054311460
0.9134541359844764	0.5025097061483110	0.9285228007820877
0.8880633361264929	0.6336637253848042	0.9231898214135076
0.6804719822826799	0.3717241233115083	0.9203259469912736
0.6782984865027066	0.5055640692460711	0.9160134711380864
0.7091795633731864	0.6356540179957524	0.9143297906826368
0.4887975624619449	0.4569970263516202	0.7056171230497689
0.4851971199788571	0.6341651978709344	0.7248488945661062
0.6426477989857082	0.9344510571527556	0.2879001620192905
0.6932292521201819	0.9343257087048609	0.1053258333503999
0.8012001123005088	0.9514219849480110	0.9897186408506149
0.9051823317061430	0.9280374319494652	0.1083735983368873
0.8948145951689143	0.9446424065518555	0.3054198968494984
0.7696649833536593	0.9654870219222438	0.2588600318206092
0.6421838998146617	0.1739462648103885	0.2488049773192879
0.6948260946881595	0.1503434968871232	0.0738940111228727
0.8108811147503086	0.1465169608450258	0.9812163158883505
0.9142006280516305	0.1702085109839936	0.0997635015365474
0.8954327652300121	0.1569015953578858	0.2948074369229812
0.7708895838742295	0.1372092690494092	0.2363011664785819
0.6738419187822033	0.0497729620003438	0.2014771364699353
0.9191693024560069	0.0491073751593497	0.1833513762926935
0.5678269715571160	0.8744256017685287	0.4235473555046102
0.5829317451383517	0.0064386415336309	0.4342511842229023
0.6038645886778076	0.1382272881112614	0.4315483217705132
0.8025523229547724	0.8649345072999111	0.3833959796867586
0.8120319124191723	0.9908708922620841	0.4442009498506806
0.8045115786318832	0.1252655166250524	0.4296213440708296
0.0114337378036403	0.9553337732747826	0.2222011167952383

Structure files (CONTCAR) involved in this work:

0.0158648119792895	0.1383234382223913	0.2166797930971870
0.8562660611695870	0.0610288992950638	0.7881020441951635
0.8078334447250554	0.0662025186479421	0.6049491799289627
0.7001474476695574	0.0535066186195634	0.4883099380457528
0.5942317513049165	0.0764574915678999	0.6034108306275922
0.6043875198138604	0.0545800511125379	0.8007057702531704
0.7291080635745868	0.0308110086308428	0.7548538504453567
0.8570560882038694	0.8269062417824777	0.7591205273255580
0.8077524351903541	0.8428282371510464	0.5794370910289323
0.6905615373889057	0.8504296357526663	0.4881596306399207
0.5868647905098433	0.8284243280528596	0.6079669415131176
0.6038045605631660	0.8553490965909392	0.8005772071723394
0.7287013499398945	0.8576849952787712	0.7375364255907649
0.8242182417836382	0.9479080996385586	0.6971989366939481
0.5797528235148042	0.9542040928308571	0.6719164428972605
0.9340335428402506	0.1248021782841764	0.9153203468173750
0.9199202900137371	0.9935429867781924	0.9356529657516717
0.8969314691402027	0.8625059777742871	0.9402361659544755
0.6983544300263990	0.1322892563010897	0.8772776860538735
0.6860052017310506	0.0074268332957030	0.9410110193292852
0.7010617445526368	0.8745313187930464	0.9322238223484695
0.4880153719410212	0.0474076118245189	0.7172981259124112
0.4840037418132637	0.8674892570069053	0.7204791252888326
0.3610790867721227	0.4285928253963172	0.7238852349207343
0.3165768277124279	0.4377122904851670	0.9083601230164143
0.2058977969600041	0.4593764223515976	0.0171557770672456
0.1059152337186756	0.4288678556139619	0.8963306276406364
0.1100649350971594	0.4521276618629364	0.6988612788826304
0.2335572532355733	0.4561773956957690	0.7589422009255548
0.3588741502851919	0.6718251006952981	0.7461669655492001
0.3031240220934123	0.6486466263768222	0.9187439528152813
0.1892988793547331	0.6462723725891887	0.0180506985747499
0.0871127210467628	0.6756570398789506	0.8985201209670722
0.1036303793707384	0.6563662017939534	0.7046625345756038
0.2303305469970082	0.6377125095149381	0.7537590786269043
0.3260173280718006	0.5480248686250140	0.7936520233833350
0.0872045284902335	0.5523417460645507	0.8280678970591921
0.4323467151025859	0.3747031589171632	0.5771815496228295
0.4036073651818051	0.5044164795332137	0.5724156274208668
0.4033789365746500	0.6381193168774951	0.5665128594854235
0.1963985969392509	0.3671030933006720	0.6208433972497932
0.2029610736072161	0.4962135778687833	0.5735320458065606
0.1912608685881567	0.6303692124390271	0.5630143665746171
0.9978891089760751	0.4565468683802644	0.7904136353930123
0.9853018479722012	0.6338988738435447	0.7862592554416158
0.1412286656799395	0.5640082428555151	0.2154444321372743
0.1847005025618882	0.5570442251154306	0.4008820250333320
0.2999887131001543	0.5691588326167797	0.4972284773017717
0.4153893519814480	0.5706389177323404	0.4021608628797190
0.3987988539225515	0.5639983934143462	0.2075162835930047
0.2709347430806969	0.5438660452591083	0.2529035206126539
0.1365660848312079	0.3259904043745678	0.2531657952800457
0.190948088888756	0.3530643043506854	0.4256750214636833

Structure files (CONTCAR) involved in this work:

0.3085662905404323	0.3539476484423160	0.5166061756470887
0.4091673560047069	0.3292197603315953	0.3934476600019302
0.3923856986286662	0.3437066318462367	0.1991121466036609
0.2682631589191216	0.3471570148908666	0.2654088036174925
0.1817034807754391	0.4477285313477062	0.2854671046968291
0.4118374072659333	0.4514592812872676	0.3140106225414229
0.0661623104763957	0.6247102455486249	0.0799398376285056
0.0832096571054757	0.4927579592610398	0.0675960201592623
0.1176589461408513	0.3630677577800481	0.0645144344657483
0.3050031918991213	0.6315147407889078	0.1133684309283162
0.3228736581721740	0.4995338650105804	0.0811000783108113
0.2944273217552559	0.3676372647561971	0.0709734805281062
0.5160625048053070	0.5330105401762811	0.2874263500920348
0.5106902559325539	0.3652562344304092	0.2782254673213698
0.4422386573357497	0.7506064769736993	0.6488182902701685
0.1948595497430037	0.7478467727595769	0.6519252530966003
0.2727100161956656	0.7492490424020474	0.0406423451292952
0.1081630169413811	0.7498678358924313	0.0568749947886449
0.0642352722176391	0.2502474105538802	0.1335433664886759
0.3065215999624920	0.2474463452690593	0.1464237862989184
0.2260082977078053	0.2504628521177190	0.5429505230817586
0.3908831388651119	0.2503210742903925	0.5491158981689026
0.5603558263359467	0.2509616054119991	0.3513375002572112
0.8004005097049356	0.2448095938121915	0.3462631837666905
0.7281092261829427	0.2494219889838991	0.9476329841394880
0.8930804579698615	0.2486859886663551	0.9427935453076728
0.9377861355281166	0.7482526837014267	0.8624113505049738
0.6861063495559124	0.7575359807889754	0.8563294030368896
0.7720636609980911	0.7465524824202595	0.4553207094633130
0.6066071459139211	0.7491325052600705	0.4518081606677285
0.8212243355155748	0.3259424571626085	0.3219099646234682
0.7989928011862110	0.4748840970783583	0.7190433353654062
0.9042572856502776	0.3932989213803266	0.6299120530420451
0.8844806364102679	0.3180989243015306	0.6448836891851669
0.9848930922260102	0.4892492367173037	0.5927874142047692
0.0165775301541207	0.4129692598456076	0.5411600856247591
0.8785699035056010	0.3858826329114027	0.4351031548510262
0.9527148383209202	0.4592912364162413	0.4779331753068565
0.9715109698715908	0.4435202324917953	0.5516655911126386

Figure S3 Mn/ZSM-5

1.0000000000000000

20.0219993591000005 0.0000000000000000 0.0000000000000000

0.0000000000000000 19.8990001678000006 0.0000000000000000

0.0000000000000000 0.0000000000000000 13.3830003737999998

Si O Al C Mo H

94 192 2 3 4 4

Direct

0.4235505408174077 0.0562340983452740 0.6543456082012001

0.3047451871618271 0.0294164526280216 0.7969487307125327

0.2810883582430784 0.0586481515442774 0.0219844976995976

0.1203416986461088 0.0656304000712736 0.0193855503425318

0.0662958723610195 0.0276429696585770 0.8071907986696747

0.1785498897163834 0.0621678836863286 0.6693621286894342

Structure files (CONTCAR) involved in this work:

0.4158391403503640 0.8261894376979655 0.6654011765494238
0.3033731971840746 0.8702018914718374 0.8080697065014552
0.2705410115199433 0.8302536553471429 0.0260216248890434
0.1161592989594517 0.8251933241656183 0.0123790670041268
0.0676013158961498 0.8701098453374034 0.7996769568336043
0.1842228473618931 0.8274776584833907 0.6726707034444984
0.0788709705408540 0.9386215799500863 0.1518693614595395
0.1943977497511732 0.9676878941843887 0.2977746785039578
0.2175728455399069 0.9428754929146063 0.5208947210949340
0.3760744813908634 0.9352621743040763 0.5149726505806581
0.4333356213764411 0.9701772627251929 0.3044393986626695
0.3187566897779035 0.9375449241635180 0.1699803297501749
0.0791884163127501 0.1724926653566416 0.1757499241546216
0.1980724221260406 0.1264521483043195 0.3068626166122924
0.2320249383430270 0.1675969436001933 0.5258459926576068
0.3868752919492965 0.1713169384641407 0.5181459197483087
0.4361865597768187 0.1286339609918793 0.3046293333217145
0.3202757372184588 0.1712550149060743 0.1732682087593390
0.5786201676706924 0.5591717071777799 0.3498871269533310
0.6922697375846356 0.5281185888512339 0.2027254468571830
0.7179669191366385 0.5565308323332346 0.9805900715308199
0.8765581411860245 0.5669635538553488 0.9816631972075873
0.9337929172499264 0.5377327710782797 0.1909376389914697
0.8165388916703744 0.5641514782466797 0.3258367203585508
0.5835090133620408 0.3265353930797488 0.3341213053298399
0.6969224515354159 0.3711251345645049 0.1966690112858893
0.7328984080764166 0.3292317819737880 0.9802271496799583
0.8890465885597388 0.3262023865930881 0.9879178908491161
0.9368947236937888 0.3791950776193123 0.1980110297655162
0.8210040676033671 0.3340592499276669 0.3304531717713181
0.9222079223317892 0.4415607790880224 0.8496189362521820
0.8052173642384682 0.4715133484439819 0.7051261724033530
0.7836035206470631 0.4470469245357780 0.4817377279383743
0.6241508090991700 0.4377303776984973 0.4885887689746978
0.5684951326784509 0.4676992792950848 0.7012095773897589
0.6845795675355398 0.4332800420220628 0.8324020762446195
0.9258612077824694 0.6720714716289523 0.8227582768444131
0.7638116560665411 0.6697726391482807 0.4683844921129936
0.6113215202195075 0.6724743097505326 0.4875821507050323
0.5639625798815381 0.6267435518248934 0.7015254698861156
0.6791930668600069 0.6769136033277768 0.8360662051477116
0.5769293807266074 0.9424290994853836 0.3545552330104478
0.6956473562567799 0.9747712686570639 0.2141261170567211
0.7135080324464056 0.9414379608534162 0.9878387832640233
0.8730164667868504 0.9295412857912783 0.9903710033591701
0.9339186578052457 0.9646242783785937 0.2033764823680217
0.8194329346757185 0.9391322671356238 0.3387537982007184
0.5820614836979658 0.1736160002782063 0.3376970949261102
0.6997549864031010 0.1318298315514520 0.2025820708955024
0.7321931408378854 0.1679831261137574 0.9845037209434323
0.8883562309796187 0.1701832438574278 0.9940719820534479
0.9363537748987071 0.1241152936629277 0.2097359724318317
0.8202337470993500 0.1764357803145203 0.3322004373108525

Structure files (CONTCAR) involved in this work:

0.9185761354786068	0.0564469723343300	0.8549637773267252
0.8066204576649908	0.0375199826232498	0.7049296867008342
0.7823016813867353	0.0617719359904701	0.4827819462662524
0.6233807408476792	0.0638219137887961	0.4925685785245859
0.5688468440064791	0.0297815008749274	0.7041953472118795
0.6852354871657711	0.0641669287221212	0.8355368361620094
0.9229996632320902	0.8255615485459895	0.8342993556690187
0.7627466069485606	0.8289068499292902	0.4821396607128532
0.6114388455231194	0.8278269214383134	0.4887260849222438
0.5606891805677049	0.8720801102053659	0.7015274400792829
0.6646410011125287	0.8296839592752351	0.8512861979012297
0.4247348732896427	0.4409474603039433	0.6511937135663688
0.3063495220154206	0.4694800521808980	0.7958837212236644
0.2826233411313414	0.4401541493337187	0.0184753566397549
0.1222364185252170	0.4312309182931033	0.0158875836134793
0.0689223116009154	0.4675257488064270	0.8033186036841804
0.1822834314297867	0.4354877286162945	0.6675470360412603
0.4197320907114156	0.6724316961909254	0.6687039817946729
0.3048970158743116	0.6291718007251078	0.8091767445204965
0.2736264555406785	0.6693661407680261	0.0276858358812211
0.1197787367892263	0.6712331362142302	0.0126849266161413
0.0730623912110251	0.6249950201748543	0.8008251613500764
0.1863873097792108	0.6702502296719078	0.6729689077463902
0.0800229449397153	0.5578823217525309	0.1505768281638646
0.1959157662890429	0.5310983525860634	0.2974279157644612
0.2225334547715598	0.5554152106147114	0.5209189836189435
0.3813253328736666	0.5628950358092647	0.5133736879555749
0.4353349059814178	0.5279126943373156	0.3030309549526103
0.3203942675562592	0.5608364276918195	0.1667806578388349
0.0794350645034328	0.3271879916951567	0.1730504420450197
0.1976653073721566	0.3719273080364680	0.3072100425818369
0.2334484910932269	0.3289313029882773	0.5238137279663028
0.3884504307811813	0.3247342429854579	0.5162129876016264
0.4380098863349475	0.3699501358884372	0.3047993292355192
0.3205223526210739	0.3285556854666232	0.1736891825891948
0.3594763694310124	0.0669444001621874	0.7272917206986497
0.3138488848920912	0.0539195483266658	0.9114774140438315
0.2003805423269381	0.0554924540097943	0.0162652529562901
0.0909318148436411	0.0663181701317502	0.9071586718926524
0.1022604469221810	0.0618034754732833	0.7108000148928547
0.2292183172417323	0.0479049276354935	0.7621490568430861
0.3587787067636337	0.8250470489385786	0.7516668031278202
0.3089244245691523	0.8566784701253053	0.9268199363269806
0.1924982863652304	0.8529317850100397	0.0187151933605086
0.0901625418167611	0.8281089216977140	0.8979026515283377
0.1055984278868679	0.8383127832334388	0.7020434495667540
0.2290080592796676	0.8488428612643516	0.7690485678443645
0.3166802062026541	0.9489662334074633	0.7845897159054206
0.0878918378205096	0.9486070015665392	0.8134129436137992
0.4335494994408169	0.1238542297719767	0.5876267371885620
0.4139705682384842	0.9924162847063169	0.5800989256635670
0.3855359954444305	0.8617246553193033	0.5656930449308967
0.1942299216106163	0.1355486666773704	0.6218647344197671

Structure files (CONTCAR) involved in this work:

0.1863540757259742	0.0038231816339687	0.5856608171346981
0.2030084851223319	0.8710360093623793	0.5744557595518611
0.9860115499878174	0.0344634155268421	0.7957096730250458
0.9875985655748013	0.8630290012183943	0.7843268736853394
0.1425684017350187	0.9283729161017873	0.2249808109477210
0.1821867478192395	0.9432161966415626	0.4117611694934098
0.2973338866707206	0.9542442843322840	0.5089292299431347
0.4082417549721886	0.9314846430978909	0.4042797854043402
0.3956216641395360	0.9402540226168322	0.2069824800653454
0.2706569507325850	0.9496820968562338	0.2664142984109841
0.1409682225639535	0.1717915998169036	0.2540975527725373
0.1958885705108793	0.1391015978567582	0.4260171886779782
0.3100448344554983	0.1445476320943372	0.5250006441485034
0.4121449058081728	0.1691049646837644	0.4033283384985789
0.3974278241805780	0.1591767869732134	0.2077015203493041
0.2713728255327844	0.1471635374384068	0.2642252232799244
0.1819267496865353	0.0479208911692983	0.2837064950136101
0.4174028748032408	0.0497830604447985	0.3173155210111078
0.0693523768713903	0.8718708851574771	0.0832762187561471
0.0862385167862492	0.0042532201727687	0.0810713761943118
0.1013323110231314	0.1367633699270595	0.0715422483361994
0.3046232323136864	0.8636955359915092	0.1235977149311709
0.3067210456544686	0.9949519981493992	0.0863607776554211
0.3045552841195766	0.1288635436420236	0.0724334664113639
0.5123276576526283	0.9576270191630019	0.2854311595576728
0.5162561755642389	0.1374966521780904	0.2901248099064936
0.6428337291374516	0.5691115730172969	0.2771487776913278
0.6797160365955469	0.5501302410670995	0.0878846563787428
0.7978882032649509	0.5556290612052945	1.0005284469672600
0.9134332710940836	0.5776351624741497	0.0890799586606614
0.8930837374804202	0.5681086430888195	0.2858740319588092
0.7696262323954108	0.5439177543881237	0.2314389451053170
0.6415745367905542	0.3234808620234616	0.2494592143977536
0.6953568492868865	0.3602795660311726	0.0771977462385538
0.8114504054586568	0.3502730607638325	0.9823980248770212
0.9159322056464357	0.3347906325896579	0.1014617739528601
0.8968601514225583	0.3521459194648039	0.2958426275304096
0.7711284791705538	0.3524361350218551	0.2380336829251869
0.6777407435327972	0.4486064317904972	0.2216323116336563
0.9188534163801824	0.4577140918628026	0.1778148972583871
0.5660717363654171	0.6289915671474403	0.4103244157651476
0.5876138133549486	0.4990902173092482	0.4306876506813810
0.6099024509664371	0.3673436110307747	0.4311917937945740
0.7951947554251596	0.6379661035037330	0.3668308961164754
0.8112690087240167	0.5088069458212948	0.4140949375884744
0.8015229096299815	0.3756414746017003	0.4298911788231611
0.0123174582746819	0.5498220719178187	0.2159468418039557
0.0165745063347949	0.3695524769858517	0.2180525483168310
0.8602739396356341	0.4324162888315337	0.7737411306806211
0.8196278371255572	0.4502506589760552	0.5894752606401006
0.7032934751763433	0.4537519509495128	0.4930496117438500
0.5932164396728370	0.4304017626979836	0.5997406284445027
0.6070324152242927	0.4373454928864478	0.7976263247256519

Structure files (CONTCAR) involved in this work:

0.7312641078344956	0.4426515464551440	0.7342604908423088
0.8813028537173004	0.6732691573862188	0.7200025939797869
0.8101645888718169	0.6508071958902143	0.5631218871482399
0.6876489908078284	0.6432522246285068	0.4856483923516018
0.5825412829101121	0.6671428191454855	0.5998384666229148
0.6042806305558653	0.6582648677942043	0.7948292462359194
0.7341899258784619	0.6730762929011693	0.7483918734565339
0.8088805824830335	0.5508374169640341	0.7229214708862395
0.5825784675956769	0.5477432009274370	0.6890560220495493
0.9330020207402590	0.3715457705703633	0.9112087995019343
0.9099497379438465	0.5017652352191204	0.9294372974167466
0.8868759478890630	0.6335662345940208	0.9124089078413780
0.6976016018036487	0.3594962393341586	0.8811913689028856
0.6990346382199493	0.4913049387334316	0.9143419688172957
0.6959362500423178	0.6258307501255497	0.9280260116032193
0.4897189727916875	0.4528193833215611	0.7209125762741283
0.4837310765743049	0.6351290359445363	0.7188494064018522
0.6414694414513264	0.9348786964196584	0.2815922970986043
0.6840251872238660	0.9619644944302804	0.0968704557369501
0.7925761701176230	0.9234184828609194	-0.0023479997965541
0.9050455242393548	0.9318166826609672	0.1019287664208390
0.8965362966523370	0.9290192508843722	0.3001251263658423
0.7701093233217674	0.9471644490165174	0.2443472269265045
0.6400600595949107	0.1746332436810450	0.2529535431450028
0.6948777472596004	0.1371415913357635	0.0823883684607040
0.8106804851580653	0.1461554087199676	0.9866082241157262
0.9136226923750651	0.1624294304289428	0.1086632254424561
0.8969632222518678	0.1566113007037802	0.3042901882000927
0.7726953975842427	0.1601956170809082	0.2360760178179745
0.6915605044300508	0.0543563057774449	0.2401259883798907
0.9178084163300319	0.0443828309274772	0.2041783280119639
0.5644939197582743	0.8727237819391946	0.4155386136828687
0.5858721460330168	0.0029373466276200	0.4346914771033086
0.6080475261247061	0.1344820409040240	0.4367315119780648
0.8092661995488920	0.8650856227726822	0.3929726876550130
0.8139320921598532	0.9999137007585096	0.4171133914201970
0.7956280400870005	0.1330126577353695	0.4278504514649578
0.0121136099474601	0.9479254238673277	0.2196823328484198
0.0163422792310329	0.1325201642946855	0.2257589377873797
0.8612242138359034	0.0762851165369530	0.7749178937706536
0.8189837969071554	0.0623501962110748	0.5900532442135971
0.7029282028763223	0.0481623808831199	0.4935694169227413
0.5949546756840752	0.0694518483284411	0.6053716057697963
0.6074380809709923	0.0565179383912052	0.8031588483552266
0.7312068336923555	0.0611694395372648	0.7356687302306868
0.8635485319351367	0.8298094654847067	0.7517899931528855
0.7943351402234274	0.8489973732019033	0.5894513339194125
0.6872855718666337	0.8585976192369129	0.4775224946865914
0.5875352773921364	0.8310647105353632	0.6040664676678772
0.5896182855492812	0.8391886320203129	0.8035823646983508
0.7181437493081462	0.8536966093052951	0.7698329237140165
0.8152071833110386	0.9583342082195327	0.7180937420545876
0.5832797985861448	0.9500712256715258	0.6891005971687912

Structure files (CONTCAR) involved in this work:

0.9341682793968288	0.1224378548419650	0.9232034865126123
0.8948140714298998	0.9959097908393113	0.9286411795785154
0.9022991763731937	0.8620881802646171	0.9380864853483192
0.6951432327882426	0.1371983125752882	0.8874800771101742
0.7061637881412114	0.0050130857818561	0.9130484896579558
0.6710715027535998	0.8766764778673719	0.9514253793963009
0.4898100929355614	0.0443866505172635	0.7217119265968213
0.4796574551253742	0.8681738671179983	0.7061793801986914
0.3590933013742736	0.4334675043137822	0.7214931001334298
0.3174000924356381	0.4426680360895867	0.9089688763582449
0.2021218118006198	0.4417174262000526	0.0086445569760153
0.0906862643478774	0.4291324993223687	0.9049524129030279
0.1057280837943901	0.4342854764299403	0.7070866548926862
0.2305605802878305	0.4511131698967316	0.7625171068230631
0.3599116663901683	0.6732395503388942	0.7504079045472849
0.3114225031939835	0.6440762754831966	0.9273918869765758
0.1961495439420420	0.6446736726791964	0.0245722426808694
0.0988555497520916	0.6680945604677506	0.8959191309086738
0.1078150495608226	0.6560875061006478	0.6998825494442952
0.2304652182254221	0.6511983796043277	0.7712160347324216
0.3175268606153971	0.5501575547219220	0.7871977399755797
0.0918956114539561	0.5461205297164466	0.8126903950577493
0.4336847187034653	0.3717336808403369	0.5881987267466551
0.4193483553690310	0.5033490257652417	0.5732974202091626
0.3944210458920431	0.6343758394659571	0.5681363361763759
0.1992698580307564	0.3620099749801154	0.6218278097521631
0.1907074631519228	0.4935694481073675	0.5833939430888082
0.2088657285532367	0.6264609222427495	0.5769959564223907
0.9892881936371140	0.4592060601117180	0.7861415678560140
0.9931064230984630	0.6316900079197411	0.7921829556891680
0.1422998054725514	0.5692044876995366	0.2263866782535567
0.1872193030170337	0.5563785524815973	0.4118126699543933
0.3023323041422548	0.5448841428088476	0.5100283447312051
0.4103971366275171	0.5691541541781849	0.4009291806001126
0.3968743141574445	0.5538917165205897	0.2038361564238786
0.2714817610622048	0.5484331291372680	0.2620292963886838
0.1399939025310077	0.3279805783348024	0.2534667317697293
0.1948590651248246	0.3567402893432850	0.4257314240733397
0.3114835159770706	0.3512938925049434	0.5175469966536360
0.4166392312174364	0.3271208690668964	0.4028739086383525
0.3974213719770245	0.3408744583824641	0.2086421109542183
0.2710213320429338	0.3518233804097263	0.2641827704228635
0.1826766631069838	0.4508322490933272	0.2867766191977603
0.4198704091190255	0.4486224284308425	0.3219530675592335
0.0716864367940509	0.6237729781687668	0.0795955615249580
0.0897382643712238	0.4921512791408836	0.0802891501425481
0.1045831504030992	0.3598043937812540	0.0682427638821080
0.3100585515828391	0.6365030030957430	0.1239503190460324
0.3058633625922804	0.5061697411696242	0.0798850279702208
0.3059268373548825	0.3713825658367780	0.0730719466191654
0.5138358014862088	0.5418542542680872	0.2818755198133173
0.5176433476980772	0.3617803908839222	0.2853700687775937
0.4372096268918799	0.7496114702306761	0.6388410056300425

Structure files (CONTCAR) involved in this work:

0.1950198376383839	0.7490020736894669	0.6432658378202831
0.2771120974219672	0.7499795981230013	0.0365313220261469
0.1122003305140226	0.7481728422347581	0.0515490812382937
0.0582582576645998	0.2496292365581417	0.1523483906448463
0.3080431804364953	0.2499199014230396	0.1480132954076628
0.2261648408397932	0.2483345364196868	0.5313560933954372
0.3919681467495681	0.2481774152131155	0.5576342716740454
0.5653670897793783	0.2504918016558930	0.3690904389231383
0.8153501984282721	0.2552174456632907	0.3597269028645913
0.7251683636819377	0.2485478567792644	0.9813743192759918
0.8963704516854739	0.2474805631985985	0.9577132613958670
0.9418701234170013	0.7480018712731084	0.8604773231146499
0.6750135648569507	0.7519465887649249	0.8849569391476504
0.7612804535154158	0.7507833992883322	0.4510864052635743
0.6091481913403778	0.7504071498984289	0.4517686855056502
0.8016805024702676	0.6344076498914121	0.6925537345313405
0.7912917378106163	0.8757967795178982	0.7159596580558595
-0.0075730848317282	0.8436440562860757	0.5063657399898827
0.9542557436406487	0.7216962167959566	0.4238020558881791
0.0939906439951475	0.6985507920860562	0.4299432111348023
0.9151196369881852	0.8137711858120340	0.4210398354149204
0.0264449428370573	0.7544579644151859	0.5241184558861472
0.9021588816166491	0.8187045930318383	0.5859362083444660
0.9201494508611966	0.7109194854385718	0.5752116119319176
0.1440097828736782	0.7102012139277439	0.4612240091771558
0.0870091657148279	0.6436931558737999	0.4325311718630473
-0.0428337123037193	0.6874840363413216	0.3593333572168549
0.0938364821560916	0.7144515450411721	0.3512164018976059

Figure S3 La/ZSM-5

1.0000000000000000

20.0219993591000005 0.0000000000000000 0.0000000000000000

0.0000000000000000 19.8990001678000006 0.0000000000000000

0.0000000000000000 0.0000000000000000 13.3830003737999998

Si Al O La H C

95 1 194 1 6 1

Direct

0.4254819013154419	0.0578109484353502	0.6405689649341182
0.3053079510188978	0.0312208259849286	0.7857424660886881
0.2805738193872762	0.0685626986019391	0.0059519064459422
0.1200031073650549	0.0701137179168408	0.0054951895017976
0.0687750006913792	0.0325908539325692	0.7939000519857244
0.1802122815238869	0.0579160862552783	0.6474941554511798
0.4202876205275777	0.8282276653293192	0.6648199308977061
0.3039763778552791	0.8734221876775260	0.8065132401359486
0.2670107365109923	0.8336887958089779	0.0246429801484424
0.1128327153806066	0.8310894191929120	0.0105173079509493
0.0640561486544674	0.8750553727491873	0.7975298776998815
0.1822690686773498	0.8321504013164543	0.6719566773009988
0.0770919929125494	0.9480322450349935	0.1439979187097808
0.1968757418375643	0.9755715216436674	0.2917158338120218
0.2199187871730699	0.9377089447347419	0.5096386535434693
0.3796756941383934	0.9344316448572970	0.5080308972875083
0.4316003822038285	0.9732575862206658	0.2981405872682739

Structure files (CONTCAR) involved in this work:

0.3202151985757004 0.9513716290334379 0.1507922720492962
0.0795977793063080 0.1745902947350687 0.1648157208265638
0.1980784023739608 0.1319274800408317 0.3067346239474371
0.2344103526459861 0.1763891409675523 0.5224047667303395
0.3883720031538438 0.1756119099713560 0.5083629139525948
0.4362078473949962 0.1308760561020129 0.2976520610423520
0.3187274273585144 0.1715069724878436 0.1685486391081326
0.5759053644373293 0.5570763901484088 0.3484829745323688
0.6956951688030720 0.5270221018418471 0.2027923583327388
0.7190953519232919 0.5650457041577934 0.9847099141013983
0.8792903722389385 0.5684873203971375 0.9848980961130651
0.9322704542309862 0.5328310655584845 0.1931932657046094
0.8202235120287459 0.5548197876476888 0.3379461896543684
0.5841853513632610 0.3293965915946921 0.3308612774124791
0.6982684255506951 0.3700091609547720 0.1851148309677402
0.7347091801701883 0.3278942025297655 0.9681473842597685
0.8887920721925269 0.3247273917622956 0.9850023147095190
0.8138575817343351 0.3323523218325506 0.3295886559601622
0.9239831666116954 0.4434769363253395 0.8524313338635814
0.8054305254245530 0.4735790307084084 0.7062662728862341
0.7766704531413535 0.4411133792364225 0.4859813323451766
0.6190164602474455 0.4381102076965873 0.4889813664266958
0.5668757864586732 0.4720662424214400 0.7001324299617148
0.6805528648931052 0.4456741256105918 0.8422877867002911
0.9212067550140463 0.6744155640654799 0.8246149671989906
0.8048848567672132 0.6314984131579872 0.6850238697078656
0.7650505240874582 0.6708258064367040 0.4668489343478794
0.6107154605772027 0.6742426588652506 0.4821938642610035
0.5643994571128362 0.6295770451406331 0.6966951107374921
0.6835071108399539 0.6725390117075459 0.8234658861904367
0.5765537942946070 0.9453407906287367 0.3520308650269999
0.6976209400510498 0.9732020934789803 0.2086936558798306
0.7208114885359396 0.9360914976330218 0.9877169766369981
0.8810369784761988 0.9342621062560966 0.9874993474464857
0.9315867081961151 0.9732360703959237 0.2008569108731813
0.8222298564045655 0.9462879527931839 0.3485850510208293
0.5806103762787491 0.1751325467749327 0.3311789038025748
0.6972155560067712 0.1311963464564528 0.1881632458690877
0.7339209952125348 0.1712112805562866 0.9700296927292296
0.8882621922946725 0.1731347701148089 0.9811030074036208
0.8179664325496978 0.1742130630181292 0.3241893094173675
0.9238831793503396 0.0553483348505079 0.8480189157431385
0.8029421560208785 0.0271333446614408 0.7029491503550467
0.7823210913475612 0.0662756918381143 0.4846264432272585
0.6226379727705468 0.0678281542662877 0.4860736180821110
0.5704056196341734 0.0305989895397767 0.6972081861532762
0.6805415922114327 0.0531339686790212 0.8449611882123139
0.9215218920216331 0.8291777420732009 0.8319270498358059
0.8024946104660799 0.8705557528802365 0.6892821060870448
0.7667273994474978 0.8272721637426664 0.4732468061294480
0.6121250488000290 0.8276511335213317 0.4852893265710547
0.5640941196079698 0.8725797656720320 0.6976306764501011
0.6816816185184478 0.8312897315346246 0.8271159805753509

Structure files (CONTCAR) involved in this work:

0.4227923309097480	0.4461570531950217	0.6497068310820598
0.3045704510208098	0.4757465100861060	0.7983882569913333
0.2818088228945094	0.4358740463785410	0.0163064156830165
0.1201756643476463	0.4351187420570788	0.0144178953984984
0.0688646224128450	0.4699301881311473	0.8007374001215048
0.1825217603202935	0.4477658427926529	0.6607165126023493
0.4211960044835829	0.6734435330972219	0.6659089454217991
0.3042812641696105	0.6334760416106420	0.8110793816661679
0.2675321461581250	0.6768550211864007	0.0259443623776452
0.1133477516341800	0.6769119537001185	0.0100442325166857
0.0652546163884894	0.6285738952611460	0.7978934334822116
0.1838384445696764	0.6731062541124078	0.6735003608226048
0.0782870997951360	0.5619927468669520	0.1461966070463002
0.1952087139695687	0.5326093340835446	0.2938810712450629
0.2206282504199917	0.5662008936169188	0.5149800604324145
0.3810879010554777	0.5663123247628423	0.5078059436435484
0.4325356494175216	0.5313146084731787	0.2944835870181614
0.3181380722827837	0.5596758980050465	0.1558243190014278
0.0791870280185884	0.3293500164359446	0.1766512550197098
0.2001847439046044	0.3739541405326563	0.3082925097206804
0.2373562569326528	0.3336087153517277	0.5264721222661390
0.3917285638749972	0.3289758266064184	0.5162308228147332
0.4409398972231134	0.3735411206948591	0.3024993364027261
0.3225691606597996	0.3300366276194339	0.1767298953377212
0.9359974263780817	0.1314675996059555	0.1970450526908695
0.9331347525512496	0.3721111598124876	0.1984865535672603
0.3606144445973029	0.0644979844730227	0.7124532425817939
0.3049737188816541	0.0723084380275830	0.8905592661000411
0.2001209108659349	0.0595625388491262	0.0136061979949159
0.0969252522166448	0.0741084294352595	0.8897015689651471
0.1050921943186196	0.0584582042204259	0.6927582030743732
0.2316668486631988	0.0362629960310000	0.7358357942187449
0.3578547094552909	0.8313194008174576	0.7417065356145747
0.3064112061200543	0.8455718751362122	0.9201253142676912
0.1897581784286099	0.8581491612100665	0.0117562167300266
0.0840597728806954	0.8338270271545034	0.8976055617203950
0.1043962715985060	0.8441192227302559	0.7024607157421715
0.2293707053850220	0.8626668367153916	0.7605266456292524
0.3235571149138585	0.9526392472904753	0.8046044066489961
0.0839632099780936	0.9533638805033635	0.8125643691289068
0.4344647027947369	0.1264340077538272	0.5760073341547923
0.4192168367316217	0.9950892034520289	0.5634400623446439
0.4004802802924435	0.8636055869054508	0.5594109487538653
0.1965777223302588	0.1328695863878325	0.6072684619703157
0.1837999096630318	0.0036439425192491	0.5568218224225295
0.1976118416693524	0.8692530198785469	0.5664266643648918
0.9892818377386386	0.0447343076392847	0.7783708095236228
0.9841750818128634	0.8672229656527410	0.7782518973264599
0.1420477880853643	0.9442720750246124	0.2159453933998558
0.1978817894712463	0.9308718190507793	0.3932796611475977
0.3001646384066003	0.9477026764617901	0.5199769083817558
0.4005423537800654	0.9308404753999606	0.3911310673603033
0.3958195310574054	0.9512335586687094	0.1944550584858327

Structure files (CONTCAR) involved in this work:

0.2701611992738877 0.9740322025365457 0.2401781398765161
0.1429996393065187 0.1696114702867077 0.2390241013254864
0.1977160691449781 0.1678944587497787 0.4150974629784255
0.3112394897911271 0.1496630331378504 0.5130460372568042
0.4134768929113172 0.1759495500989281 0.3930627579680880
0.3962100618814658 0.1564904873877453 0.1987262247965770
0.2714150802498569 0.1389291266775823 0.2551662707532972
0.1785078510827213 0.0531096849705831 0.3183694807477727
0.4191479983157612 0.0526503459312611 0.3205943146170934
0.0683069751596650 0.8770769361683157 0.0852703083610749
0.0836505849607207 0.0075349067447222 0.0612999566058046
0.0974414880432511 0.1398842467984847 0.0582371617848175
0.3023201309745211 0.8761791454189817 0.1131310905545775
0.3157492837788267 0.0038981526919426 0.0581471896045802
0.3025710774676614 0.1380282087434700 0.0605655400275556
0.5106426745987550 0.9575787606387077 0.2840970354114527
0.5159432341325801 0.1399183787975093 0.2790362850104850
0.6430875832015299 0.5593735403484835 0.2811597303340582
0.6929009374436950 0.5696454149433235 0.0993963792002166
0.7993602828830695 0.5552336503883560 0.9806930114665937
0.9052135599578867 0.5773448182291808 0.0985617718998914
0.8957053152155521 0.5589141960422072 0.2956042234222556
0.7704816577635518 0.5302198550693596 0.2491774864527281
0.6450059858065852 0.3283615604056941 0.2514442659384786
0.6962778894253252 0.3395549158101052 0.0734325902126692
0.8116743792648707 0.3522928283215621 0.9782198527263020
0.9147166970093341 0.3224856534549110 0.0976708685591514
0.8927473822137997 0.3482765715524706 0.3125634222354007
0.7725598222434685 0.3612886818954362 0.2335000431947799
0.6769115998526822 0.4487582921047102 0.1826538179760466
0.9178623146839768 0.4551538752852569 0.1731619626376834
0.5668665105675789 0.6279584626238339 0.4071014575533721
0.5783574667322157 0.4967391880828263 0.4307337240407443
0.6083236003301441 0.3667335677142072 0.4329027017202792
0.7985496140217611 0.6287508208071519 0.3765977960053856
0.8172681196100100 0.5009790929471366 0.4303999246196278
0.7883429461355228 0.3691812325703993 0.4318464723359206
0.0117337636666133 0.5474091020425679 0.2109766168055820
0.0170607308702599 0.3596649463799989 0.2417958695283656
0.8598918936785348 0.4372514895037808 0.7774493036497053
0.8078484674084297 0.4331712352070475 0.5990585223847725
0.6978363363323458 0.4590120871923035 0.4906099026274156
0.5914486787085773 0.4303593640831288 0.6021152231720450
0.6050361075653019 0.4445208277979854 0.7986934425256189
0.7308654012324103 0.4673117264766830 0.7519573912078156
0.8613319773502940 0.6743614540129479 0.7430270259556887
0.8049391709530008 0.6559069967644999 0.5699085034861691
0.6876840954145900 0.6477536050731907 0.4811666554948845
0.5821671428139418 0.6701991193412736 0.5951683144928975
0.6062424546969247 0.6606440796752003 0.7900321404084978
0.7317984433477290 0.6436167658556967 0.7350950765629046
0.8240885767606861 0.5519819832697697 0.6901079956258888
0.5838477176657653 0.5510133541054490 0.6818293531828502

Structure files (CONTCAR) involved in this work:

0.9331819576158940 0.3734082934326468 0.9124656729525287
0.9159454702793938 0.5055483190058084 0.9300628927535766
0.8969062236430217 0.6375602455896626 0.9262437301113019
0.6983114937494629 0.3708139700996808 0.8808142971369698
0.6847241859694067 0.4997885745188092 0.9327295344063807
0.6980499778540141 0.6339607274630971 0.9280513416089126
0.4875133876349019 0.4613899120417357 0.7191293754807571
0.4850163133756304 0.6375299512129189 0.7196342608135002
0.6414279872533242 0.9396684726985317 0.2801405333939345
0.6997937610337065 0.9316602081932985 0.1044434966969015
0.8010817339483157 0.9446159852563182 0.9749011986459259
0.9018281538243059 0.9338534073854035 0.1042276280187451
0.8968987287076416 0.9441490409061721 0.3015531879347900
0.7703329839171089 0.9686480758075618 0.2613942417620169
0.6422349970253093 0.1715549139423982 0.2531720283452062
0.6947791900180051 0.1596111637168742 0.0749112407428362
0.8110584519094827 0.1466841003629614 0.9829500206527215
0.9180865926320705 0.1691758651987968 0.0933347934899328
0.8956699621161203 0.1665660241093042 0.2893521370197654
0.7711343446733860 0.1433630749141794 0.2357581455114605
0.6794282345435769 0.0515792423754719 0.1884846815139121
0.9151950312568178 0.0528569705433381 0.1889705511936735
0.5673424537468934 0.8756473435657784 0.4138807188186125
0.5833941042204868 0.0063993965677424 0.4321011355717577
0.6002206505766301 0.1384060896901567 0.4355522245777395
0.8049958665864382 0.8718933269261674 0.3900978166832672
0.8201801543517264 0.0008911281934331 0.4389167496824213
0.8059424323918107 0.1346703324313870 0.4288310692435477
0.0113636435720055 0.9609274091470725 0.2120120107342933
0.0157955566548708 0.1382592622578965 0.2180894077859782
0.8581227667318466 0.0583373735638136 0.7778827885223427
0.8017632670227515 0.0726045268858760 0.6020439780870753
0.7022549567691274 0.0560850152737003 0.4708910755517716
0.6032769783659682 0.0710415902292164 0.6035494631927668
0.6050092669584906 0.0539077534048742 0.8011901454680709
0.7300921479269187 0.0288278552099121 0.7557602919819707
0.8573915697951338 0.8338791587385540 0.7587300695023235
0.8032325733889538 0.8340102466965726 0.5811197822778044
0.6896259736706679 0.8529132896965016 0.4824524663662494
0.5852998289569280 0.8295413467340081 0.5995150889415924
0.6041670342299451 0.8438273412376929 0.7946808822781983
0.7289281618570790 0.8631087268242211 0.7398442601576117
0.8209900746873279 0.9495772700034668 0.6757693063390868
0.5825635620982819 0.9508331256431848 0.6784520916300657
0.9319850266752189 0.1259079459550116 0.9071423903812071
0.9191900337782584 0.9947956238555532 0.9293616148052085
0.9039156784471218 0.8628858061295707 0.9395454395048493
0.6989099254014686 0.1283725383697949 0.8815796684437287
0.6846960369435908 0.0013821091291547 0.9386487915314587
0.6964474825518768 0.8672557745372945 0.9337449774600397
0.4914935940162337 0.0472611782480790 0.7087898419311525
0.4842469761427070 0.8649011251022884 0.7169193638949638
0.3566086661139232 0.4439528490007518 0.7189514375823191

Structure files (CONTCAR) involved in this work:

0.3087356149853547	0.4336835073362537	0.9019851522180307
0.2009717558212745	0.4341019569434921	0.0209874322925499
0.0960800588979042	0.4305317166960924	0.8991044851614596
0.1065369227218579	0.4417870523162213	0.7017795833613750
0.2293074362898552	0.4704118497877020	0.7542730221935052
0.3584855641598655	0.6714202447807831	0.7419053806494250
0.3074989756571179	0.6662232247908464	0.9216089606073152
0.1907272110347158	0.6512190485407647	0.0123529505651539
0.0851469809376773	0.6713811918218259	0.8968270139799031
0.1061558726436678	0.6581981804598203	0.7022480091073430
0.2299929802657172	0.6437145836564366	0.7639894773346143
0.3226478570046662	0.5541894642260666	0.8177772139955913
0.0831850911568825	0.5498773370706559	0.8150730670638446
0.4328996913521075	0.3733798813875195	0.5969868954518363
0.4172599852706186	0.5032870124089742	0.5630316857220317
0.4024248352263289	0.6360882833969339	0.5617464440076891
0.2055392601789830	0.3750668737830590	0.6187803796832745
0.1862972761429348	0.5036469596257868	0.5729257834743925
0.2024340548273829	0.6370074431501294	0.5684187217204307
0.9897589313985584	0.4556666557376333	0.7837761473957011
0.9857431927327351	0.6367466532271350	0.7761679995421018
0.1415217807332854	0.5687969352816014	0.2214517444261431
0.1909693361651201	0.5683121794726256	0.4023978256324598
0.3009713152476715	0.5553980625336919	0.5140447201248539
0.4054448118442111	0.5710045491598140	0.3926521977862508
0.3948271598190328	0.5577828348240647	0.1947997768486693
0.2702631227248156	0.5419998104638533	0.2502965313644346
0.1460733383902252	0.3301100295676128	0.2460806770922926
0.1968206765347215	0.3503933198360210	0.4241531479417999
0.3149474238867914	0.3558877042233430	0.5103538785899459
0.4254774607956027	0.3355100017623254	0.4069486772641102
0.3999888706714500	0.3374054274819477	0.2122130719668738
0.2747253328612660	0.3615577585995597	0.2638262586701416
0.1788649535856011	0.4525872793079191	0.3007563940440733
0.4185017487222711	0.4515919549730322	0.3104751241413207
0.0685862033829126	0.6320412174046169	0.0856142061928210
0.0915153355472655	0.5034820328440114	0.0640164702964234
0.0903183511266100	0.3709447741939425	0.0739023971102657
0.3028715343347757	0.6345697440957619	0.1146084009315240
0.3079395319171764	0.5051481376402679	0.0670463030951363
0.3115644993235159	0.3702063648177112	0.0726648541340801
0.5115857219037195	0.5456311888212659	0.2769478209217753
0.5206915144706729	0.3679662094786737	0.2804488772205881
0.4387341441101902	0.7508283172938692	0.6400522895756287
0.1967468590815851	0.7526991123740632	0.6585598894659941
0.2701898637206895	0.7553864461568019	0.0570025081103965
0.1089971330748743	0.7539907457858698	0.0484767768508478
0.0630236690294390	0.2527163356560146	0.1440213527184991
0.3049010303728524	0.2515159682926917	0.1592109668504902
0.2332253172577767	0.2546907829577031	0.5546681526795334
0.3946507408810653	0.2512831506450248	0.5523196734280685
0.5640525332682924	0.2527726989394567	0.3582213191277472
0.8002143578199625	0.2525909690337845	0.3437469567381458

Structure files (CONTCAR) involved in this work:

0.7298961053459821 0.2493863979081343 0.9371975731736963
0.8920442822762671 0.2490520747898179 0.9376949872807808
0.9401804198423391 0.7512766511208203 0.8521047966099319
0.6970635157334247 0.7518717504445039 0.8404119566247021
0.7695807659850639 0.7496050080788359 0.4374277094048971
0.6061751038456240 0.7513257540055442 0.4437342187903573
0.0231326733818003 0.4703854130906223 0.4661096513380517
0.9118742182858344 0.3371511380497211 0.5703547430637282
0.9947228061382849 0.3707239592549290 0.4327305326673983
0.0244377450271377 0.5188018305647784 0.4574596363719924
0.8739493152583920 0.3627521576467188 0.5974076249422543
0.0902092898395111 0.3030798973649599 0.5855055770892545
0.9305009922887597 0.3098248016480784 0.6239109049629351
0.0892583106977149 0.2553440380383848 0.4731587049039723
0.0257796371082866 0.2437070389200379 0.5630447605412990
0.0570171878703502 0.2826606921696393 0.5268897987770742

Figure S3 Cu/ZSM-5

1.0000000000000000

20.0219993591000005 0.0000000000000000 0.0000000000000000
0.0000000000000000 19.8990001678000006 0.0000000000000000
0.0000000000000000 0.0000000000000000 13.3830003737999998

Si O Al Cu C H
94 195 2 3 1 4

Direct

0.4227694072502425 0.0550218810075512 0.6403500735474557
0.3028122997893631 0.0269104231506635 0.7846884412212297
0.2798109521282683 0.0649220015169598 0.0048199231254185
0.1199879057015123 0.0667692386707382 0.0046960089554461
0.0694617700935074 0.0296569702011831 0.7933902236534824
0.1789590440033714 0.0528510806624009 0.6451418134325757
0.4210725021001617 0.8270730703550716 0.6630423760127705
0.3039288126545516 0.8696162625758087 0.8046333359467942
0.2673364130376318 0.8294160329364912 0.0238823487784492
0.1128638347572027 0.8271079814139711 0.0104728469486719
0.0655452418974057 0.8725181152720765 0.7974366921436451
0.1820620566893099 0.8285337691305792 0.6678707167206722
0.0767968290950029 0.9450007391710510 0.1421045607801903
0.1970574594260274 0.9732719955792748 0.2874418734957205
0.2186343495549480 0.9344036238495792 0.5063371904403268
0.3779718471507066 0.9317017352862665 0.5073033131915280
0.4298127504780542 0.9703031584348784 0.2973094208333437
0.3206518839660127 0.9483195281307077 0.1473801332638487
0.0793150624548741 0.1714004016586732 0.1622310818266478
0.1969773702180828 0.1299318255330213 0.3045100200201815
0.2325584017873888 0.1725512880308786 0.5208725629004465
0.3871383794541460 0.1733056219533203 0.5067731851636541
0.4350301417107777 0.1275565205222390 0.2964040906474270
0.3180212912946054 0.1694157679665134 0.1668619539086870
0.5753516132453400 0.5562406722650935 0.3540737094170446
0.6972872433545071 0.5269736341886025 0.2189472421356655
0.7141967444772203 0.5507577675143317 0.9872050454438959
0.8722967542727800 0.5683726952490359 0.9930006329061650
0.9286282510362484 0.5279088299134495 0.2045734326090825

Structure files (CONTCAR) involved in this work:

0.8203971024675761	0.5629221430412896	0.3498037713760220
0.5810907100668445	0.3251145597573584	0.3287179945491635
0.7025669049196207	0.3689663145701917	0.2039013413343455
0.7321411244834375	0.3292331102489510	0.9849153224312273
0.8886595527228237	0.3305250780613271	0.9966440623845326
0.9360440035666693	0.3696315037532666	0.2097832355859458
0.8220033714254446	0.3258777041997743	0.3401957684587752
0.9243166893175344	0.4480660708683495	0.8605325813376092
0.8066387346159045	0.4665210890687404	0.7148993189627667
0.7804334101316577	0.4397114010247773	0.4926148268771701
0.6203817155487535	0.4311938465359464	0.4892053666777938
0.5642342971777317	0.4642555171858662	0.6990611935773173
0.6781170180924695	0.4327750680143972	0.8380197113797154
0.7967778130832411	0.6246817128908470	0.7091205409062256
0.7670787801205331	0.6705348323363702	0.4863255451067991
0.6120591388882256	0.6723411816563559	0.4878117529715498
0.5630930596863168	0.6221233438996858	0.6988007471491353
0.6718236626810644	0.6649618866900279	0.8375460832134275
0.5758753342713406	0.9410940461223704	0.3482550353710090
0.6935728534977158	0.9712231042433014	0.2042818809033287
0.7189420877302936	0.9502250031999044	0.9809412322027086
0.8769583803570421	0.9471209315108222	0.9812300817068137
0.9329986171650034	0.9684948951142078	0.1937074124330500
0.8164640652998294	0.9296007891577649	0.3239911325691813
0.5804630646153223	0.1714742440517465	0.3214955853726983
0.7011146048757276	0.1282759840978566	0.1955583471176069
0.7357819961088484	0.1682723559065499	0.9776387472972609
0.8933175400769768	0.1776729270174450	0.9767644255156220
0.9370933167372471	0.1264362489887584	0.1939190160596733
0.8226958831623626	0.1722674727994672	0.3296393186344951
0.9242293269267982	0.0652615070264672	0.8400605266896364
0.8067753888809782	0.0303450042563686	0.6982772995023366
0.7831832202668030	0.0525827664075436	0.4730684413468044
0.6232818831333444	0.0657896666705152	0.4809256185857564
0.5671767992266625	0.0341179259443614	0.6921887589187947
0.6830472033606841	0.0658264375735312	0.8240163068889367
0.9179803841662066	0.8338955145466721	0.8252051548302417
0.8018875788231774	0.8723693537054573	0.6927305883001525
0.7673738926161342	0.8312123262356823	0.4772614975915833
0.6112001957860775	0.8271114223330279	0.4881130759736833
0.5647814323357555	0.8757298062085690	0.7023080957280221
0.4200027953464973	0.4438913922492242	0.6470655288237831
0.3001183483155606	0.4733092315004358	0.7904148202281528
0.2796331382894829	0.4355075486281761	0.0115003975861396
0.1204359985820547	0.4327766916180856	0.0106796317107783
0.0700891986856511	0.4701436309170834	0.7998496014434778
0.1774082601227258	0.4467526224417958	0.6496405606327266
0.4192724938082418	0.6718990601408511	0.6623992396810681
0.3027241172728925	0.6300262825778786	0.8063048445824115
0.2677421770411831	0.6727936174865313	0.0258503944153444
0.1140794651307006	0.6734106957037733	0.0110183189565873
0.0639123680037442	0.6282172602459528	0.7994632573626831
0.1807910468674137	0.6695858635709444	0.6680042395651163

Structure files (CONTCAR) involved in this work:

0.0740767237230051	0.5561363945235825	0.1413587365508990
0.1947379838715817	0.5274947370430172	0.2860026690245894
0.2162850549414764	0.5633833583155270	0.5074255858208069
0.3757496318011010	0.5655930966067754	0.5094470387827292
0.4301199326533961	0.5282697727012364	0.2989134550067086
0.3210107938316379	0.5544604636014083	0.1488764842111003
0.0791280914706931	0.3259727759324715	0.1664102806518081
0.1970970212205716	0.3694557330257416	0.3054063066576022
0.2328086753072213	0.3288933689700942	0.5237310552446166
0.3876631144262638	0.3261185439827757	0.5115093925817306
0.4372968598620963	0.3704593721471340	0.2993378456638339
0.3193377241002032	0.3285433768190454	0.1706731120458056
0.3568948831672653	0.0608776737035764	0.7102317317863971
0.3010173102012120	0.0697592440978202	0.8880627963981723
0.1996677446915313	0.0545020139078425	0.0167654205893618
0.0987014599661352	0.0714192584166830	0.8883029217715014
0.1040692586773680	0.0553528400403190	0.6907970765145031
0.2294958258756042	0.0289593662172429	0.7332738551094905
0.3593647120534790	0.8286690244762396	0.7415577655710355
0.3044589563917443	0.8404803532244183	0.9176164388876814
0.1897634492787655	0.8533167357236650	0.0144565854609068
0.0862721408372560	0.8303677828821213	0.8966713241938835
0.1049376713133996	0.8416566244632708	0.7013598624834188
0.2304490289893243	0.8588726424208960	0.7549949805990132
0.3226797233727962	0.9491089226310864	0.8065475372222146
0.0859766323567288	0.9508478864518701	0.8131828821708027
0.4314475280701171	0.1238292621352388	0.5761467658445256
0.4181234967607834	0.9920246587195881	0.5630391242457520
0.3975963150912512	0.8600810360985509	0.5572650256222599
0.1972337255102838	0.1276871389678806	0.6064453176019532
0.1806261765692292	-0.0006428125727354	0.5533722306182797
0.1963483348720025	0.8653035668032316	0.5614899139764732
0.9901851814223026	0.0428473896141261	0.7788253874671133
0.9859559316044838	0.8674965119994832	0.7798435221799382
0.1428797142810135	0.9410821788866125	0.2114377779844825
0.1983215464317476	0.9286910414341633	0.3890763386717862
0.2985169599476325	0.9458910607845027	0.5195861467545981
0.3981173713697470	0.9282546161615504	0.3900687880268147
0.3957028325175020	0.9481345445969405	0.1925011739662864
0.2702238491590863	0.9722340173169670	0.2356343489033759
0.1427817305412232	0.1688770173427200	0.2365504204809841
0.1947068023259839	0.1635230673759530	0.4145320294636288
0.3097394491966882	0.1482538424445011	0.5083583882649431
0.4142467342667959	0.1727966577000641	0.3925337536105806
0.3953736107010464	0.1547739473406561	0.1980581287806182
0.2707736834405682	0.1386695089607872	0.2550701722769920
0.1777158284547279	0.0507992139225736	0.3125159219348042
0.4164687253978890	0.0496837017281007	0.3189673926742747
0.0673877788798354	0.8738193484126899	0.0834552968961824
0.0812940355681336	0.0050658239233910	0.0597624091171096
0.0984247413532322	0.1375152746288686	0.0556540507793515
0.3033532350997872	0.8727672112118660	0.1107035223241225
0.3170112448599747	1.0001920493213035	0.0537574126259671

Structure files (CONTCAR) involved in this work:

0.3018973425675336	0.1341344134150559	0.0600875565061074
0.5086707934365969	0.9546739212321191	0.2842596930188530
0.5148391583909804	0.1340727419893243	0.2763910793792801
0.6384526138619260	0.5655090918594052	0.2786776999918920
0.6893233076911629	0.5442842752199926	0.1012401395693744
0.7942673103115495	0.5486721842777319	0.9732056678717521
0.8916982269220569	0.5633395036961035	0.1100691191911111
0.8960103924984752	0.5569829538717985	0.3069417600852877
0.7694691560388478	0.5550690339315696	0.2549532993024653
0.6423686177539419	0.3247790287656400	0.2495994060741046
0.6988592690774660	0.3630209382609953	0.0836131754398919
0.8104087766820645	0.3509077372289633	0.9843036416553476
0.9098304608053548	0.3275432549943713	0.1135818041571901
0.8993549586309734	0.3409206180513402	0.3094144635660908
0.7746414017312112	0.3424261106172390	0.2435637772152260
0.6922529956421115	0.4467913996797374	0.2386732813860118
0.9158925055018965	0.4479496750041945	0.1945937044377419
0.5649718807969253	0.6243314140210287	0.4192218174874742
0.5867696691027215	0.4933215065762274	0.4290036981469268
0.6055571901779111	0.3612302923163139	0.4312171068504087
0.8110342697041449	0.6376422483012096	0.3960834438112707
0.8067848871753950	0.5054652600606481	0.4325567962449209
0.8009582118002946	0.3714319217708377	0.4348943039019717
0.0073101874822340	0.5460497090271614	0.2084541299869682
0.0164315642642135	0.3628388697117872	0.2218522056115469
0.8606465688174498	0.4313958778589418	0.7891785127726656
0.8155358076089837	0.4381887294915855	0.6018311519957723
0.6998371406990676	0.4443386067034279	0.5014974986742069
0.5863873335793079	0.4248974884981075	0.5983163136752147
0.6029361045048823	0.4313014700994983	0.7937469976259913
0.7308671908674363	0.4483201629785317	0.7492611450206129
0.8469168329799509	0.6728470816008174	0.7659733773182692
0.7928268359247428	0.6404496763150062	0.5907839371653831
0.6892368088945796	0.6494482400761546	0.4698218710743093
0.5928630448533665	0.6642936610879570	0.6050904990187798
0.5954363031442337	0.6519929493579421	0.8018848954137500
0.7210884421627586	0.6314526956793223	0.7564375547714044
0.8192172512634132	0.5464530718657238	0.7205340607169973
0.5833466206847528	0.5434340544218451	0.6874765002968286
0.9336155320840991	0.3863479733760771	0.9393514151509295
0.9157994706210411	0.5177681435473023	0.9240867417763282
0.8905749617463367	0.6464183552831493	0.9617184332657970
0.6945659759917933	0.3604687391348746	0.8881714901928305
0.6807723939118174	0.4923929523394089	0.9213811873884462
0.6819926383996343	0.6241761568609766	0.9485857215886923
0.4847423636275404	0.4551692383011324	0.7183489040002484
0.4827649641368266	0.6299319040877881	0.7059511522892241
0.6375145477306391	0.9328199606770511	0.2700721621321034
0.6789570386702872	0.9609817099336041	0.0857222004735814
0.7980813260794229	0.9625619860590531	1.0003385461869956
0.9132242364652948	0.9339720588865760	0.0878082223859160
0.8930345254060859	0.9323099801457434	0.2844482075651015
0.7666437013677685	0.9388614942702457	0.2280676006074482

Structure files (CONTCAR) involved in this work:

0.6375240689215214	0.1711649159800700	0.2349237005379394
0.7041081210481513	0.1309389842700773	0.0747379375673412
0.8154943109435219	0.1538899961729451	0.9716528623081645
0.9208367518396343	0.1628736666091611	0.0883669392860484
0.8977657282283165	0.1636463516629746	0.2847711407963612
0.7701366444473817	0.1597972459641064	0.2385735406890884
0.6931211001467938	0.0508130908672152	0.2330698997757902
0.9142351601842083	0.0480967075568728	0.1905763409887600
0.5659236477425492	0.8732011167397249	0.4139963489148227
0.5882958056013998	0.0035657210394999	0.4234526402382918
0.6083061841890969	0.1352168902363154	0.4215282145630058
0.8034902165012436	0.8568674304932480	0.3751161622917546
0.8032239265169085	0.9891352407976861	0.4038571883571376
0.8093404196695666	0.1214221509135488	0.4214393835932305
0.0123029043685530	0.9571607705700496	0.2135066600465539
0.0170084080971582	0.1320441607434975	0.2145108410740885
0.8617891852915972	0.0710725666688661	0.7636849623211956
0.8194244525421579	0.0457400839397345	0.5808533815809480
0.7030484207639093	0.0540146541659163	0.4880633297310000
0.5910807416186029	0.0725932269467513	0.5911572282820603
0.6062201368193902	0.0676214584863353	0.7864976520997248
0.7324582249597916	0.0570230265474511	0.7284776805443827
0.8657136248182381	0.8295993094801777	0.7327914411989001
0.8025125498578164	0.8681157087040916	0.5709960260840747
0.6885229014540843	0.8505724957321722	0.4740470688121038
0.5887041685049488	0.8335174850744488	0.6035126532972090
0.5994404813826654	0.8485273432518470	0.8023605996621780
0.7334444223456934	0.8444928412985344	0.7379587320848543
0.8139576845425208	0.9511697384149880	0.7239339868967077
0.5834419461371056	0.9546461907058854	0.6821809722681302
0.9364166365799752	0.1379510537537692	0.8927258513026968
0.9106368832354006	0.0124972041631188	0.9302877475033217
0.8860713843761198	0.8817089755178784	0.9122087770857679
0.6993495055236489	0.1362902166316987	0.8805322388807991
0.6910744129032913	0.0010671899532201	0.8976214850390734
0.7085480156573746	0.8709917446230275	0.9471243856651942
0.4878840261128226	0.0462438751291319	0.7110960454261511
0.4834906501620885	0.8680100201155072	0.7101994431722521
0.3540473637351619	0.4384177425290285	0.7165477424633095
0.2970365637971966	0.4301906960621537	0.8934081409786341
0.1997264375875677	0.4444118286386419	0.0296283654437095
0.1035646202380453	0.4290350797609194	0.8926864298398273
0.1025139295393041	0.4435032104284955	0.6957638821554548
0.2273924841106544	0.4728978067150685	0.7372679643956271
0.3597771125225536	0.6694370139088918	0.7440955934443543
0.3015868918459043	0.6622854108004221	0.9171501722857370
0.1905272115695546	0.6468705477840826	0.0235924260646237
0.0923704229904824	0.6704081141173608	0.8954218103901154
0.1038239609530777	0.6564765472076147	0.7011042997570021
0.2302089409596869	0.6389241952210720	0.7536016268916287
0.3215748665157225	0.5505935310272327	0.8132007014446830
0.0844195469236170	0.5494636906736015	0.8163649750853489
0.4301030897400417	0.3739972202384766	0.5861225661958483

Structure files (CONTCAR) involved in this work:

0.4152303172050765	0.5057646305979856	0.5676297381919063
0.3942653453457455	0.6379789971040386	0.5582395522268710
0.1984799908815531	0.3722597485762635	0.6121762979389354
0.1781785021692030	0.4991275266108902	0.5563698529065372
0.1951930912620269	0.6331213271831262	0.5613494474191747
0.9906008389102176	0.4545781623348676	0.7925157301616489
0.9850286038405379	0.6373497486930129	0.7893364194606615
0.1384399276407016	0.5605420779253359	0.2141218847881789
0.1949308060660213	0.5684436644230166	0.3907272642073156
0.2962845955782813	0.5510604179113234	0.5188258709843678
0.3984141949543310	0.5682848352387551	0.3933684422462155
0.3955884534848181	0.5531007191193311	0.1959198666222019
0.2679562146141244	0.5334933188432869	0.2352051350627349
0.1431919973830166	0.3277386166565515	0.2400576361937835
0.1940312787611482	0.3416012189344952	0.4188921698826702
0.3104011560861763	0.3517466901582199	0.5101095620865431
0.4180164621568442	0.3290515992457456	0.3994543593877790
0.3968850937799531	0.3399688096017229	0.2039607156089183
0.2715304542176858	0.3583141637515181	0.2590733328491622
0.1775214689232344	0.4486597482907691	0.3040963590747394
0.4172657779353446	0.4485729846433504	0.3158790783852554
0.0657647558339756	0.6265900052928877	0.0803930095080919
0.0798137656099489	0.4947310203867520	0.0619169472369170
0.0967112802867281	0.3626265757074695	0.0612529501624401
0.3076578144726756	0.6302012742619549	0.1096657179306306
0.3171086580351858	0.5013493328234717	0.0567094166032858
0.3051350730659527	0.3671426770860068	0.0657646433205783
0.5092791486375817	0.5437352452044329	0.2870970833328406
0.5173033814351393	0.3638698028237217	0.2794917882665067
0.4406318896564165	0.7490819046421214	0.6412738865391747
0.1957093835090447	0.7490126359329846	0.6532774409123835
0.2713967348809324	0.7512470013474178	0.0569932686039592
0.1069298723955643	0.7502878941338244	0.0509127094923154
0.0592984461284264	0.2490023997090267	0.1413971978099290
0.3048042525199379	0.2493032101651523	0.1542068631735932
0.2281756495596057	0.2504644222518549	0.5554642298058821
0.3927134454158177	0.2491809879486478	0.5508858042207349
0.5613436501038411	0.2479430586104331	0.3523352119093467
0.8136021996162567	0.2479888307557180	0.3727267115321095
0.7222761028830751	0.2485762276075876	0.9840106323091491
0.9009565713405128	0.2567057365930764	0.9495358565470537
0.9318698793137211	0.7616739620525708	0.8744299864714246
0.6859472713270219	0.7411329348152277	0.8710886942251672
0.7768875185037140	0.7506829033299411	0.4831407145555855
0.6014337168194043	0.7494094795036736	0.4533770358931185
0.7759164314062410	0.6705749678661987	0.0852568015798898
0.6787388731556095	0.7741629091585867	0.1119341169784948
0.8328702476102405	0.7995477171617676	0.0928912195305877
0.9173673687236459	0.6791550324289298	0.8389856662307762
0.6800227884978431	0.8267494868258313	0.8354157435423444
0.6888827223830623	0.6988686799535758	0.0448782023036522
0.7492538013706180	0.8174476167321609	0.0580466595553251
0.8605505700619253	0.7211135421369727	1.0457389678951079

Structure files (CONTCAR) involved in this work:

0.9421091738681975 0.7448489318804086 0.1227664981997722
0.7768361897911026 0.6675117452538954 0.1583702108573951
0.9631243172856370 0.7897309986320207 0.0881470793093713
0.9230959429452861 0.7525191731770735 0.1985082413518168
0.9686929559947048 0.6975897773703637 0.1090611570210945

Figure 1(b) Zn/ZSM-5

1.0000000000000000

20.0219993591000005 0.0000000000000000 0.0000000000000000

0.0000000000000000 19.8990001678000006 0.0000000000000000

0.0000000000000000 0.0000000000000000 13.3830003737999998

Si O Al Zn C H

94 193 2 2 1 4

Direct

0.4222315956906888 0.0600205156779385 0.6487854637370913
0.3045012476925999 0.0322728876529955 0.7920110987578940
0.2818657752749729 0.0569911233374105 0.0173973885070961
0.1220366809981945 0.0646375585515379 0.0127024921004119
0.0675227261455376 0.0317126074237008 0.8009059730707019
0.1799319270717094 0.0652367480117991 0.6643628476806259
0.4185470336617413 0.8276324771860039 0.6690150291323881
0.3005674918896972 0.8733884740772896 0.8006464007003021
0.2670572896507950 0.8306460767130091 0.0197645765926929
0.1111488062166020 0.8264922470011626 0.0122511798790656
0.0657960190755553 0.8745829848196881 0.7984341708504152
0.1788158747427852 0.8289575359443325 0.6643465807818393
0.0758808265854396 0.9415247346645308 0.1483358592874305
0.1945178006034802 0.9702573503470594 0.2901488647036715
0.2162536364009456 0.9438179629746244 0.5158842037005352
0.3765283622632671 0.9356409060964369 0.5137380583773019
0.4331462081474707 0.9684316074021273 0.3016654043894743
0.3197667874931087 0.9357082933593539 0.1643855778715639
0.0813835300565583 0.1738802783358495 0.1671514063743340
0.1982414818409581 0.1288746277472329 0.3005557469396014
0.2313949460795215 0.1697710701341047 0.5181122059719335
0.3870875865329422 0.1737303182847238 0.5092430094284298
0.4354348396722320 0.1269186706316908 0.2959778521220139
0.3194348723868560 0.1724839917400661 0.1664440985485536
0.5775657651960358 0.5556291375728190 0.3562433140995118
0.6911664267681564 0.5272240292931422 0.2018331748169959
0.7149018885076122 0.5687466265068272 0.9869202444663995
0.8746660661026374 0.5716225208334758 0.9876157290602383
0.9260979495963239 0.5304817072750423 0.1943521716043006
0.8123324354244109 0.5522662515616440 0.3416848915342858
0.5735169538511834 0.3290087480807520 0.3326970397492731
0.6947120263311936 0.3726039350798545 0.1937292376226636
0.7304165988855472 0.3273558047000320 0.9795838798106099
0.8849556184572327 0.3263097782193150 0.9928689801521209
0.9405473387596138 0.3761665441566485 0.1916250414106703
0.9202498587157568 0.4447731311709951 0.8602290136918966
0.8010556064841640 0.4734520932184035 0.7195371546317918
0.7773510899729130 0.4373875225389444 0.4942691282497138
0.6195229526841475 0.4289410070526531 0.4903103121484984
0.5697252864861174 0.4696337751174794 0.7020700685261435

Structure files (CONTCAR) involved in this work:

0.6764133516277968 0.4477438730034380 0.8566076602795012
0.9214669997805226 0.6777647209649632 0.8343511058374536
0.7709815808687911 0.6690080225214183 0.4669765620662024
0.6157341753338719 0.6731970324963737 0.4882693268855781
0.5611492054323972 0.6279263991548523 0.6978929749763659
0.6733194123714217 0.6744063445162389 0.8258554458958441
0.5777571908336669 0.9451275416304852 0.3586403039453238
0.6983344431163763 0.9739883057462562 0.2153940557534988
0.7191879195250289 0.9380997500026527 0.9935420117796910
0.8789899937396792 0.9346240901775669 0.9951795297196204
0.9312709894759058 0.9705212528316134 0.2048150446026911
0.8223692928731829 0.9465585664451398 0.3552303047466858
0.5782648871081011 0.1737933433582603 0.3298724062502489
0.6980681020436651 0.1321315831276810 0.1939929607452378
0.7325360200974381 0.1712790532729801 0.9728420857873586
0.8872924436894705 0.1734922280885325 0.9857008005114680
0.9362552082056899 0.1283030779676535 0.1987948867280135
0.8205991310862721 0.1726659023863183 0.3318686542863619
0.9230733049166269 0.0549406207224494 0.8571264073934006
0.8022985938807640 0.0263524798759124 0.7115502993782129
0.7807058194754772 0.0654282421397593 0.4930427937157971
0.6205386738203155 0.0697215408780324 0.4903912479196337
0.5677486792877054 0.0322706343191112 0.6991474816920152
0.6782999630398039 0.0534983648656173 0.8498241909314678
0.9232556154012808 0.8302079554486773 0.8383935143947663
0.8036875550047045 0.8691853224296789 0.6967808285260174
0.7706093449475496 0.8270704852665202 0.4789466854090999
0.6157371629899228 0.8268491375358838 0.4905538744257796
0.5639416821093322 0.8750842979576171 0.6979636621705632
0.6788885371370207 0.8332667001956593 0.8329208894178796
0.4234652054761412 0.4420111021516682 0.6455736933925373
0.3055060462636973 0.4694686426822835 0.7891408450671514
0.2810321597832238 0.4454465570042859 0.0144755492645434
0.1231238978403628 0.4370074258667705 0.0135697377099462
0.0645280945443856 0.4686704025337660 0.8022392663690922
0.1783069114589197 0.4355665477073838 0.6647917674434514
0.4154282229323188 0.6737329992368452 0.6674559110768287
0.3002362316956070 0.6278885093265238 0.8004922719581689
0.2670545181388161 0.6694130549711498 0.0195621097078843
0.1114691977166761 0.6725498131392876 0.0100580794430295
0.0639651950583390 0.6276676152699711 0.7958462783338168
0.1790492403077475 0.6716485362035711 0.6639356336453339
0.0724103620807574 0.5585036693395222 0.1487071009987147
0.1916736213115570 0.5310096529388600 0.2898985405040328
0.2148379708835843 0.5558542154887833 0.5164235562236970
0.3736924408231050 0.5657196715652351 0.5149697218740601
0.4300429532120291 0.5317971560847691 0.3051893086063832
0.3189859494504368 0.5645530454816490 0.1638548127195897
0.0852896405331839 0.3270328733602879 0.1624379592929331
0.1974473789059755 0.3726241340314367 0.3007199567281833
0.2306292763022742 0.3311991622399076 0.5188040934000143
0.3856283271663632 0.3277286193349838 0.5070205376009413
0.4312017504912988 0.3743163985736111 0.2944024371849986

Structure files (CONTCAR) involved in this work:

0.3169576304332402 0.3301209392345960 0.1630237535487157
0.3587223656454850 0.0708019817664016 0.7225417309613033
0.3156900957622607 0.0541181000854965 0.9073263126121001
0.2014694580022333 0.0496410518277391 0.0090307507805459
0.0922788615215330 0.0704922368026509 0.9007997727055749
0.1032587155745487 0.0648003206176115 0.7036596478675229
0.2291474352821725 0.0531605449446985 0.7595300734138597
0.3600719251571762 0.8286895275674412 0.7529316903414988
0.3004737337639526 0.8623528345471941 0.9201450794160656
0.1884318844502374 0.8507861514668343 0.0232013947121354
0.0885540179934292 0.8324259036250212 0.8965023360515790
0.1022021044804586 0.8419745553429002 0.7008840857966960
0.2286852041928969 0.8506518023776347 0.7551834000309082
0.3147653360751561 0.9519197268266414 0.7754799055505985
0.0881297034459647 0.9527335876210766 0.8102015081921634
0.4326065859911166 0.1275548349030401 0.5821801810371060
0.4116508639051411 0.9965851461718144 0.5743632821214293
0.3926385566507050 0.8646450357017890 0.5681127624408192
0.1954376058232014 0.1383944389262191 0.6159524024455030
0.1894370672022659 0.0059833146323479 0.5826630962469151
0.1943124748748417 0.8723736762686833 0.5644056871104496
0.9874920273267214 0.0404833937223294 0.7866959331002470
0.9851708131433190 0.8702011041306292 0.7856540247623970
0.1402405985583643 0.9318461768280892 0.2207397710351577
0.1828513811729400 0.9495469705943889 0.4058055944296852
0.2968069848859707 0.9485107605107119 0.5084383986728466
0.4070006952843161 0.9314184886093124 0.4021890139225116
0.3961003407665309 0.9362092428980964 0.2049128268972668
0.2697944826198376 0.9485099660564884 0.2585575068107487
0.1404422413693772 0.1744774899081883 0.2501117663730343
0.1948100693676932 0.1388311928206161 0.4202990189850294
0.3097965283596899 0.1484590163450085 0.5158629256792612
0.4132829893513745 0.1682802211058344 0.3951448218388698
0.3964697100573019 0.1585307388306861 0.1998482780531862
0.2713666078167078 0.1522735662563915 0.2603824351428251
0.1847739541166309 0.0506483399918972 0.2724395884360487
0.4158154922844701 0.0482302379552537 0.3091962595633008
0.0649181240030691 0.8733735420284694 0.0832559402259112
0.0850142106396892 0.0042180987168053 0.0720176133513232
0.1070036022697562 0.1357531209601619 0.0672312736196569
0.3048555913644419 0.8624080330962021 0.1158676923341287
0.3107145419176899 0.9947755551483510 0.0821459281121412
0.3010041653530507 0.1284423376725704 0.0683219407073512
0.5126876188772537 0.9556957263504177 0.2880000615734754
0.5155702201259444 0.1339343706190223 0.2792202812682633
0.6386590132598495 0.5614166257833324 0.2779420969758885
0.6971091164094629 0.5755245385964121 0.1048037957531898
0.7951544586835529 0.5611254688682505 0.9694128408848198
0.8906773482061220 0.5747511235228481 0.1073207956845904
0.8884851293199330 0.5397953200416695 0.3024937125785803
0.7639059838739380 0.5249673752585823 0.2557960421762397
0.6394846249252858 0.3363920050133776 0.2646688345712629
0.6924839208949362 0.3345185882002784 0.0858754840375916

Structure files (CONTCAR) involved in this work:

0.8079063705919342 0.3520017550135217 0.9902940388763549
0.9106907063796019 0.3251113486786326 0.1086096212627749
0.9073939712203527 0.3603215570492993 0.3009986217585421
0.7675480605425844 0.3690974938506221 0.2434686409429070
0.6709082432544325 0.4506098653406876 0.1748848754077875
0.9216891337266477 0.4524860792498498 0.1593574919469989
0.5707683029520310 0.6266966927603298 0.4147895786972767
0.5907337291962007 0.4966125507184569 0.4380401562205084
0.5846951937944592 0.3629851788306233 0.4424432677399063
0.8012408901177149 0.6311172409417073 0.3684218601403327
0.7983735792468115 0.5124771017208428 0.4487761536616065
0.8260585463652147 0.3825151620402347 0.4419874976327511
0.0036837158115028 0.5510840078089642 0.2129027900832914
0.0207905685406650 0.3689914699494892 0.2017794707944781
0.8551078629624997 0.4346530145184768 0.7888145177369164
0.7928884081181152 0.4354639313164801 0.6125868129133044
0.6997693228960616 0.4238372963606204 0.4695283550358950
0.6050721631105732 0.4302397676100408 0.6091931297145007
0.6028182398900656 0.4449887140409938 0.8064213815439789
0.7288776133236812 0.4747485349962287 0.7727071808275185
0.8599443447067168 0.6799906406682691 0.7588305176790908
0.8164450917998599 0.6442584152622473 0.5633956446344370
0.6935042130288354 0.6472840306745177 0.4861661187480175
0.5865558342097501 0.6692333633243549 0.6005016048081002
0.5948717762313592 0.6606629476322714 0.7970326144422794
0.7196882663263811 0.6494246805468322 0.7345835347442190
0.8265942219962670 0.5498375756829550 0.6959861958074886
0.5818464963038498 0.5494705559295309 0.6854012848811611
0.9306647628835962 0.3770701253502733 0.9266925735345733
0.9130212388976404 0.5085987337958969 0.9353121870324804
0.9016046864352836 0.6411593931369645 0.9398214835936168
0.6948149043298066 0.3728486339598961 0.8943811454327057
0.6774483173715082 0.5009010627107842 0.9483618904815497
0.6888161485068142 0.6350789322963676 0.9300794459712814
0.4909487719813600 0.4518026733636337 0.7104680208382886
0.4804020480393461 0.6329939714721716 0.7074703844310430
0.6434840386903038 0.9402410984809662 0.2886756001044574
0.6986846894691171 0.9331324341728343 0.1104799622989280
0.7994743298353564 0.9470352510715555 0.9804124961371704
0.8979596344237919 0.9290111419561236 0.1126674416415457
0.8975463586595543 0.9488303467766809 0.3101684349877789
0.7715798602780165 0.9681993350409052 0.2662678508084296
0.6408432628217565 0.1735082296470160 0.2534705538959203
0.6964789164902270 0.1577752278598359 0.0792356892337898
0.8102625399500956 0.1475062658848867 0.9806613413223219
0.9139036122449814 0.1697233644614941 0.0997617024138263
0.8972228448465285 0.1559349461004115 0.2965514541019669
0.7709419957681319 0.1451972584140380 0.2432501105837006
0.6800637239320614 0.0524837235607058 0.1975040903807217
0.9192690352574912 0.0495838445238686 0.1815446244358590
0.5702758922446216 0.8750677405167442 0.4203784325301584
0.5819165759072276 0.0071036868165700 0.4377258776934955
0.5995237211704861 0.1393310007094944 0.4354253427132667

Structure files (CONTCAR) involved in this work:

0.8082266627946429	0.8704934346332525	0.3936706418667235
0.8161259181517537	0.9981217639539232	0.4486677377289938
0.8056561376983331	0.1321978174122681	0.4355025916557771
0.0102677566043715	0.9541095842745673	0.2164010037507755
0.0162186741083722	0.1378930309835619	0.2157608872650771
0.8569844273148522	0.0574232944225426	0.7876271738729012
0.8012140628811142	0.0713696423106965	0.6102937407928358
0.7002660054454186	0.0570940815838562	0.4806658386885861
0.5984776720289414	0.0757679895419821	0.6068274870630225
0.6033849542813555	0.0526151412415472	0.8037246170233201
0.7289378847056724	0.0280685334479576	0.7628485652783599
0.8598658319475593	0.8325005932221931	0.7637156352032842
0.8062760027202351	0.8349472323506361	0.5869288671733329
0.6932545985984154	0.8518355888632748	0.4865792368709800
0.5890505082949089	0.8290424295048533	0.6049076870278027
0.6031279308793860	0.8528594733086650	0.7989998247743293
0.7301028669284819	0.8586908822920358	0.7458051070838162
0.8205913561229105	0.9486939225228181	0.6861820177416126
0.5794663486089955	0.9533316503785144	0.6727340341383186
0.9325993527126903	0.1272873076314925	0.9121733332561316
0.9182578913890594	0.9970063451453018	0.9428268877747478
0.9024019648872051	0.8646686538457734	0.9439455305229617
0.6957296337103257	0.1294723209689207	0.8847419805781431
0.6821784286703518	0.0033754777205409	0.9455871941582666
0.6956701724675354	0.8694896042053821	0.9386543411928143
0.4888291876713122	0.0477559812307062	0.7149522221099645
0.4842676839095913	0.8644428183946208	0.7148442668131464
0.3604169393341384	0.4311167827079251	0.7204711147723251
0.3156042757394789	0.4476899622315189	0.9048258558922712
0.2010957681279478	0.4584104290534740	0.0054011647575516
0.0901614552203566	0.4325070364911656	0.9037205268424124
0.1023158518484131	0.4349311289488834	0.7072016588292578
0.2301170479393559	0.4486817555061040	0.7562332673046038
0.3589663018542694	0.6744639600983119	0.7545606884781448
0.3002616096802685	0.6371094035891228	0.9202363523231012
0.1886016651494795	0.6483338852608419	0.0234949942833375
0.0901930746432329	0.6681612619160285	0.8935888449796976
0.1021251050387419	0.6575422131324582	0.6978238418568125
0.2278752060632101	0.6499843585216484	0.7560802595390043
0.3156461975552686	0.5498763370728441	0.7727107018601226
0.0817907064092664	0.5483622602089862	0.8079229088687351
0.4324906965142208	0.3760707411694955	0.5749834223260948
0.4137020139543242	0.5076011809934778	0.5750409417793924
0.3843682052204085	0.6381165219793808	0.5683373898653774
0.1930794180536455	0.3625348186070853	0.6154708924746155
0.1836960144439810	0.4950638307070180	0.5822280266966572
0.1964617466157275	0.6283622169023397	0.5644332350500211
0.9849051158698073	0.4559688149457901	0.7887874299901808
0.9840198359603255	0.6371904557488242	0.7824201762334085
0.1348113104769866	0.5691909723505203	0.2246197345811769
0.1820531259413970	0.5518536241938882	0.4058589812853279
0.2951215437883731	0.5461985021498369	0.5108148155434877
0.4035118543677815	0.5715506264090703	0.4031055474741675

Structure files (CONTCAR) involved in this work:

0.3946126386250672 0.5639073998166306 0.2072077045892172
0.2662595403180718 0.5524370197948962 0.2548374291876291
0.1400299759995964 0.3258446870494138 0.2516436542663501
0.1952613559536682 0.3624727485292812 0.4202791465304450
0.3087515961282249 0.3533185123066740 0.5188207108253194
0.4078349484381025 0.3302043093491031 0.3905261104314700
0.3937628039325921 0.3469476461445009 0.1943068966304640
0.2702730603734247 0.3508453627187705 0.2582184906766551
0.1818501923879189 0.4505699028166915 0.2730062902964272
0.4114108054674217 0.4524093277864870 0.3149058009791721
0.0643564575627626 0.6239873133457996 0.0773057576903496
0.0828784238397897 0.4920229833164358 0.0800387237777304
0.1166033723142696 0.3629470217898821 0.0639765868946156
0.3053742862128180 0.6379582264868832 0.1153302418302728
0.3126030540530677 0.5051204509726049 0.0816069912400729
0.2956564774023182 0.3724062150335896 0.0642196164628948
0.5100358068208083 0.5408959156547845 0.2936163421817095
0.5110994758510585 0.3661992984219894 0.2771239150039856
0.4358755966227194 0.7503560283961320 0.6402897737052544
0.1893524422943793 0.7503003846669222 0.6366010642599970
0.2760570643499688 0.7499779024025252 0.0204944620995534
0.1026838307727773 0.7492199061545166 0.0486675229358994
0.0637939328353231 0.2507624765394045 0.1356077535020178
0.3087110608285292 0.2509512743042997 0.1374589573330978
0.2230935754765913 0.2505144000989211 0.5207611977746226
0.3927882111928688 0.2510806136547014 0.5464893269166907
0.5560413448172967 0.2506393667993306 0.3518825809168249
0.8120446496648209 0.2512743224127766 0.3507687158188352
0.7275054084075252 0.2499502795431543 0.9425131699982220
0.8921090976668662 0.2510159876648129 0.9478567456160170
0.9460099876452364 0.7536546577640559 0.8616944239831241
0.6848556358855677 0.7534186761669736 0.8498779357498694
0.7759873995867964 0.7486285336733370 0.4467111728951567
0.6110298765359677 0.7502411118147339 0.4493102058457430
0.9360285405464893 0.4975130542617143 0.5153702015760789
0.8224576200824829 0.3348931679795021 0.3283149264224365
0.8000090870480385 0.6358886402201445 0.6963214477525461
0.9257223077509795 0.4184275279130043 0.4283374774303687
0.8782922131611326 0.5611525886095515 0.5614789117031607
0.0345494630853952 0.4246758578370449 0.4469638086174773
0.0719820983274333 0.4452921595330606 0.4989136687178296
0.0502067024040226 0.4382353005199771 0.3710143376400958
0.0381147823186014 0.3697912720205833 0.4568296332109122
0.9914107604529701 0.4698654186585214 0.4921681110281060

Figure 1(b) Fe/ZSM-5

1.0000000000000000

20.0219993591000005 0.0000000000000000 0.0000000000000000

0.0000000000000000 19.8990001678000006 0.0000000000000000

0.0000000000000000 0.0000000000000000 13.3830003737999998

Si O Al Fe C H

94 193 2 2 1 4

Direct

0.4240509578453535 0.0559207755249671 0.6444932144151279

Structure files (CONTCAR) involved in this work:

0.3060830112265017	0.0279877266182693	0.7912800510676774
0.2810634372913808	0.0634771710321883	0.0112490700472714
0.1203722503776186	0.0665777538862354	0.0079950024320218
0.0678951362047197	0.0305958303722109	0.7957650711128798
0.1821784621723393	0.0561326114204041	0.6553986294031272
0.4204499163476471	0.8271722399523213	0.6651560666966095
0.3053174470983875	0.8695921031570149	0.8086547895008827
0.2688412269469111	0.8292693264294727	0.0269901183000025
0.1145609015564627	0.8266603229817331	0.0126480396333224
0.0663623234852506	0.8717654399174359	0.7995123173850265
0.1840580848029733	0.8286600491736247	0.6728358793674271
0.0793290880787312	0.9431254695028931	0.1459241913938104
0.1970544600916301	0.9708155661100928	0.2928865339863242
0.2200696950161380	0.9368264813425401	0.5119458646419518
0.3799267362928466	0.9330424319346345	0.5081787634763955
0.4347096605652798	0.9696132240277837	0.2980892667582966
0.3208599566805538	0.9447308235341098	0.1572479904371988
0.0817253681583180	0.1720330327223909	0.1677002764618798
0.1986408950419688	0.1288075181468127	0.3081034797482373
0.2350286529080525	0.1716828531252809	0.5244019517036477
0.3896698888494333	0.1731923391807326	0.5093753426962585
0.4383488686688359	0.1277990870372472	0.2978881234633143
0.3193337457194613	0.1695946758109956	0.1722490631219212
0.5779804883204218	0.5550486109454096	0.3548840525803852
0.6958152133798692	0.5267977043985760	0.2054926685183534
0.7180630078261626	0.5575672881331108	0.9887668041012615
0.8770615430392681	0.5688623613164427	0.9941245658482067
0.9346993850989903	0.5304466237741350	0.2028058446140454
0.8187596766719508	0.5560812926651908	0.3391591237323556
0.5799799216551116	0.3280085946475076	0.3386777594212245
0.6995494989953590	0.3683685643565860	0.1978164027391810
0.7316010309566214	0.3219559117662397	0.9821565146138402
0.8861316001062225	0.3291266946557995	0.9956680144620489
0.9372551027402810	0.3725264339870591	0.2055567457315471
0.8208832547256343	0.3312157139550165	0.3352488147813527
0.9232489120419100	0.4470047545048139	0.8578466994418575
0.8022955328730537	0.4702155263309368	0.7153500273582092
0.7794954144068915	0.4387997998297987	0.4904436809784781
0.6184158619645928	0.4335821929931683	0.4963104873209192
0.5669459366242537	0.4702736902122679	0.7103599866049737
0.6785102170545330	0.4354391014645709	0.8499056592185659
0.7991917209949093	0.6298427205796608	0.6916328498879515
0.7664714574827188	0.6670145836553824	0.4720002233136956
0.6116877044301661	0.6720502692338054	0.4863692896226773
0.5647467650367699	0.6289763366191647	0.7041876086587552
0.6816119212708439	0.6709609053395176	0.8291085310785770
0.5791714514276984	0.9412856307529925	0.3496930599916792
0.6952646409961597	0.9724880153817610	0.2051989430645612
0.7226025806155428	0.9417986572915604	0.9845359441137677
0.8797779798080757	0.9443572243977043	0.9863751424416251
0.9358780148643724	0.9686899241585737	0.1984737920325074
0.8191549684073538	0.9363445208025296	0.3300118779526362
0.5824278969638813	0.1742016468520395	0.3249509499746335

Structure files (CONTCAR) involved in this work:

0.6982159715285716	0.1304983308314904	0.1901871042226124
0.7384255176707063	0.1634349932957350	0.9721999034268236
0.8932725937210535	0.1750542781863139	0.9828440740856125
0.9399542636738347	0.1271182742560856	0.1977442401807293
0.8205034198771215	0.1735204245082245	0.3223040489612501
0.9242288305663159	0.0630423695004030	0.8435471831570427
0.8096302674170101	0.0289306330540891	0.6961351548543885
0.7839888469704694	0.0585273175279139	0.4759494703338447
0.6239869014765979	0.0662147553429836	0.4825488357828700
0.5682996013446387	0.0321221667555426	0.6927653142431216
0.6850675581330806	0.0542548574481964	0.8259835239167453
0.9179827527698062	0.8319235038839176	0.8282215402901099
0.8070603964468392	0.8714305142409745	0.6836296288135979
0.7685219525174388	0.8278214347959002	0.4704878630895988
0.6132845608907328	0.8263303481895650	0.4891769004309509
0.5643223953660831	0.8741612202907895	0.7005643830902673
0.4236984658852660	0.4428687496161847	0.6517783215446137
0.3059116030523798	0.4723384655523180	0.7967637438798946
0.2832788147835284	0.4378523248826326	0.0180120716052687
0.1229220989439496	0.4332811364931591	0.0156346814114408
0.0694719568811941	0.4680672746121832	0.8043336762217255
0.1820283698505371	0.4431044173757838	0.6632133676073163
0.4204050261267511	0.6733814003189570	0.6694701439262617
0.3063852520880597	0.6307177363010905	0.8127476335759288
0.2687776141384446	0.6710408815272100	0.0299708929956011
0.1146987311535501	0.6726845607894180	0.0118750662906628
0.0667357456035764	0.6260115712882129	0.7996108936027702
0.1858216053290642	0.6697960973605822	0.6746041867640609
0.0788270704700234	0.5577293829571560	0.1488736820648485
0.1959480386998772	0.5287952121765428	0.2950123158232958
0.2213439100908773	0.5605705885992389	0.5159158477747279
0.3808114377842413	0.5642245450703930	0.5128717276708048
0.4347243680035626	0.5299772711325955	0.3013844311829849
0.3209911554347650	0.5573668156367897	0.1626218201401799
0.0814863532811279	0.3259964861256721	0.1728603400634428
0.1973737750819072	0.3705416810254316	0.3114828350702614
0.2361177350421821	0.3302499001432591	0.5294358361142735
0.3909266760982872	0.3267876890167707	0.5161032859524095
0.4381267092105492	0.3722039564179800	0.3020337907053834
0.3193739784217841	0.3284056890201730	0.1761617141460500
0.3585295407092886	0.0628812467503435	0.7150818665935649
0.3100780604860690	0.0663354078659623	0.8981341946129174
0.2004509665171208	0.0555168751766691	0.0104761562281499
0.0935424066566578	0.0708462527933267	0.8941185352003610
0.1061608401680141	0.0576766535880829	0.6970265159837369
0.2307500063016003	0.0346983713713154	0.7473976047976701
0.3595957409503421	0.8274662628771182	0.7451948746875889
0.3081604499683688	0.8440563212829929	0.9234159495098591
0.1913924445962657	0.8533195396381688	0.0159400386866563
0.0877921320500775	0.8305371925644199	0.8987362444788060
0.1063005426708082	0.8419814889639938	0.7034308232660240
0.2307010671776242	0.8566303488053877	0.7638308984904021
0.3240939118992403	0.9488843555744962	0.8035271433567347

Structure files (CONTCAR) involved in this work:

0.0825117896963523	0.9510283996367292	0.8133884658533573
0.4336512063445074	0.1246500148557532	0.5806331434147984
0.4178843786274218	0.9933133600849019	0.5670226075344538
0.3961372744290642	0.8616599395615023	0.5611486705085748
0.2011498698894989	0.1305422832712466	0.6155527407390550
0.1865068959045617	0.0019067470636184	0.5650851446755346
0.2010581192632386	0.8677918537199639	0.5695865522247873
0.9889457534412665	0.0442610645709979	0.7763529409176452
0.9867663495950284	0.8612027295472819	0.7822892442390524
0.1457237490955763	0.9366266384298769	0.2144082266832964
0.1912745406402790	0.9315780293743743	0.3987793872849599
0.3003125647549125	0.9478675933715603	0.5109841217534300
0.4062355725541706	0.9285339485989458	0.3939406624236347
0.3974123216067162	0.9456193447772691	0.1965724573017575
0.2728123106097096	0.9644945672929355	0.2507964468086438
0.1455987781235504	0.1704687644929192	0.2416043052840171
0.1948985219863140	0.1569387568338697	0.4213694154494548
0.3122602137487593	0.1479479643911347	0.5105586788875611
0.4174609871515428	0.1713297375524405	0.3956504048286388
0.3971398021901112	0.1556335936456385	0.2013774635751372
0.2733571370950231	0.1397199957763819	0.2627376288368737
0.1786695225974206	0.0497916988149046	0.3063408850600567
0.4214786642833631	0.0491942771518007	0.3176515992077890
0.0687798109836148	0.8731347002148183	0.0850851604642733
0.0849979263989407	0.0042432920497344	0.0658125513881216
0.1003325190816724	0.1366768913011309	0.0619395032091742
0.3037962784393012	0.8697700509766534	0.1178146876754544
0.3126366315626717	0.9983667032255726	0.0668135510642527
0.3017660844070030	0.1326789098077375	0.0673441234869869
0.5134774366716135	0.9538132906079090	0.2812935350765446
0.5178443041433528	0.1364596968336166	0.2767751889762963
0.6448754930903448	0.5584617205250638	0.2865882657622771
0.6867974746004262	0.5667719475413475	0.1000752891730938
0.7984943967894721	0.5495895056284797	0.9961281427515463
0.9067098265039277	0.5718008711228068	0.1065076686798458
0.8961939471908282	0.5546449632035645	0.3031814986291646
0.7722378179641350	0.5361820737007237	0.2437621726759673
0.6461425617566751	0.3322795409758070	0.2700036715852772
0.6950449568697596	0.3329632308027969	0.0891560359261074
0.8077010524449720	0.3508513213024643	0.9895794457086088
0.9116246770763802	0.3284648380534274	0.1107725196169963
0.8982790423215220	0.3470061276907962	0.3053989141906908
0.7741313835814976	0.3592757337551764	0.2442765316946348
0.6810271349159920	0.4475307012302866	0.1882031605066749
0.9213062059974074	0.4510742333717800	0.1828580333025086
0.5665946521601510	0.6262786030946348	0.4117966254092901
0.5832355231517716	0.4958841319826214	0.4381933920066655
0.5950231019963081	0.3631463015959656	0.4460154262135245
0.8005509014958530	0.6317566089142017	0.3750954727429481
0.8084248290228171	0.5029835521101148	0.4295559292466173
0.8029562416593257	0.3686990386318545	0.4394188829862091
0.0135077231222364	0.5461407155413924	0.2188420133586579
0.0169663667785589	0.3629772029656798	0.2225403338231435

Structure files (CONTCAR) involved in this work:

0.8591812495940019	0.4362412670468622	0.7855163250695463
0.8091204984117737	0.4407566305944099	0.6029839214708548
0.6986501648397530	0.4427906609366118	0.4899479463414738
0.5944357849387608	0.4321701182802935	0.6114408834290336
0.6024605448457387	0.4389616649312190	0.8088780807010297
0.7287639993033955	0.4506514983318047	0.7574618911399343
0.8533883163019115	0.6755667736589817	0.7452096087254206
0.8030925643779899	0.6393970165872565	0.5714426644350777
0.6882506751340761	0.6455781984299838	0.4782120476002786
0.5861116261825033	0.6653277838070805	0.6007030068891186
0.6031290294720211	0.6650490814257426	0.7982065983738440
0.7241091581204196	0.6509309245010648	0.7303466691400987
0.8113960639504844	0.5509195878912425	0.7187188219270110
0.5847270401453937	0.5498824945158537	0.7013846159970822
0.9300942987571621	0.3821097620131141	0.9311478886930501
0.9166075865207900	0.5149278357378247	0.9255547670447162
0.8875166888712412	0.6440854938823367	0.9462377520190112
0.6915436361793551	0.3610917868799319	0.8947347086618297
0.6876080234246869	0.4905914402804064	0.9383765942058113
0.6992689967525167	0.6242302513401290	0.9251585448500447
0.4873374295028258	0.4576655734721153	0.7235572298881612
0.4847283133461534	0.6363058063904846	0.7196768438486554
0.6435192169001196	0.9320969420468261	0.2764911398196687
0.6835413524930661	0.9490984283691813	0.0902136004258810
0.8008216745579465	0.9607149926934171	0.9984092631885182
0.9136661395906673	0.9326667420705795	0.0944871364609000
0.8961194364787624	0.9358575343962016	0.2920069223310247
0.7717415002323067	0.9543546045864714	0.2347164627249017
0.6407626124421048	0.1769718295531246	0.2402982204608999
0.6968333950685238	0.1389177430395702	0.0699042084069237
0.8172052355083602	0.1457233737092756	0.9860469541495852
0.9258441711273919	0.1648133250202876	0.0924078913065334
0.8975054951137946	0.1627561391439794	0.2868422171921028
0.7716788980867073	0.1533229909038536	0.2294757393862184
0.6827316133656910	0.0526838488878256	0.2198306422718943
0.9188473716110767	0.0484979965396151	0.1905158945962224
0.5690173183709627	0.8733365026715274	0.4150857274509264
0.5880910180764184	0.0045341938941136	0.4246267304555100
0.6093229410095833	0.1360562667782997	0.4241607453490230
0.7997642314099682	0.8621884683124218	0.3708075458840272
0.8106603694893463	0.9928361083127946	0.4164538739112446
0.8039765562428123	0.1274864329055835	0.4188588832860858
0.0150015399964419	0.9558825553324913	0.2173661722251455
0.0193550638826532	0.1338872195466925	0.2221004254722454
0.8586712224577314	0.0683517678047316	0.7729733787679141
0.8191474279820327	0.0601721662743260	0.5851488778839765
0.7036671036635295	0.0528124076025165	0.4875280797541888
0.5927678335652010	0.0725499806871644	0.5936141786264260
0.6083682527390246	0.0611740473584557	0.7892336089978358
0.7322439324735018	0.0391327947951761	0.7297687730713165
0.8643308445273541	0.8269519923636558	0.7392183325403515
0.8113279146906816	0.8535352908851409	0.5654889581371360
0.6908773491152588	0.8505798338330386	0.4828515677821996

Structure files (CONTCAR) involved in this work:

0.5867026242190957 0.8301911723974221 0.6029094279457717
0.6014879518806706 0.8475938918428522 0.7994543492576128
0.7347146378309044 0.8554275155847272 0.7284274172555087
0.8286496371618675 0.9498770669065087 0.6993837185485852
0.5825821055048916 0.9526143701336449 0.6770846471106476
0.9358476746148419 0.1349362984595760 0.8984690654196782
0.9159827210483464 0.0063391951236784 0.9303143588899735
0.8895638128860310 0.8760539086188183 0.9215534435254514
0.7083188145271448 0.1241832632297536 0.8767572291115244
0.6888873766949239 0.9915069142385763 0.9037102717545847
0.7149543725078468 0.8641798810776150 0.9435670854840693
0.4895282300906296 0.0457390729640427 0.7140681010557507
0.4834457764544177 0.8669616004348339 0.7131188206503842
0.3570070387419522 0.4361842801440245 0.7197860544827672
0.3113836353535174 0.4352980939110543 0.9044052061327001
0.2027417287679278 0.4463464588060933 0.0195065358173858
0.0972556423814198 0.4275564269822864 0.9014018935574789
0.1057556850955726 0.4400481118762657 0.7039619002137653
0.2299107161538784 0.4652893231134803 0.7558326402384833
0.3608980249546603 0.6740219884795341 0.7512902691695226
0.3094749987052304 0.6543091828965896 0.9282831963867221
0.1916486321800223 0.6464931850077253 0.0178910347626559
0.0892562745597168 0.6694292517604506 0.8975940348271174
0.1086988384856322 0.6537331067641636 0.7032295185226833
0.2322650612982345 0.6447438348117663 0.7676922308728568
0.3251936708596338 0.5514625977425138 0.8048357634863986
0.0855123207128382 0.5473590765483022 0.8196298539907345
0.4347934038580878 0.3725289662881289 0.5921851947749978
0.4184524622437199 0.5034016225398957 0.5707036713153949
0.3957868191482882 0.6349175251437233 0.5688708779661878
0.2028880712357663 0.3691345334088224 0.6233070203747666
0.1869890887742019 0.4975957983611086 0.5732638107823286
0.2062256864638261 0.6310134104670770 0.5722527053820016
0.9900391081960397 0.4539247570377411 0.7904713284545508
0.9885153701753528 0.6356438824958444 0.7806993990362540
0.1442520647078155 0.5656483253436630 0.2194685845745199
0.1902577057846327 0.5640786331372657 0.4039359979958492
0.3014529106437888 0.5480843266544111 0.5111874223037989
0.4098196939986061 0.5701270563024544 0.4002721608453863
0.3972275904316958 0.5591447803708450 0.2032837499749470
0.2720171392149690 0.5367487578027876 0.2546285264645459
0.1420867028041501 0.3259649602276509 0.2532132102608539
0.1960041300084807 0.3494557248444883 0.4281179326808994
0.3138107259581139 0.3529105423847549 0.5169199773575296
0.4200431453048661 0.3318367290006863 0.4036081942851129
0.3969491078393704 0.3398852998487947 0.2088266766168922
0.2714157459234878 0.3564767976824786 0.2655258093180299
0.1775064388705563 0.4493087687270606 0.3000345106799092
0.4178755575363177 0.4506022589328121 0.3154050175944534
0.0685641365887327 0.6262657819127991 0.0843097465188376
0.0854360309934706 0.4949222417491387 0.0719899503057030
0.1046392300244338 0.3630743425176888 0.0706317447330506
0.3027163971789675 0.6318922802444322 0.1228354655983306

Structure files (CONTCAR) involved in this work:

```

0.3157708825264977 0.5027841780645497 0.0729174472959054
0.3043779902073963 0.3682736735374817 0.0727837054336792
0.5141984027391204 0.5410703595725729 0.2831949594714152
0.5179820229509172 0.3647738889592975 0.2812157254338254
0.4397620706390319 0.7498146445894878 0.6397919467874559
0.1968915264204824 0.7493712037196464 0.6545704011386468
0.2723415461774010 0.7503747786625301 0.0545045616965784
0.1089653056696548 0.7496886914770967 0.0514038311784024
0.0620635977619388 0.2493842077945292 0.1444736071211312
0.3055435807167682 0.2492114065090199 0.1573372526795194
0.2310005942493176 0.2506215346050518 0.5519113325024068
0.3954717515069573 0.2491981171294495 0.5523183948921764
0.5621131004404371 0.2497936107851173 0.3580270444097378
0.8089103672547359 0.2515037232671052 0.3525714360092438
0.7302972554478744 0.2431984498844917 0.9534424044328389
0.8950809520267060 0.2537749488795881 0.9515416270538465
0.9266583261551147 0.7567913426493278 0.8779168530798855
0.6990829095088917 0.7472985850852731 0.8694203841721007
0.7741239019607632 0.7472039733645326 0.4585388172725917
0.6063248004268521 0.7493978103608916 0.4500214461112833
0.8216493959736468 0.7801498487339268 0.0978548022631675
0.9187518906270902 0.6734384462193436 0.8267283247576808
0.6840074986277694 0.8321231722208610 0.8257333425030232
0.8643243320688230 0.7389045325540911 0.9970969802706318
0.7437515711963345 0.7725060202073003 1.0033034054016483
0.6998291837403188 0.7441206934340113 0.1482231080420904
0.7178112123600519 0.7100233111570179 0.2072994843866929
0.6614391384247985 0.7156221716474397 0.1068848739528634
0.6767730133385508 0.7885424295733533 0.1828084882588411
0.7704895937935965 0.7606141260977268 0.1338120651690392

```

Figure 1(b) Ga/ZSM-5

```

1.0000000000000000
 20.0219993591000005 0.0000000000000000 0.0000000000000000
 0.0000000000000000 19.8990001678000006 0.0000000000000000
 0.0000000000000000 0.0000000000000000 13.3830003737999998
Si O Al Ga H C
94 192 2 1 5 1

```

Direct

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0.4224751064944764 0.0582089579760333 0.6482505988448554
0.3051207303668143 0.0290087195617479 0.7931755222206042
0.2814524247497194 0.0573973157256899 0.0162989618795743
0.1214164180986371 0.0631223049634646 0.0113074932842919
0.0669223026077090 0.0287309634525345 0.7993065700657161
0.1805494581053215 0.0597185765146836 0.6620036393638562
0.4210586796117458 0.8273792794891354 0.6729645934929676
0.3032647339271743 0.8700315238843989 0.8083834216216683
0.2674528456943518 0.8298960438734234 0.0277306072912525
0.1124505573841544 0.8265301934469979 0.0177770132809332
0.0639579713410862 0.8701897284650328 0.8028638430733057
0.1810528510654405 0.8265842575537866 0.6741154559770649
0.0767500653049010 0.9421782647996908 0.1512610840714638
0.1948151667405718 0.9704763692902777 0.2957671635278590
0.2180479700265464 0.9382154233583777 0.5179303203505103

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Structure files (CONTCAR) involved in this work:

0.3786845039150170	0.9326906207685125	0.5149901467597305
0.4342185013805983	0.9682222875078706	0.3037753536085566
0.3200282821116666	0.9394160834073464	0.1651351481320687
0.0813118590442458	0.1741485534633937	0.1638170113074113
0.1960369655204118	0.1297737458785334	0.3062805556967226
0.2315816424982818	0.1709386974304211	0.5238811299341821
0.3863400128356535	0.1732257192263343	0.5100806284895897
0.4368354195432406	0.1269395918461324	0.2990171157796848
0.3183845367040073	0.1686879183189364	0.1712097795859973
0.5831953767062337	0.5552568766818329	0.3496180640719931
0.6963803731759126	0.5310721501115045	0.1914543249162704
0.7176297046096674	0.5658230151860708	0.9754691359545897
0.8747493280430428	0.5634328986163116	0.9831919134723643
0.9295891105823697	0.5289274234624258	0.1933330404714893
0.8163406028003912	0.5576992609636363	0.3337783296729415
0.5763924201944893	0.3310802830823562	0.3305467218630859
0.7040836178877745	0.3761033776440643	0.2042006195776160
0.7334801682940665	0.3274410026968021	0.9884525668124082
0.8859601151235060	0.3266050071817459	0.9763503839331134
0.9394213617575031	0.3720842867302931	0.1870132864334544
0.9301195014562779	0.4439302711558807	0.8480338242690565
0.7822574991670229	0.4378100131228906	0.4827342912800723
0.6237862474110160	0.4306458073576230	0.4891464729431200
0.5706642935749431	0.4676887811834138	0.7027998807845720
0.6716724157778741	0.4382953430654104	0.8589800952237170
0.9194907519258515	0.6733772804177975	0.8303095524831754
0.8012170660731257	0.6404694255766763	0.6903330518860091
0.7682399301935874	0.6698165386337281	0.4694492751003814
0.6132406908769990	0.6713898614908126	0.4845730634401426
0.5670269607829281	0.6261421693539696	0.7023241946083006
0.6839872366683757	0.6824319006965448	0.8236576961361263
0.5780499376759148	0.9441264888623706	0.3601423071420847
0.6969676725841920	0.9745223496693687	0.2175877973904832
0.7203412945220409	0.9437761934927233	0.9951345237576632
0.8801310419596937	0.9347859129940768	0.9951776272936463
0.9326301196905298	0.9719548768069252	0.2053976173645000
0.8216128279004651	0.9453988826071209	0.3527661310713929
0.5805577792776491	0.1756014814619576	0.3291209361008327
0.6974453526054334	0.1314399481629434	0.1933796530083313
0.7328606173178903	0.1711426877560820	0.9724797647215574
0.8873953917170143	0.1732253461051501	0.9846131565389676
0.9356232392405768	0.1304950801542015	0.1986269266042245
0.8189029372794504	0.1719484932374687	0.3312357357975975
0.9239081070695679	0.0548546268371425	0.8563404424549302
0.8036304086477715	0.0270400702835780	0.7125958357892047
0.7816146140564718	0.0630395234963458	0.4927104579314897
0.6214340547000350	0.0696416335272230	0.4897587505968302
0.5681487121619340	0.0333709771845097	0.6984906801475560
0.6792991455028208	0.0568886201469749	0.8477016781902679
0.9195348701204301	0.8265879457446027	0.8395164695301152
0.8031576069193223	0.8695526230490959	0.6963943992466767
0.7683199377256933	0.8281104791359981	0.4781230482026006
0.6136053856950670	0.8264825907099662	0.4939637333617700

Structure files (CONTCAR) involved in this work:

0.5637187618341964	0.8769570077764658	0.7004710105017460
0.6792509798977191	0.8376189530282354	0.8349600801368843
0.4221006717419525	0.4417574385675413	0.6444426696508797
0.3106216301150390	0.4677590512495958	0.7967912764932081
0.2854655464136731	0.4407357189139128	0.0189968908024840
0.1296626824026698	0.4363748034825995	0.0099410185093868
0.0770610100476022	0.4730138955937023	0.8020467523636666
0.1882363480440679	0.4438108465208395	0.6598870872091426
0.4248616399459207	0.6731587360373648	0.6710205699064669
0.3045208645859788	0.6263559559364951	0.8011125237272010
0.2685328637023648	0.6698913682550508	0.0219296086785847
0.1142286652619126	0.6735959287711895	0.0141292787474871
0.0664985543365332	0.6298448784508097	0.8043766182347797
0.1804964218685262	0.6684875249986164	0.6665384105486180
0.0755289478668218	0.5551185444109756	0.1425436133009946
0.1956986396773009	0.5279084336145872	0.2862144340608820
0.2208830446637998	0.5640977598562603	0.5077412118454913
0.3811484475325984	0.5705533537146452	0.5106274651850807
0.4366451546477451	0.5285300035869391	0.3023296406790820
0.3252245024175405	0.5595413846145840	0.1604834286347590
0.0860262861000736	0.3276120525679738	0.1578604405651143
0.1961498948541907	0.3682970286196736	0.3062412761928500
0.2317807778323777	0.3306409793227688	0.5239996610650843
0.3862177892707989	0.3269307308616438	0.5068148689094621
0.4331429247514615	0.3719609486496760	0.2942967655701555
0.3157912154805621	0.3261860080362467	0.1706853936351138
0.3579919999573624	0.0666696044665282	0.7206397408806617
0.3135178780192889	0.0583829821023577	0.9051729936705232
0.2010462409960014	0.0488481531836566	0.0112634071010096
0.0934874659110034	0.0674268839511196	0.8982339144989793
0.1039460265393060	0.0589346799758076	0.7012307172009286
0.2292185767890602	0.0433313003985494	0.7561883245484917
0.3603420847604207	0.8258875312801244	0.7533224659683373
0.3054307874948255	0.8537065821553346	0.9266939417199840
0.1894799551342845	0.8527795930268502	0.0214984113823892
0.0856076433878104	0.8309573303158054	0.9039695018451430
0.1036402026121706	0.8371112067728722	0.7084805003763154
0.2295603567274656	0.8513575393758769	0.7649148776542720
0.3197224361998203	0.9487722626283307	0.7889836253566518
0.0834676054661527	0.9491149894284270	0.8113846218146490
0.4313272347204031	0.1264916785441030	0.5828854356501874
0.4140669109403488	0.9945430744091862	0.5734811378417699
0.3962945921151518	0.8619651033581216	0.5693849357440598
0.1969196242832587	0.1338323276881853	0.6181769674310899
0.1890800094606553	0.0036703772717846	0.5752336348919711
0.1959761465421719	0.8691015735637018	0.5731536894957923
0.9875322390656230	0.0416839527568795	0.7837468584453032
0.9838489678192125	0.8623688318311605	0.7868019999807749
0.1423550615387562	0.9339702702254111	0.2213627142022840
0.1869586051265212	0.9377736770844419	0.4060418470042835
0.2986429731734962	0.9440773944237096	0.5142541602193925
0.4069075895255462	0.9289289620265796	0.4019636494017426
0.3964277629815239	0.9396533397969709	0.2052290892024336

Structure files (CONTCAR) involved in this work:

0.2709576461515967	0.9585840888742643	0.2578189077690500
0.1414218013594659	0.1732139197057036	0.2450915120815335
0.1917599886136588	0.1514362106977023	0.4225752092067562
0.3091190866546584	0.1472705649755203	0.5136837678476504
0.4140943443461348	0.1694292321599189	0.3967524239047094
0.3958122490491487	0.1551294730551210	0.2025283126067384
0.2708119597387723	0.1450995176836653	0.2639178933225769
0.1785919452337658	0.0504825795715123	0.2955528955128054
0.4195215304794896	0.0481497402916037	0.3169083889206623
0.0661971820411140	0.8722435899155824	0.0903929276241988
0.0845498044840172	0.0027181272006808	0.0708477325903067
0.1045363060527988	0.1343483395648800	0.0639519059592051
0.3026940446282721	0.8648599763777637	0.1235022426776218
0.3125788664398785	0.9939408701262639	0.0759115577480171
0.3003323481544791	0.1275880348872481	0.0703950377013209
0.5134399620088427	0.9543763825997381	0.2884005090698621
0.5163770285477032	0.1370950148548461	0.2801855126444825
0.6438356524836475	0.5622420877260177	0.2708152253801387
0.6917899523933295	0.5755323357774283	0.0897737565125907
0.7962782149765860	0.5434244879970584	0.9768021799073938
0.8999693127727370	0.5707246454718399	0.0980015071879124
0.8938315962915655	0.5509487876073196	0.2981790192183250
0.7710067333508970	0.5393426882126815	0.2377706142359299
0.6413921522893604	0.3412737927733141	0.2616201052835326
0.7190999262624276	0.3290203937031066	0.1072362133654793
0.8095301579288668	0.3545127512676819	0.9653915177023330
0.9122570709445105	0.3310513633318801	0.0897746042834432
0.9097238897414911	0.3401952287322015	0.2870286606520024
0.7693655189164960	0.3799372453855431	0.2731191384315407
0.6818029755209253	0.4520505115105921	0.1688291147792930
0.9167708650286642	0.4501683770487829	0.1712831972968886
0.5705598067939545	0.6269839855931250	0.4048317679159352
0.6014513688895181	0.5002177689023143	0.4355666956364947
0.5861715391597140	0.3673010177438216	0.4389104691941279
0.8022251525927639	0.6332646346410050	0.3734374459202811
0.8013598511921806	0.5072805885094855	0.4277741820322206
0.8338242935660896	0.3769518175669637	0.4497930130203363
0.0086488184844080	0.5446965904742430	0.2091462947942198
0.0208370114176899	0.3705176338829080	0.1897369580006401
0.8740898665402372	0.4411220295956276	0.7571155588542920
0.8060691672881384	0.4423172527136688	0.6011398019652633
0.7043319182519074	0.4202291005305708	0.4760434636099291
0.6058579427502707	0.4324205058924390	0.6065792152744434
0.5988606524073948	0.4341278003129264	0.8046483858218546
0.7302956796900092	0.4381661665657814	0.7773361657041082
0.8658041622990503	0.6769178231349587	0.7402192765469422
0.8086959550008541	0.6485424081177225	0.5698019801009335
0.6906959562145735	0.6460175774364653	0.4810821026954035
0.5840529761438302	0.6616149435741302	0.5963041326650801
0.6081549240614301	0.6620370041331642	0.7922103109976949
0.7322764514814624	0.6776832077821853	0.7255331608151927
0.7988340724543521	0.5633693739140719	0.7244299043440556
0.5880390911364731	0.5474694203991128	0.6979138376580204

Structure files (CONTCAR) involved in this work:

0.9333726028125119	0.3715796978109622	0.9027282811951904
0.9160301051923212	0.5034447285765522	0.9267148964177460
0.8892705470388439	0.6338354422783460	0.9265834108221986
0.6788292545412085	0.3734539845871483	0.9318360978350564
0.6731791766745353	0.5075196722864320	0.9241630783117911
0.7102335338654834	0.6359094075267854	0.9150536694063324
0.4906840534464637	0.4568469527821100	0.7033283364895658
0.4873642156282867	0.6345645935340729	0.7240743495726831
0.6443050422684510	0.9374281110814248	0.2912108190382899
0.6964561049711893	0.9367990562624883	0.1102243514349141
0.8009819270969178	0.9512698251608408	0.9868643194336966
0.9029243685151352	0.9298072592931992	0.1110653045595423
0.8969790062643475	0.9477968724932071	0.3082528570357229
0.7715781681546319	0.9693975173995075	0.2640874087445160
0.6415153766664061	0.1764371779909210	0.2497468474377675
0.6961143892463471	0.1521181072118326	0.0764540708115751
0.8105166931460331	0.1469434339243944	0.9794427615310581
0.9129801020578349	0.1718949452519336	0.0993851685052987
0.8962445859483705	0.1585080707811554	0.2958276106404954
0.7709448749556549	0.1435300591891665	0.2410240231962502
0.6761659537774262	0.0528708362530998	0.2054346341149966
0.9194157525701061	0.0511059021881620	0.1830361638510395
0.5684237007507403	0.8751778217055498	0.4239426990244418
0.5824283141291451	0.0073703741181500	0.4369300097969819
0.6030592120405515	0.1392083769092894	0.4326868271724935
0.8045711826295595	0.8694772702219156	0.3889425514468512
0.8159539363029767	0.9952862677336397	0.4482924773726010
0.8059291977336346	0.1291390073048369	0.4334062609098977
0.01182194996433360	0.9567216437612798	0.2201662048376270
0.0156591942332251	0.1404487608984718	0.2147480319749966
0.8570040581811812	0.0602883994604127	0.7888795150485863
0.8044372706683901	0.0694092515960110	0.6089937004653818
0.7009748676022338	0.0551226536370943	0.4841177775198344
0.5975781242525408	0.0769800162941304	0.6053721930952991
0.6041115604524557	0.0541027363441189	0.8027653034730037
0.7293102977917232	0.0302002211548457	0.7606606743597070
0.8573658280716970	0.8288868313971223	0.7624337942705511
0.8061676896606519	0.8402221830893942	0.5837329204586909
0.6908380161572814	0.8520674035744527	0.4891127703147600
0.5871052245488402	0.8288395745491108	0.6086526161607860
0.6030623676176556	0.8552513179307452	0.8016128294854020
0.7289275326245962	0.8589289281491026	0.7435597866923397
0.8228213464127523	0.9487240424088268	0.6942807503935714
0.5807900445168149	0.9544463192579793	0.6723791161166300
0.9342323179078676	0.1254647108343482	0.9155201247783891
0.9204093106823070	0.9944136583341906	0.9380563597680616
0.8985941835971187	0.8633652285765276	0.9432685054321674
0.6966314524421269	0.1335828226186503	0.8793816701680326
0.6851728431330253	0.0096925294725266	0.9464730961312292
0.6973556510726838	0.8767221525430565	0.9369850530672920
0.4890868189057291	0.0479095461329499	0.7152144134080980
0.4839500135884268	0.8684878729821723	0.7200074866604610
0.3627930519685666	0.4286105438991686	0.7249124808632400

Structure files (CONTCAR) involved in this work:

0.3166317407242117	0.4357515245112096	0.9075431322320693
0.2068125133540262	0.4614133937688669	0.0151296014456967
0.1065847045728855	0.4290753904317536	0.8938994553465189
0.1111259005988866	0.4529154235443358	0.6960337599746321
0.2347219013324948	0.4568614810638483	0.7571223120536581
0.3604402216389470	0.6704897827696992	0.7441438372305826
0.3019768684096701	0.6513244051302972	0.9155804469938119
0.1906865041571380	0.6460502422173749	0.0216429617549006
0.0905578825053105	0.6752290506475018	0.8981678742194478
0.1039929612773625	0.6564267789504076	0.7041807212463728
0.2316159243087440	0.6367748009066430	0.7491274901108550
0.3266534615169092	0.5478310439358283	0.7964765187694347
0.0870544744629369	0.5521165592260557	0.8266745070869600
0.4323574871565155	0.3750741371453622	0.5761927388174560
0.4030060727272266	0.5049498153139521	0.5739637595598360
0.4068307616935819	0.6384435543878373	0.5647911067019181
0.1981006332372724	0.3676985161969052	0.6195675930008971
0.2046775318054788	0.4964907079161064	0.5712197788650795
0.1894757208309451	0.6303665620209825	0.5602522006216230
0.9984093395814292	0.4557510805658083	0.7857993408737316
0.9862559151766569	0.6352003393422170	0.7891429018486916
0.1401106563002989	0.5628140420681966	0.2149929523342553
0.1868848880327924	0.5570328467831790	0.3984645977190003
0.3008537939379217	0.5723572546580866	0.4985016798997723
0.4156519026592835	0.5690738281213198	0.4020370361489729
0.3998672063178205	0.5632526315519952	0.2073492918993110
0.2708870540998035	0.5445099128329250	0.2482506407826205
0.1384374132650235	0.3256513285519678	0.2504592390864983
0.1905810609458441	0.3528587658410978	0.4247814290746734
0.3093230461501004	0.3538338182248015	0.5121874843682402
0.4121288327994222	0.3286995778912180	0.3922820089052750
0.3931954904548946	0.3429433247243351	0.1976697024688528
0.2699449436392462	0.3464555193305226	0.2670119265523717
0.1833603803766194	0.4473440064827738	0.2839087710583261
0.4134565403658680	0.4503837001709943	0.3126051893692137
0.0664285022763931	0.6239712144854933	0.0783442423926618
0.0833848858023055	0.4920888420659493	0.0656103303900299
0.1213397245026069	0.3629960484441793	0.0613714241576007
0.3087917870225461	0.6314231336076590	0.1096446590441434
0.3250249591075799	0.4992149153497006	0.0787630915024907
0.2933259811802980	0.3681544482566648	0.0724392553443824
0.5169412571356219	0.5331029649538408	0.2880084667665928
0.5125386130298362	0.3643901137852806	0.2732707296884722
0.4437150199843711	0.7508802758595062	0.6491186922964627
0.1948457636287691	0.7478259821792618	0.6501972426966244
0.2736865160812274	0.7495980918011179	0.0421894940207341
0.1085444838787601	0.7494411029707355	0.0573690867923022
0.0657760451177321	0.2510126470108135	0.1301419673547047
0.3065279217136848	0.2473213376966333	0.1457607580083786
0.2265221078704959	0.2508807798350566	0.5431878259432353
0.3909411470629047	0.2505209439573423	0.5483609407333369
0.5610787402950456	0.2527509251601601	0.3538520869473345
0.8053508006877907	0.2494623091012813	0.3536284365466212

Structure files (CONTCAR) involved in this work:

0.7275953920410455 0.2507062007963207 0.9490720696933677
0.8916748004373773 0.2491022519641215 0.9398728305558016
0.9379531806977296 0.7490783411525264 0.8657268662259989
0.6853706646037928 0.7589986024062624 0.8630392447734736
0.7722694115162619 0.7495485870846462 0.4485259395127302
0.6075176634858355 0.7498958491607205 0.4532433345876490
0.8292204056980603 0.3309902293991626 0.3322762514663355
0.7948056438200898 0.4786886295295543 0.7226123543994351
0.8830583594953294 0.3839162335281219 0.6350546453952962
0.8796330100223739 0.3086857134900834 0.6634321072703337
0.9689640343300709 0.4541597624605470 0.5855167286006363
-0.0101482309850990 0.3846369943444344 0.5063626023969712
0.8926182747414301 0.3956043847004313 0.4876807989305228
0.9436849110449153 0.4567459465124153 0.4629521943713741
0.9505236320711836 0.4207458641249623 0.5250895707475980

Figure 1(b) Mo/ZSM-5

1.0000000000000000

20.0219993591000005 0.0000000000000000 0.0000000000000000

0.0000000000000000 19.8990001678000006 0.0000000000000000

0.0000000000000000 0.0000000000000000 13.3830003737999998

Si O Al C Mo H

94 192 2 3 4 4

Direct

0.4238057369159199 0.0556641141216816 0.6539201333236233

0.3045510856640627 0.0288483804001982 0.7954091861024485

0.2816914096651573 0.0583120535931331 0.0206840018932936

0.1209353560783491 0.0660973542241235 0.0182362195599321

0.0660895877307872 0.0279762563977765 0.8070812084120190

0.1781873775617015 0.0621245640725604 0.6685407398058060

0.4169421767915013 0.8262161039028902 0.6649051528636958

0.3044646877636845 0.8696228886145124 0.8074657856180668

0.2708391068397729 0.8303806720617880 0.0254127663875445

0.1162115785501436 0.8252327727373509 0.0127595030989115

0.0676444443935749 0.8703349615116184 0.8003525449038394

0.1844649272056199 0.8269672231929588 0.6720943014221402

0.0788902199575717 0.9392251972856281 0.1510638679471225

0.1944427508183942 0.9675845330881940 0.2974472405164822

0.2174609403453819 0.9428226951109976 0.5206208422992459

0.3757293786233523 0.9349366555803849 0.5150607474873302

0.4329410230547366 0.9698013983278779 0.3049102431055295

0.3188171693095911 0.9373418664595159 0.1695062522561936

0.0797130357267514 0.1725668449101515 0.1753241814929526

0.1988241249099780 0.1264644111229638 0.3059509927653276

0.2324304943415167 0.1677842542937355 0.5256537156486044

0.3874146803614788 0.1711305530930090 0.5184675119962675

0.4361831546155991 0.1281649701026991 0.3049636526624563

0.3212404049217328 0.1708335929499591 0.1716292226788375

0.5793184843929474 0.5591313453848110 0.3497744102123150

0.6931921261204425 0.5276213027000866 0.2027324246972763

0.7181699280344629 0.5558916942158949 0.9804117982660007

0.8766492337956304 0.5668675991392950 0.9824092790780758

0.9340790630517440 0.5368625154204467 0.1911575439343347

0.8171863707434086 0.5640969775979812 0.3258177719959812

Structure files (CONTCAR) involved in this work:

0.5836637124432176 0.3264490383904173 0.3334456889648672
0.6979224548159930 0.3705108955290792 0.1973294047726577
0.7329946170720758 0.3291487756262661 0.9804422112298016
0.8891355541444725 0.3261781251830111 0.9871738381376514
0.9368941743929595 0.3785107017365117 0.1974026349943392
0.8217912680880619 0.3332651927717141 0.3314543649984873
0.9225965859745937 0.4418944417385194 0.8495979486418256
0.8052906348661394 0.4711952444918999 0.7048863047436066
0.7838009251026195 0.4468449414309263 0.4816870298951976
0.6243854728828954 0.4373584680277231 0.4883424979495441
0.5688016068324618 0.4678776657322777 0.7005621292611149
0.6847599195255930 0.4326597457311422 0.8319103611915424
0.9260598996231661 0.6716832959468506 0.8241509955526709
0.7649628815952850 0.6699282865718938 0.4686697248981144
0.6125818976381813 0.6727028355292192 0.4874407687657336
0.5648815119772544 0.6268616332562404 0.7009559465272508
0.6797873651886782 0.6769156683844693 0.8367882883376401
0.5768765576979366 0.9429036083229558 0.3554595543589393
0.6963815084203265 0.9748432727713210 0.2150404805483354
0.7130550732310773 0.9413474028719158 0.9883634053092177
0.8725573662865629 0.9294191513941635 0.9905037973073954
0.9336063884110345 0.9660060949525925 0.2022356654714034
0.8198649918809816 0.9387316603893926 0.3393785470754438
0.5820500857198299 0.1734007640112868 0.3378329365870391
0.7006210233783787 0.1319852064437884 0.2031297345824561
0.7325503125781546 0.1678888307652880 0.9853314418736909
0.8887156883845817 0.1708304770633434 0.9940493091575174
0.9367116221870899 0.1252304991383694 0.2087252905472303
0.8206387656276763 0.1764602323219047 0.3326309178420599
0.9182996717192851 0.0564188505039154 0.8552798854056133
0.8065162908854790 0.0376700053708765 0.7048289104384009
0.7816356692953131 0.0614255774440053 0.4830896244127816
0.6228548215023698 0.0644107940348753 0.4934289850335133
0.5689077147548585 0.0299912338528911 0.7048338714139373
0.6851561347779660 0.0642144584089424 0.8359377902531158
0.9230664643789485 0.8253857794946868 0.8357055622861516
0.7641271181303223 0.8287298689955619 0.4821561688944130
0.6133506529083453 0.8281377079392068 0.4883944439397858
0.5624840537301717 0.8722976550102287 0.7008559784840345
0.6646118715056830 0.8297975861046022 0.8526005503762573
0.4250048196890154 0.4408869023540907 0.6508674939727135
0.3070067528601126 0.4693998012085523 0.7955281043524258
0.2833487849705225 0.4403113821154846 0.0180716577166717
0.1231598723603809 0.4308949385241922 0.0152360797353912
0.0694517409749525 0.4669959269372207 0.8038888805121043
0.1827817164571754 0.4355566930146095 0.6677321953839115
0.4204807891602410 0.6724411302798705 0.6686876138909807
0.3053773961077036 0.6289365867705036 0.8077055002588167
0.2739550291571885 0.6693511168619850 0.0272210684849071
0.1200942911394053 0.6713541003498784 0.0136561443175499
0.0736232272822794 0.6243433798280883 0.8024907137470196
0.1856216368138475 0.6696630740482374 0.6709683387550393
0.0801514721491502 0.5573752465667201 0.1494374682175768

Structure files (CONTCAR) involved in this work:

0.1964997040559502	0.5304320429553701	0.2955891721978773
0.2219835088822440	0.5552052933856184	0.5195639104562330
0.3811183844854808	0.5630648367003903	0.5131338305593001
0.4356903937779881	0.5279765119146510	0.3032206360104948
0.3211188073234861	0.5611640558724050	0.1662900476992049
0.0800270246756806	0.3271143676361917	0.1735267678327859
0.1982931668065573	0.3713942158941525	0.3069548422354815
0.2342248464891337	0.3291205618656572	0.5240725456056678
0.3894385336880575	0.3244812227043903	0.5164921152237542
0.4383132105237269	0.3699998748177079	0.3047765128432333
0.3211270065418852	0.3280839726636013	0.1728808706958186
0.3593298716371801	0.0664689191334091	0.7259930302862285
0.3142769632582564	0.0526327936708999	0.9101566838173248
0.2009912207293001	0.0562706405750188	0.0146659225248446
0.0912285650323281	0.0672635828408020	0.9062061432048388
0.1019482455598847	0.0615118388605152	0.7101212836505199
0.2290473922154992	0.0478875711232330	0.7611393804770462
0.3617628987321380	0.8252954872732224	0.7539314869468724
0.3090337632639335	0.8578308961374264	0.9266926129448801
0.1926657171585019	0.8527298435241213	0.0186743260726359
0.0900891193786158	0.8280342803102874	0.8983253692758869
0.1064076500536909	0.8392618215069539	0.7031020557753429
0.2310258446060978	0.8456585730621110	0.7676636530267575
0.3158703460640253	0.9483790900036190	0.7817822604186335
0.0874149142026921	0.9488883247255354	0.8146591375197797
0.4341713746335825	0.1232763532004330	0.5872557393181139
0.4144543904155606	0.9919326735051763	0.5793538029025126
0.3844584111471894	0.8614737313711670	0.5664356205317921
0.1938481167779843	0.1354531396343235	0.6208170395237292
0.1856620676131318	0.0036799124054388	0.5848706617844405
0.2032601849224404	0.8709331131714731	0.5743138882456152
0.9858107204487412	0.0346820539625238	0.7959378450885090
0.9875879139638595	0.8625803387473746	0.7843705495367443
0.1421930418673758	0.9286815202822987	0.2248879291088445
0.1823501403413816	0.9426482464401655	0.4112724404124221
0.2971707716423099	0.9547090200818162	0.5092442903704302
0.4073747789846054	0.9305709502721985	0.4040446329858324
0.3956112344283668	0.9404250676863762	0.2067110015816278
0.2705674993578017	0.9493090238554511	0.2657815868300270
0.1415346165836383	0.1717527487762066	0.2535930477860427
0.1973343007378679	0.1394157089770477	0.4249948050218386
0.3104679772516986	0.1448714050239827	0.5264496538715898
0.4118183204401527	0.1689673907529574	0.4032046181706186
0.3981024922709653	0.1586622002068858	0.2073891548294880
0.2718402854396033	0.1467422184066207	0.2619383871909278
0.1823488124101689	0.0478695413252815	0.2838010950308675
0.4169973577284378	0.0494086426051722	0.3182215652792834
0.0693932496206300	0.8720550784663881	0.0833589769356994
0.0872614514965567	0.0042436424079037	0.0793596931680706
0.1018250603052334	0.1368947728106104	0.0711226207676172
0.3049597386771984	0.8633414690558108	0.1233313157395999
0.3064376265280098	0.9945395218634699	0.0857067045998469
0.3061890609693387	0.1283589896303958	0.0706127392914387

Structure files (CONTCAR) involved in this work:

0.5119449858904828	0.9571988949924911	0.2866308080375656
0.5163041480747292	0.1367220635461739	0.2910514999735114
0.6431484617505876	0.5685669425121738	0.2762860329497655
0.6797960336402603	0.5480698254740912	0.0874316346933530
0.7980113931143460	0.5551176996218908	0.0008829685435497
0.9136063691210139	0.5771558985250540	0.0897059695898785
0.8938329037449949	0.5664777948912851	0.2866994599367893
0.7702454256503923	0.5450868149080961	0.2307406394668826
0.6416284943706522	0.3232673434293456	0.2487342643749282
0.6963241415772359	0.3608818332807317	0.0776430380473247
0.8115508585731964	0.3502244504645567	0.9810154936362656
0.9155818435694193	0.3338459649702058	0.1011716681184799
0.8974004440525666	0.3515975783968389	0.2958240734008065
0.7716058731639269	0.3499047907311858	0.2386715700830864
0.6801299913565687	0.4480683277166888	0.2239707133837310
0.9187717971035326	0.4569180299166817	0.1767312376513469
0.5674654976931967	0.6291665193212304	0.4100236997953016
0.5882436545696584	0.4990094682800168	0.4305012891034914
0.6101468663985254	0.3670601931348352	0.4306538614428953
0.7960259695553347	0.6376430388830480	0.3675699780827332
0.8107881700591901	0.5084833569832413	0.4135457794108234
0.8020485607677087	0.3755032226804840	0.4300460572881421
0.0129184262832526	0.5480934678179377	0.2152524952719633
0.0166849805800750	0.3693021344952174	0.2170366443047528
0.8608912787308961	0.4328053705453937	0.7733936477011258
0.8200960824210590	0.4503787114585568	0.5892082652718382
0.7035109574129887	0.4530186421626926	0.4936778599170477
0.5929711113877590	0.4300669193798048	0.5992187609951259
0.6072665634522186	0.4373223499408359	0.7968756712690984
0.7318867798984983	0.4409116934255910	0.7340191958872812
0.8819674541470414	0.6723099817736935	0.7211909662361811
0.8114167938287349	0.6523374574973283	0.5640193202153874
0.6888234857911044	0.6433237234855140	0.4865228634829922
0.5832953948560657	0.6675273634901943	0.5994574675765549
0.6051682231062555	0.6581014122480608	0.7944443628496797
0.7352611504420160	0.6736126756218557	0.7497511713450608
0.8076914460692239	0.5505862872381208	0.7225772104478356
0.5833828863005407	0.5478315916437848	0.6880471687541505
0.9333700354202836	0.3720142578447845	0.9115172483199857
0.9103414666263777	0.5022357500457955	0.9290733971586236
0.8865997419580033	0.6338448127225100	0.9138567666675985
0.6968656805639715	0.3590326510605015	0.8818102737864062
0.6996698527525642	0.4911741748277816	0.9128443337816294
0.6959712393168974	0.6255481223202187	0.9287675492939135
0.4898634056430138	0.4538297260209531	0.7203780003883994
0.4846224130227662	0.6352043718453320	0.7183614345311556
0.6411132776281060	0.9361587878045623	0.2819460540409102
0.6846188759939319	0.9627208220396579	0.0976454779494508
0.7921352103621989	0.9228616672789606	0.9966710742335394
0.9040686802711624	0.9319201596826796	0.1022326202026610
0.8970025896777887	0.9315963786179918	0.3001895802054436
0.7699980594454604	0.9452343562839899	0.2453177183718555
0.6399334204846447	0.1736039645712266	0.2530117266035999

Structure files (CONTCAR) involved in this work:

0.6952899345225222	0.1365220209290400	0.0828847802829244
0.8111208801214886	0.1463904638579667	0.9878955299048429
0.9145312194189346	0.1652622266960354	0.1087421719737001
0.8972247137967279	0.1562730295455019	0.3042332380817839
0.7728013285501422	0.1626659714040398	0.2359193471430414
0.6946009541434464	0.0544862444608773	0.2415772379585341
0.9176588362535530	0.0457771433969678	0.1999179582488345
0.5653942139721689	0.8731547854416543	0.4168275993589681
0.5851736795216729	0.0037378780944158	0.4352151754462504
0.6080554911439019	0.1351944366872493	0.4376519756141458
0.8114303939842028	0.8645424536061337	0.3938106682304435
0.8125379720943204	0.9988943300543985	0.4183592105724143
0.7951800780639515	0.1319770283211296	0.4265415582095212
0.0119605947658059	0.9495742994974132	0.2179733190396064
0.0167435471595890	0.1328365876807188	0.2254026420205181
0.8610246998072865	0.0763453011202777	0.7751703772596574
0.8186477866911619	0.0629793202622117	0.5901373460676139
0.7022684383720260	0.0483526573825527	0.4950413288194326
0.5941407594386040	0.0702202516212702	0.6060293292758241
0.6072223366223619	0.0574257036082556	0.8036047694530217
0.7310616384595173	0.0608334218087630	0.7360643332122598
0.8630860603866574	0.8302224068521062	0.7539716635245163
0.7947143428321497	0.8478136766673998	0.5904098984199173
0.6889428744741120	0.8591197219815823	0.4752550651316461
0.5912602083436336	0.8314398641782627	0.6045712955269665
0.5898582534056989	0.8392704571493746	0.8037957542851530
0.7185555672920160	0.8546122828785430	0.7723474140438222
0.8154109319410950	0.9584391002440437	0.7169476834704521
0.5847198256083128	0.9505061874518671	0.6897629335809446
0.9341398003170455	0.1220388656023051	0.9241944314648711
0.8944458827571707	0.9955872883600684	0.9283514013922998
0.9028433516580998	0.8619769344392229	0.9393946232392317
0.6958497872671434	0.1370975104260908	0.8880108211851406
0.7054153043554222	0.0046656392481538	0.9131682455439142
0.6700777635635037	0.8765539448341181	0.9532099900544158
0.4896114080095312	0.0433948532412355	0.7221241294928347
0.4814463978966615	0.8684208168200673	0.7021589431442548
0.3594810167184505	0.4328035103868682	0.7213325683436248
0.3184655720942327	0.4431646831798288	0.9088136018190673
0.2029501444531228	0.4418533889188156	0.0071703862170456
0.0912199273492028	0.4273525089540518	0.9045351337097142
0.1061833940929978	0.4345577829239207	0.7069584407518722
0.2310425350430185	0.4512534689952624	0.7627158657271645
0.3610876802929357	0.6734314036367208	0.7511671324846189
0.3101869212207243	0.6432520163208915	0.9261802214671149
0.1963944530044329	0.6449810073633800	0.0271270561841809
0.1006687752437011	0.6680508802874429	0.8962598162595610
0.1076126948636237	0.6547285904957220	0.7004181151971894
0.2315049040985163	0.6508621673542160	0.7672323907523058
0.3184423381393725	0.5500265225306918	0.7854792465275094
0.0925254289313748	0.5455245029823841	0.8151045746558465
0.4347390035104298	0.3716333875330336	0.5882000203303155
0.4184552698677180	0.5029251176960770	0.5725299539104722

Structure files (CONTCAR) involved in this work:

0.3944699681262613	0.6342360810708021	0.5686060777025344
0.1998793619718957	0.3620992056827028	0.6220655594836807
0.1912055538360855	0.4936435545380936	0.5835772488205367
0.2060749579793605	0.6267746569500984	0.5730182441529611
0.9898558194941911	0.4592072390243123	0.7863330844353134
0.9936487861460043	0.6312151417827738	0.7953851851425109
0.1426963977709593	0.5685069548592557	0.2249626704817471
0.1867773215200365	0.5546789165390260	0.4103624880257964
0.3018990897347424	0.5460982141469595	0.5092529153639475
0.4103889255606731	0.5693561112272421	0.4008085963038878
0.3974317719543565	0.5538002123032165	0.2037474514414616
0.2719296784677824	0.5493307586362437	0.2614760901730643
0.1395910926428658	0.3274610708774775	0.2557117710450221
0.1963412981765275	0.3579931494699795	0.4259906731200163
0.3124104485583521	0.3508718347889432	0.5185084333375684
0.4171213963984461	0.3270706224319703	0.4028649500322540
0.3977542331951323	0.3408690397072204	0.2086323251351452
0.2711442164530727	0.3501235524109227	0.2634192403745270
0.1841719854929332	0.4501581641720336	0.2837258387815722
0.4201187581410992	0.4486771276730345	0.3221371996911733
0.0714983652106235	0.6238945356201191	0.0797486352716691
0.0903853336362284	0.4924608989267423	0.0777952624462420
0.1065526131271193	0.3599831882378112	0.0696899512987063
0.3114841149206894	0.6367958038390320	0.1228055478290393
0.3061769758581461	0.5063213758678968	0.0798679004688305
0.3065090028230993	0.3715656435309046	0.0728466869352486
0.5141491073386074	0.5420712691942594	0.2824178709633144
0.5178917651862948	0.3620225535063685	0.2849719126243794
0.4377529768945501	0.7495304688907883	0.6380392291597405
0.1926947557330123	0.7484733054582484	0.6402843660219747
0.2778690167615950	0.7500291197908616	0.0344273558023211
0.1121435054708262	0.7482997349888850	0.0523508234954605
0.0589897517474029	0.2496895237990497	0.1517554598120962
0.3093658662697503	0.2495158058683212	0.1459057585569128
0.2262456324422274	0.2485411638809564	0.5309889636731854
0.3932451283187178	0.2479479762756096	0.5579466060086029
0.5651713990316315	0.2504309828946214	0.3680393376614642
0.8169104486214044	0.2547931134495833	0.3630793554769376
0.7251718855933409	0.2484580436669569	0.9827665254186997
0.8964758783312439	0.2476802543123083	0.9553923929720074
0.9420793340054687	0.7478401390367697	0.8611621871075820
0.6750369204633456	0.7519505690027655	0.8857622929000299
0.7621453439582055	0.7507590100852959	0.4508700978653932
0.6105637092163826	0.7506748656584482	0.4515973277299979
0.8021959019036947	0.6344246771186042	0.6930817359690914
0.7910252141435609	0.8760767407202231	0.7160698612940151
0.9931685239834210	0.8432495340340102	0.5112564088176720
0.9540434067148090	0.7248853152226310	0.4211899712992947
0.0971185340996367	0.6986658185065130	0.4010272501747775
0.9163807794784522	0.8138726671351926	0.4227861517076291
0.0260669717712653	0.7543380545802030	0.5235053964883425
0.9040474266255829	0.8179396946626692	0.5938000345487607
0.9202759628306072	0.7128906158776508	0.5765415520421180

Structure files (CONTCAR) involved in this work:

0.1425726951779219 0.7162520228065027 0.4399336961441082
0.0978986235713108 0.6435967123953009 0.3997103222246360
0.0183493076951096 0.7059378637006717 0.3951488280951000
0.0994418207395799 0.7183411139612129 0.3242569270399442

Figure 1(b) La/ZSM-5

1.0000000000000000

20.0219993591000005 0.0000000000000000 0.0000000000000000

0.0000000000000000 19.8990001678000006 0.0000000000000000

0.0000000000000000 0.0000000000000000 13.3830003737999998

Si Al O La H C

95 1 194 1 6 1

Direct

0.4254519941532713 0.0578418464708669 0.6402422588410760

0.3050809546166097 0.0311823653866767 0.7852092278776617

0.2805172942811598 0.0685345938645099 0.0054591294972926

0.1200689130129357 0.0698131435889365 0.0048856791005454

0.0686919424760870 0.0324884571032805 0.7934875965313802

0.1798460614364751 0.0574504029174367 0.6466130327764051

0.4202767497452671 0.8283172416923062 0.6644090181952201

0.3038062257859197 0.8734125795668451 0.8060310670223797

0.2669766013598812 0.8337796099814079 0.0243039376716032

0.1128705412516683 0.8312378248577721 0.0102050578771745

0.0639952047577727 0.8750110117875199 0.7972239666157467

0.1820764413405974 0.8320646186191053 0.6713079642001752

0.0768780939038537 0.9480383014810900 0.1435229192728007

0.1969179817775475 0.9756066914578315 0.2908991022719816

0.2197193945482964 0.9374716295345300 0.5089226169868295

0.3794138921017130 0.9345116976988248 0.5077639580617918

0.4315178500391587 0.9733973217873503 0.2980308729515060

0.3204305862520244 0.9515251393973873 0.1500341269546292

0.0795097590259784 0.1743570484389940 0.1637844876762663

0.1979224592231816 0.1319621950568152 0.3060413082011037

0.2338975732633661 0.1761821705420613 0.5218468829795477

0.3880507394785691 0.1757491270386017 0.5080744054670731

0.4361645017507635 0.1309999238027819 0.2975298602030927

0.3187348823696876 0.1714919053594041 0.1681249287868438

0.5757620544008765 0.5570160648042912 0.3488285263900953

0.6960188958271029 0.5270268568545863 0.2035033915323150

0.7187169513637590 0.5650538693257725 0.9855390208613590

0.8789231585564067 0.5686404512058779 0.9849933826796390

0.9321670222371773 0.5331821277153327 0.1932307774507764

0.8204812015972297 0.5546042992233188 0.3388686390025813

0.5842890508663622 0.3295139462250693 0.3313197043630229

0.6987664008617716 0.3699391974707857 0.1854840897954688

0.7344145011110079 0.3280012750736840 0.9683321074788767

0.8884610632511504 0.3248358566088344 0.9848532816351419

0.8137154252245685 0.3330257041527883 0.3308345432990805

0.9236382576847783 0.4436221892670186 0.8525614187849030

0.8050737258283446 0.4742167685890327 0.7069458940827809

0.7761284149327002 0.4413769439182195 0.4868423574060404

0.6187790246177483 0.4384752044833850 0.4889585585853102

0.5669656966032576 0.4721166207845659 0.7003757567106185

0.6802528192187147 0.4461607414162935 0.8436749413129002

Structure files (CONTCAR) involved in this work:

0.9211147910784776 0.6747059533399555 0.8251232311900726
0.8050167774502741 0.6319578980335525 0.6859431761800304
0.7653293021543917 0.6708176544078298 0.4675533784577306
0.6109272667829462 0.6742272087849720 0.4825169247440191
0.5643060928937290 0.6296935872703728 0.6968922155576588
0.6833211883191594 0.6725832450194137 0.8238854623931170
0.5765883696176135 0.9453792885284233 0.3520598262960586
0.6977246663863880 0.9733665593178205 0.2088104372509172
0.7206548121445664 0.9362509528967099 0.9877160834322720
0.8808347219474664 0.9343555876581053 0.9873041285420289
0.9313945701415601 0.9732111883735635 0.2005539959134056
0.8223192711394954 0.9463080951481032 0.3488127299514225
0.5806263819431763 0.1752465599232684 0.3312809959993732
0.6975169496548578 0.1314840801358757 0.1885675167925890
0.7338781768543302 0.1713995355640577 0.9700775311011605
0.8882237106146696 0.1733472271301503 0.9808753024412531
0.8184682044931975 0.1745164581202005 0.3247350381813707
0.9238363282750796 0.0555036027186627 0.8481876479290159
0.8028757795362543 0.0271785722531416 0.7033490166150373
0.7825383724426969 0.0663478830321667 0.4847578821507730
0.6228769968923886 0.0678460352239382 0.4859694696718053
0.5705826600530494 0.0306412994198785 0.6970074381380148
0.6803633497225184 0.0532750406260452 0.8452199430874908
0.9215057228965607 0.8292050202273975 0.8319198443998782
0.8024472353850817 0.8705359934568226 0.6895358332184546
0.7668084509103197 0.8272750817177150 0.4732928848151145
0.6122326637931367 0.8276305519504856 0.4851007795248861
0.5641976169932365 0.8725887496587117 0.6974245841856359
0.6815488208551226 0.8312761521685567 0.8273826215867358
0.4226933126757157 0.4462940679163332 0.6498478977224473
0.0795097590259784 0.1743570484389940 0.1637844876762663
0.1979224592231816 0.1319621950568152 0.3060413082011037
0.2338975732633661 0.1761821705420613 0.5218468829795477
0.3880507394785691 0.1757491270386017 0.5080744054670731
0.4361645017507635 0.130999238027819 0.2975298602030927
0.3187348823696876 0.1714919053594041 0.1681249287868438
0.5757620544008765 0.5570160648042912 0.3488285263900953
0.6960188958271029 0.5270268568545863 0.2035033915323150
0.7187169513637590 0.5650538693257725 0.9855390208613590
0.8789231585564067 0.5686404512058779 0.9849933826796390
0.9321670222371773 0.5331821277153327 0.1932307774507764
0.8204812015972297 0.5546042992233188 0.3388686390025813
0.5842890508663622 0.3295139462250693 0.3313197043630229
0.6987664008617716 0.3699391974707857 0.1854840897954688
0.7344145011110079 0.3280012750736840 0.9683321074788767
0.8884610632511504 0.3248358566088344 0.9848532816351419
0.8137154252245685 0.3330257041527883 0.3308345432990805
0.9236382576847783 0.4436221892670186 0.8525614187849030
0.8050737258283446 0.4742167685890327 0.7069458940827809
0.7761284149327002 0.4413769439182195 0.4868423574060404
0.6187790246177483 0.4384752044833850 0.4889585585853102
0.5669656966032576 0.4721166207845659 0.7003757567106185
0.6802528192187147 0.4461607414162935 0.8436749413129002

Structure files (CONTCAR) involved in this work:

0.9211147910784776 0.6747059533399555 0.8251232311900726
0.8050167774502741 0.6319578980335525 0.6859431761800304
0.7653293021543917 0.6708176544078298 0.4675533784577306
0.6109272667829462 0.6742272087849720 0.4825169247440191
0.5643060928937290 0.6296935872703728 0.6968922155576588
0.6833211883191594 0.6725832450194137 0.8238854623931170
0.5765883696176135 0.9453792885284233 0.3520598262960586
0.6977246663863880 0.9733665593178205 0.2088104372509172
0.7206548121445664 0.9362509528967099 0.9877160834322720
0.8808347219474664 0.9343555876581053 0.9873041285420289
0.9313945701415601 0.9732111883735635 0.2005539959134056
0.8223192711394954 0.9463080951481032 0.3488127299514225
0.5806263819431763 0.1752465599232684 0.3312809959993732
0.6975169496548578 0.1314840801358757 0.1885675167925890
0.7338781768543302 0.1713995355640577 0.9700775311011605
0.8882237106146696 0.1733472271301503 0.9808753024412531
0.8184682044931975 0.1745164581202005 0.3247350381813707
0.9238363282750796 0.0555036027186627 0.8481876479290159
0.8028757795362543 0.0271785722531416 0.7033490166150373
0.7825383724426969 0.0663478830321667 0.4847578821507730
0.6228769968923886 0.0678460352239382 0.4859694696718053
0.5705826600530494 0.0306412994198785 0.6970074381380148
0.6803633497225184 0.0532750406260452 0.8452199430874908
0.9215057228965607 0.8292050202273975 0.8319198443998782
0.8024472353850817 0.8705359934568226 0.6895358332184546
0.7668084509103197 0.8272750817177150 0.4732928848151145
0.6122326637931367 0.8276305519504856 0.4851007795248861
0.5641976169932365 0.8725887496587117 0.6974245841856359
0.6815488208551226 0.8312761521685567 0.8273826215867358
0.4226933126757157 0.4462940679163332 0.6498478977224473
0.3042261787490625 0.4758880224869603 0.7984077222598476
0.2813963577251558 0.4361101111512201 0.0165043016592257
0.1198232249830572 0.4354402776949460 0.0143321699115422
0.0686597072780710 0.4701235754540891 0.8008781393714632
0.1820998521359889 0.4479839691118302 0.6601674022300500
0.4210942875069603 0.6734616756644344 0.6656303189564590
0.3041318909665863 0.6335913642982707 0.8110244844544774
0.2675261862949375 0.6770433511610490 0.0257945670339033
0.1134305658396919 0.6771280157017044 0.0099009096332857
0.0650456484780955 0.6286682541744515 0.7980561249351161
0.1836170963997195 0.6730124335114375 0.6733389395833927
0.0780989679216372 0.5622259436245376 0.1458237138848159
0.1954095062119863 0.5324176073761606 0.2933290238059958
0.2205109091634313 0.5661516992978300 0.5145000338664980
0.3809565605956458 0.5663156605358909 0.5077367825767093
0.4325483409080382 0.5315374932369561 0.2942158106116465
0.3182662760287779 0.5597929374876643 0.1552994752559986
0.0784921744311759 0.3291247092753861 0.1757488606740599
0.1995269742662120 0.3735603501219729 0.3083721819296227
0.2362876361506862 0.3332541616356721 0.5263743279104220
0.3909467797105141 0.3291028722284301 0.5159158221771784
0.4409488567201567 0.3736599395051780 0.3023726237299841
0.3222952259477671 0.3299500574746830 0.1770108707260498

Structure files (CONTCAR) involved in this work:

0.9359021849824539	0.1314316606761874	0.1966693773212564
0.9322752645741137	0.3723500473645168	0.1978957002813405
0.3606625993410782	0.0644058089011359	0.7123555020530864
0.3041937442173551	0.0726081063869239	0.8897386867363298
0.2001360723121122	0.0592319346513621	0.0139702345876803
0.0975073610017112	0.0739748581090961	0.8889035527257879
0.1047994117465344	0.0582274111583510	0.6920843109007319
0.2316460288919702	0.0359251230374405	0.7344551096151457
0.3578708263737150	0.8314962437743126	0.7413502323078360
0.3060829891958251	0.8452607960702323	0.9194743383086238
0.1897577084249788	0.8584225505596138	0.0116804366159222
0.0842343050952668	0.8338419251523693	0.8972570427268221
0.1042763010674409	0.8440712082316252	0.7020725053982930
0.2293187312789620	0.8627153055258842	0.7596156195428904
0.3232558417112059	0.9526751364549129	0.8047728566412214
0.0839827930082751	0.9532920173907906	0.8121690216872536
0.4340390911927776	0.1265899015413440	0.5758076479730174
0.4190008536203066	0.9952126051052789	0.5629825964582656
0.4002974061805483	0.8636762745535902	0.5590348984188495
0.1959335188073931	0.1324789363599359	0.6063000186675300
0.1831146238400824	0.0032576131460617	0.5558189440959542
0.1973386500965790	0.8689468220072553	0.5655365855035204
0.9892389533923748	0.0448198083394289	0.7784888747885147
0.9841161177250960	0.8673272816639745	0.7781627090592392
0.1419311885030228	0.9444487912939109	0.2153411947434717
0.1982227882468442	0.9307621773604551	0.3923341020106419
0.2998940539433655	0.9477955214630003	0.5201338063741336
0.4000524188581464	0.9309953777630160	0.3907864940878637
0.3959047849840365	0.9514912315695301	0.1941123464859336
0.2701012838529768	0.9742782086001013	0.2390719011229072
0.1428587691154468	0.1696253926887479	0.2383065058957952
0.1971563594761642	0.1681305613924040	0.4144201077288815
0.3108028622816715	0.1500072210521384	0.5126986381529774
0.4130986646030383	0.1760922051655594	0.3927968566125041
0.3961667885002920	0.1565188866109440	0.1984894640470286
0.2713254916339942	0.1391039372431488	0.2548417202144735
0.1785511665877596	0.0531218833456385	0.3179217839649744
0.4190241935736750	0.0527870809727619	0.3205306960273724
0.0681440208317711	0.8770583052288886	0.0848776501329315
0.0833818593929004	0.0073992746315667	0.0605774762301475
0.0974741079954051	0.1396820168080656	0.0573609858535690
0.3026667936006581	0.8763038063879028	0.1124111106468463
0.3161514487186821	0.0039292473656049	0.0571709511309372
0.3025408505596419	0.1379539923272338	0.0602091257285214
0.5105399446330863	0.9577020942352329	0.2844203479572893
0.5158567735865850	0.1401098855185745	0.2791357009584239
0.6431078721084214	0.5588259215168575	0.2819494475095651
0.6931965300561714	0.5701521051231004	0.1005270186978491
0.7990333398364096	0.5552450651660499	0.9805574983090232
0.9047020067289063	0.5775869448321159	0.0987603400262147
0.8958860287835431	0.5587769669664747	0.2959793779791880
0.7707714752894500	0.5304002936105195	0.2498194961957594
0.6454627222680092	0.3287296040007988	0.2525002778462941

Structure files (CONTCAR) involved in this work:

0.6961187878069254	0.3394193571424990	0.0738234673921203
0.8113971976748696	0.3524146738288331	0.9780862593652536
0.9139560032954723	0.3222319797926888	0.0978853841065859
0.8926926480381699	0.3504376856652175	0.3136745446437437
0.7733219766155582	0.3606200351015915	0.2327339226280720
0.6775992500865660	0.4487540411646130	0.1828268635452700
0.9184448872135368	0.4554902375759352	0.1725158008791696
0.5670886475663908	0.6279318284976466	0.4074859787891849
0.5770101833768012	0.4965433691630227	0.4308882894860697
0.6076457344688079	0.3668248357378760	0.4336539026329322
0.7989534669052714	0.6286208042262498	0.3775664179143112
0.8176957599575839	0.5006090182243805	0.4307456844041325
0.7858107532924414	0.3697587488288332	0.4310667357202903
0.0116688249623644	0.5479625391918943	0.2108278778423022
0.0161428441228469	0.3584325293888631	0.2415896496980340
0.8599189957799578	0.4372604616978863	0.7772265123153365
0.8053563001373231	0.4348812032037725	0.6001056131846565
0.6971764885464764	0.4603489632271889	0.4889172221883573
0.5916514320400937	0.4305868982864714	0.6023831594685567
0.6049304973594587	0.4447893713768046	0.7991591082200865
0.7310129199384033	0.4692887917379736	0.7550771432278878
0.8611818981376136	0.6754621468367048	0.7437488023777968
0.8051703136951893	0.6562400534143792	0.5707342171479610
0.6878946789069164	0.6478533771883843	0.4819281312743306
0.5820931468902776	0.6703328068566565	0.5953649319690051
0.6060338472646456	0.6608147068432504	0.7902774489758353
0.7316892287784382	0.6441386254241012	0.7353256693974121
0.8247996327564192	0.5527374459683484	0.6924064466409738
0.5836125671184901	0.5511435682386575	0.6821171480804135
0.9331331085908577	0.3739404125144138	0.9134909900123344
0.9157925734526066	0.5059062385703185	0.9300449264142374
0.8967639005529620	0.6378574265681457	0.9267093617336194
0.6978415937935487	0.3710513092637341	0.8813679655627271
0.6835913496433292	0.4996364570014223	0.9351544115933358
0.6976039823152005	0.6337791768476341	0.9283360813738414
0.4875221708118387	0.4611066930980590	0.7190480120616545
0.4848337628107957	0.6376187527419900	0.7195314328350916
0.6413022085309247	0.9398480961542790	0.2798651153866297
0.6999189698856039	0.9318577978996193	0.1045383328241491
0.8009213690713832	0.9448079276055393	0.9744796292708974
0.9015486768235298	0.9337388222983810	0.1040987428171693
0.8969343220776209	0.9443176877699030	0.3015187908842947
0.7703426961736280	0.9685631325375684	0.2617205440969989
0.6422522967309844	0.1716612643100419	0.2532758541717698
0.6951083313153550	0.1598017525750958	0.0752832160444683
0.8110558810623772	0.1468154540716671	0.9824895861001642
0.9179143640999856	0.1694013714979311	0.0932803392040986
0.8961076635916682	0.1664672337213567	0.2894665566923492
0.7713159322559341	0.1438973069764550	0.2364141356055839
0.6798544111662390	0.0518189059055120	0.1888455351350680
0.9151211444399168	0.0528295378615204	0.1883914046712775
0.5673827098222561	0.8755844135480425	0.4136829790693546
0.5835130652089972	0.0063461534729273	0.4322697941732105

Structure files (CONTCAR) involved in this work:

0.6001008835593833	0.1383561509483556	0.4355986454846281
0.8052489866917403	0.8718567605272760	0.3902599249917315
0.8203594959167465	0.0008712117086368	0.4391722006272504
0.8063779629328888	0.1346594974817990	0.4290605692832100
0.0112081740668865	0.9609395844099438	0.2115655193804529
0.0158133330973967	0.1382161532409820	0.2174834983128630
0.8580773982426576	0.0585013177915168	0.7781523627688550
0.8016054515252339	0.0724080818647709	0.6022843529568540
0.7024591270660007	0.0562470009201629	0.4704305227812368
0.6037238651008924	0.0710154883832903	0.6035338299370887
0.6048811691465128	0.0539889740110796	0.8011517735018961
0.7300386127230415	0.0288841808175557	0.7562341872380424
0.8574491221905745	0.8336653810445720	0.7586541825540719
0.8031415234301623	0.8342226943006559	0.5812448746072951
0.6896849755983265	0.8529681828836424	0.4821453635584847
0.5854372151914154	0.8295719043874757	0.5993443086254246
0.6040668889135310	0.8437736273520661	0.7945819963929088
0.7289106429991714	0.8629591425311270	0.7401340924673055
0.8210239196732577	0.9495660667557799	0.6765633070229577
0.5826697135276526	0.9508515562277312	0.6783936955247611
0.9322063439725787	0.1259464228379197	0.9074871823790293
0.9191967063722800	0.9948620736769577	0.9294441365606784
0.9037684082315403	0.8630030948617965	0.9393711247171546
0.6985585095225456	0.1285008207408601	0.8819406328059762
0.6843250259566953	0.0014732504948509	0.9388680833658640
0.6961903353640863	0.8674130104089144	0.9338983770263224
0.4916063834050946	0.0473705538268735	0.7080561582695323
0.4842737576162626	0.8649808475937752	0.7163315764537416
0.3565858872438559	0.4442745965762664	0.7193606144871336
0.3074915011424451	0.4334114831739557	0.9017458720520828
0.2005698099879073	0.4344372598597045	0.0226379711752097
0.0967260140570485	0.4305490980666750	0.8986169035659718
0.1060747207413818	0.4424348624246178	0.7012251992455590
0.2292280832973403	0.4707193799683136	0.7530771489497002
0.3582918024391703	0.6712349460085316	0.7414564694400132
0.3074756210294779	0.6665855161319312	0.9213955307007462
0.1907751257045935	0.6512694885964520	0.0120929495296649
0.0851758478952182	0.6715920397599799	0.8967567945364595
0.1059727297377853	0.6580048698245992	0.7021508779285416
0.2298601096228181	0.6437094764733123	0.7637591371637922
0.3222006699316906	0.5542431329426418	0.8185352098575026
0.0830823227011138	0.5500198847906810	0.8154621450179689
0.4318183300911576	0.3734506943098989	0.5969643213072051
0.4171968046734186	0.5034135668156345	0.5631454493839647
0.4022607119524771	0.6361834504894962	0.5613876392325634
0.2042221321580540	0.3749031980511999	0.6183024883339070
0.1856329856124471	0.5033739562275819	0.5715136708099674
0.2020052143946146	0.6367589298950657	0.5682224575252798
0.9896807344697330	0.4557688764850446	0.7842586036874574
0.9855427804789492	0.6368218296800769	0.7764615635869964
0.1416526287611914	0.5682024042824181	0.2207059997215411
0.1911702966892845	0.5684219722987925	0.4017246744992103
0.3008006362738361	0.5552125451676521	0.5145459745987931

Structure files (CONTCAR) involved in this work:

0.4048452850898985 0.5708435154926023 0.3923981458843364
0.3948647742329000 0.5579358660620984 0.1944277613920878
0.2703981671703043 0.5415117748559517 0.2496306735056456
0.1450140886420857 0.3302007645398124 0.2461583068181813
0.1946628206983920 0.3494359244782566 0.4243206165738196
0.3137717393493420 0.3553530662821662 0.5096460047355461
0.4248349317487018 0.3359069509487260 0.4068539986421112
0.3996706800220905 0.3375039557764298 0.2123782582980158
0.2741141751200140 0.3604826236746911 0.2647648060150597
0.1790374998902970 0.4523922263837267 0.3015105963807907
0.4186686839801355 0.4517672324695942 0.3098933153531523
0.0687203346445521 0.6324727783113684 0.0857615865639667
0.0907655999946507 0.5038440164484735 0.0631986411497951
0.0895236779820606 0.3714023703638744 0.0737284436872802
0.3028199301502427 0.6347662577878950 0.1145362398943292
0.3080747837986749 0.5055558358132350 0.0660944206208719
0.3111568507632831 0.3707069450228664 0.0734893559098114
0.5114509372275636 0.5463768374671591 0.2768558119643941
0.5206318498248697 0.3677329794025444 0.2804654605936170
0.4385450511463527 0.7508740299959399 0.6397490290578859
0.1965637670050276 0.7525740138981649 0.6581143152102078
0.2700970798330477 0.7555403499595765 0.0570204490700591
0.1092119681707524 0.7541858808516043 0.0483016634580698
0.0631164547938792 0.2524940127361363 0.1425995394932948
0.3048868165404263 0.2514893142627003 0.1585298578271937
0.2313117951874739 0.2544193387910059 0.5547777952418425
0.3939223441696917 0.2514287302387647 0.5520245646272841
0.5640054975259093 0.2528401950380645 0.3583382359299749
0.8016128807025793 0.2529783129760895 0.3441511596180883
0.7296780839658545 0.2495056755086270 0.9372457639615372
0.8920681012344271 0.2492145498468979 0.9375883846367897
0.9406305247664744 0.7514629270577767 0.8525921474538114
0.6968307428917885 0.7519093049839591 0.8412631341120401
0.7697076349438400 0.7495773441057643 0.4377275273764710
0.6062840416092613 0.7512640173542032 0.4437447819484714
0.0205028564625011 0.4687272182221571 0.4628763853349526
0.9134438470327426 0.3315514391692710 0.5542689593484280
0.9932092422465625 0.3695358395714570 0.4314023168022724
0.0274757494552585 0.5169618839065127 0.4633981011080003
0.8919310753152242 0.3519015570550169 0.6120942130373770
0.0704839643433752 0.3065721394179419 0.6146459387620283
0.9612525292600339 0.3066100388647953 0.5724571829350960
0.0732917476882119 0.2648550946108199 0.4977462666827427
0.0233233362937703 0.2325993262664057 0.5931591306043815
0.0389528484642291 0.2805675280975644 0.5590403584447161

Figure 1(b) Cu/ZSM-5

Si O Al Cu C H

1.0000000000000000

20.0219999999999985 0.0000000000000000 0.0000000000000000

0.0000000000000000 19.8990000000000009 0.0000000000000000

0.0000000000000000 0.0000000000000000 13.3829999999999991

94 195 2 3 1 4

Selective dynamics

Structure files (CONTCAR) involved in this work:

Direct

0.4215703113503950	0.0545690962273506	0.6397872959642331	T	T	T
0.3016288954356063	0.0270693091261372	0.7845152817928720	T	T	T
0.2789502840393868	0.0651815892416149	0.0043701136411149	T	T	T
0.1189504234775317	0.0655483484167682	0.0037711300291386	T	T	T
0.0654541328760021	0.0256411774804883	0.7920570322185867	T	T	T
0.1772636573418263	0.0512201254185066	0.6446655394481180	T	T	T
0.4200532160614323	0.8279282144166816	0.6619839204305303	T	T	T
0.3036447631279683	0.8701030678429589	0.8048459466996954	T	T	T
0.2682551785575650	0.8289020328658807	0.0237649698209634	T	T	T
0.1137597887176617	0.8265588806297749	0.0111425537500581	T	T	T
0.0636357514628860	0.8647455228266869	0.7950274761703934	T	T	T
0.1840838881665544	0.8282407928051260	0.6673503033875724	T	T	T
0.0759139325212377	0.9443295054976744	0.1425481102900756	T	T	T
0.1968357518778120	0.9726602795472317	0.2866704972650986	T	T	T
0.2193188895265167	0.9339597073060658	0.5048630228939136	T	T	T
0.3785245866940916	0.9312556081328036	0.5056450563845554	T	T	T
0.4308246467538860	0.9709131302697809	0.2962081972405186	T	T	T
0.3208625998711635	0.9485284399460495	0.1462815696200369	T	T	T
0.0796517435708473	0.1713078700493375	0.1592479704283927	T	T	T
0.1968406313875529	0.1295647115711663	0.3035787317279027	T	T	T
0.2296837093139869	0.1720122602158716	0.5210868579140541	T	T	T
0.3846443738293341	0.1727377221279617	0.5064539599225258	T	T	T
0.4343022292548316	0.1279305711944984	0.2965951390799569	T	T	T
0.3178790973732130	0.1693160556612949	0.1669748088409657	T	T	T
0.5748457321496585	0.5558577429746957	0.3599634938654732	T	T	T
0.6951339770482345	0.5270409519226008	0.2232751653203190	T	T	T
0.7144179840119441	0.5513305722268040	0.9944202607217065	T	T	T
0.8732499963890091	0.5673222367019100	0.9918591559893919	T	T	T
0.9326220876783012	0.5308457156997117	0.2021037978032887	T	T	T
0.8215934094447541	0.5608368578675947	0.3473431799861931	T	T	T
0.5814342406949343	0.3250682025574973	0.3317552074760358	T	T	T
0.7000297076454742	0.3696247577635736	0.2047337954097370	T	T	T
0.7332528668923001	0.3318739422630179	0.9863645775694713	T	T	T
0.8880725359488826	0.3318927616013622	0.9985151886149950	T	T	T
0.9367118454585850	0.3724809061181678	0.2094277266913162	T	T	T
0.8214844451641889	0.3282790616964212	0.3397580004205897	T	T	T
0.9250040729334286	0.4458569296418947	0.8592398064769537	T	T	T
0.8080130196726584	0.4672679843071737	0.7157129213010051	T	T	T
0.7814296735531351	0.4401215074500274	0.4922619462487758	T	T	T
0.6218698187043845	0.4311826792852460	0.4908350163930111	T	T	T
0.5665611487752534	0.4644942038729731	0.7001741808255313	T	T	T
0.6792957380435157	0.4358035020886503	0.8411499145861941	T	T	T
0.7979528626048482	0.6234309873889641	0.7035503629412220	T	T	T
0.7648601754236166	0.6696856201649021	0.4828808587776820	T	T	T
0.6094221083090147	0.6742630652322469	0.4898412362884410	T	T	T
0.5683918560182373	0.6227431157933658	0.7025350789326010	T	T	T
0.6771893430712809	0.6663449797131397	0.8448791957575538	T	T	T
0.5774741771808768	0.9420758645456285	0.3441894327274660	T	T	T
0.6959485050651432	0.9738389338986877	0.2035087121066101	T	T	T
0.7182985746053089	0.9528388239447244	0.9756909116594616	T	T	T
0.8785972417206425	0.9497529322206442	0.9815473851999831	T	T	T
0.9315357264885771	0.9686632293549855	0.1968912773931583	T	T	T

Structure files (CONTCAR) involved in this work:

0.8165326506253203	0.9309295569428984	0.3288953599769202	T	T	T
0.5799114077161768	0.1723739747983078	0.3238434206861524	T	T	T
0.7001277277903143	0.1310110089078332	0.1945952922494383	T	T	T
0.7355554370209397	0.1703789897329708	0.9774510734528939	T	T	T
0.8916373308300999	0.1782801614669203	0.9785950782980042	T	T	T
0.9375450735323717	0.1269077068951097	0.1944740026355990	T	T	T
0.8223110660082404	0.1737663304533971	0.3268284781594106	T	T	T
0.9230867183352858	0.0680390988904505	0.8433414734580084	T	T	T
0.8054403075969758	0.0340949081586396	0.6990401024339984	T	T	T
0.7831195454387586	0.0551080442208449	0.4749863236114827	T	T	T
0.6232336965093956	0.0656790922083149	0.4814177134575717	T	T	T
0.5657366257252527	0.0360766503109661	0.6946468721998159	T	T	T
0.6814156303717388	0.0705354488819944	0.8231876155217931	T	T	T
0.9145585624614566	0.8324702744914643	0.8270310988796190	T	T	T
0.7980456553888704	0.8756181618454767	0.6919281865713541	T	T	T
0.7682997709225531	0.8278714561116034	0.4780566568182855	T	T	T
0.6084795850341359	0.8266786383033341	0.4866909349599982	T	T	T
0.5620213056946662	0.8776561965296443	0.7028076778416088	T	T	T
0.4221106729314437	0.4430794249248562	0.6468048715112094	T	T	T
0.3025195976874488	0.4726754953854879	0.7910356911487366	T	T	T
0.2813663979546272	0.4354395046247553	0.0116637466018326	T	T	T
0.1218006834833597	0.4335351121474384	0.0117711509036849	T	T	T
0.0707000601454155	0.4714386711657982	0.8006826872363544	T	T	T
0.1789861959345246	0.4474845021916022	0.6505979789720554	T	T	T
0.4233387405512636	0.6726093757084584	0.6653690704664290	T	T	T
0.3064257173189544	0.6292631296278045	0.8079038232862674	T	T	T
0.2691892108010157	0.6722064945088251	0.0269884750124745	T	T	T
0.1153981587028967	0.6736214505718728	0.0131401379461517	T	T	T
0.0675679047052477	0.6304875132220884	0.7992341873981467	T	T	T
0.1856969424185761	0.6699714474255396	0.6676630562631906	T	T	T
0.0770797126872858	0.5569128970583848	0.1440299499317935	T	T	T
0.1976297186888973	0.5269204373565287	0.2865200053617004	T	T	T
0.2196489967689544	0.5636738779832020	0.5080464180245521	T	T	T
0.3790041822186824	0.5659012354052543	0.5110507554933001	T	T	T
0.4314334246987906	0.5288406142828386	0.2999339527583275	T	T	T
0.3230527838510909	0.5537975059324328	0.1491507263298554	T	T	T
0.0795951535703820	0.3262545040065215	0.1666716974447142	T	T	T
0.1974718451285195	0.3692815944740127	0.3059355181574013	T	T	T
0.2319408759023331	0.3285123120677757	0.5250109224452852	T	T	T
0.3869724257522085	0.3254983757506282	0.5126416221332780	T	T	T
0.4374618740054753	0.3709914779344320	0.3012935714203061	T	T	T
0.3201877763047964	0.3286112649719377	0.1717634720146964	T	T	T
0.3552756034326769	0.0603394117896507	0.7087410801110783	T	T	T
0.2999275015718764	0.0706548866418455	0.8873867816112193	T	T	T
0.1988229639795187	0.0542304505140911	0.0160855663650475	T	T	T
0.0980015354061805	0.0649488006643110	0.8869434027564288	T	T	T
0.1022502734542643	0.0494794086649075	0.6901581918255584	T	T	T
0.2282539589066876	0.0287191017063216	0.7330648454531757	T	T	T
0.3578240657148292	0.8290852633002479	0.7395531629730007	T	T	T
0.3048871013275828	0.8395059175053345	0.9169204922650219	T	T	T
0.1906863148697532	0.8529903811031926	0.0149200001390710	T	T	T
0.0880989082846611	0.8277181549221961	0.8965350222559557	T	T	T
0.1064207948386094	0.8385600159115750	0.6994875062673466	T	T	T

Structure files (CONTCAR) involved in this work:

0.2297800130756835	0.8607802667989566	0.7557745334766965	T	T	T
0.3219612192650724	0.9496361848932643	0.8082855335328739	T	T	T
0.0727365128868867	0.9451901581978951	0.8092488166766540	T	T	T
0.4295775644513931	0.1227948445174721	0.5740954534194258	T	T	T
0.4184672609658874	0.9907314300974682	0.5637543059582465	T	T	T
0.3965216828765372	0.8589277680687979	0.5548537470337438	T	T	T
0.1931936722428644	0.1268220201541464	0.6057756711389785	T	T	T
0.1810122785061830	0.9986259401041060	0.5519804578139839	T	T	T
0.1979123860931735	0.8649564734176538	0.5609473857968202	T	T	T
0.9873032159284310	0.0449156776030104	0.7786679828988292	T	T	T
0.9866195915666757	0.8437443257052720	0.7739797790804275	T	T	T
0.1418714656487630	0.9403481632394406	0.2121252617109393	T	T	T
0.1985062947831216	0.9276965901940859	0.3879383085156990	T	T	T
0.2991384735255159	0.9462748782371515	0.5164986939278424	T	T	T
0.4002657671211113	0.9281225159740263	0.3890321812442920	T	T	T
0.3959198247492527	0.9491883739606621	0.1916878333354204	T	T	T
0.2696915698030308	0.9717492959421100	0.2339273448829668	T	T	T
0.1438340454454763	0.1674912044687935	0.2322219571553155	T	T	T
0.1928522465314068	0.1634273354667538	0.4135753944864092	T	T	T
0.3071199837786884	0.1478638590915310	0.5098647083674929	T	T	T
0.4109525877712799	0.1729689430740712	0.3916781676792652	T	T	T
0.3953544706953713	0.1538061956299890	0.1967333209170628	T	T	T
0.2712187948774504	0.1389193447164240	0.2562270537983529	T	T	T
0.1780136377936809	0.0502863003991971	0.3122047694424098	T	T	T
0.4169107866725654	0.0498801627608071	0.3196368707614418	T	T	T
0.0675490370637764	0.8741614806482242	0.0814118466612994	T	T	T
0.0803547472682075	0.0056062246857932	0.0625250868211844	T	T	T
0.0970231931238257	0.1374500016760262	0.0515260724597252	T	T	T
0.3048349348393408	0.8727307766884230	0.1095150058672024	T	T	T
0.3167327090531458	0.0005368377476859	0.0527220779498504	T	T	T
0.3004891806298434	0.1342893258082739	0.0604210151787520	T	T	T
0.5097803565072840	0.9563465813289551	0.2815192817697535	T	T	T
0.5141458532325743	0.1355689926486386	0.2781804483182626	T	T	T
0.6400483454501695	0.5667145521057464	0.2889879237834029	T	T	T
0.6852299684311250	0.5482968807311325	0.1068189096490341	T	T	T
0.7946763973260936	0.5457734731659875	0.9898213620710743	T	T	T
0.9023890645048817	0.5688328406238580	0.1043049812140125	T	T	T
0.8967678055218297	0.5593169088702872	0.3023485476330605	T	T	T
0.7701653986117262	0.5485005824391684	0.2546660993516562	T	T	T
0.6419289831551351	0.3229565934681046	0.2511598610777502	T	T	T
0.6969276443497425	0.3630427485981966	0.0844231168617672	T	T	T
0.8107428869961520	0.3563585084813414	0.9890940859299430	T	T	T
0.9106460456304633	0.3288012216732252	0.1146731413252541	T	T	T
0.8982917098073544	0.3462786370838866	0.3092467828242198	T	T	T
0.7733374994058948	0.3469991247890688	0.2448629335237006	T	T	T
0.6846840774952450	0.4468807964811582	0.2376370426531401	T	T	T
0.9185737010068863	0.4509500517674237	0.1896091129301090	T	T	T
0.5623898001162577	0.6219065329879543	0.4288137834454577	T	T	T
0.5838920907142607	0.4914963162647930	0.4327709558339626	T	T	T
0.6079832494366071	0.3608136073345626	0.4334395396149315	T	T	T
0.8087216410392750	0.6345027185764243	0.3949648530986792	T	T	T
0.8127725868919901	0.5029994755270116	0.4311523690454692	T	T	T
0.7998008098139379	0.3699643545616632	0.4380537940634493	T	T	T

Structure files (CONTCAR) involved in this work:

0.0116678425538771	0.5462188413793930	0.2139748010839751	T	T	T
0.0168765904148911	0.3629856057261838	0.2225425723194115	T	T	T
0.8615527818468246	0.4290827048043056	0.7873132396624188	T	T	T
0.8141758693067921	0.4386302066247359	0.6028296052325927	T	T	T
0.7008833214054746	0.4485923951519366	0.4969292040772624	T	T	T
0.5914833643685528	0.4235657228604834	0.6021942957196198	T	T	T
0.6040471854299102	0.4338049474992223	0.7975977521503403	T	T	T
0.7318776783010313	0.4535160341169869	0.7530593508681004	T	T	T
0.8536679687887139	0.6756711158179245	0.7373496698299826	T	T	T
0.7795589883161216	0.6316271579930512	0.5866940423641858	T	T	T
0.6862890245872169	0.6596601399673742	0.4576041749753849	T	T	T
0.6004031395171394	0.6650041705148930	0.6101220211616663	T	T	T
0.6019459038700153	0.6481891468603994	0.8074696323534791	T	T	T
0.7293025322800012	0.6313644288355400	0.7691080189192721	T	T	T
0.8246535080024934	0.5468250747798420	0.7212780836575139	T	T	T
0.5849443148599706	0.5435602820410350	0.6862004558234411	T	T	T
0.9351533665776517	0.3839709946202551	0.9373885698396229	T	T	T
0.9141068954475914	0.5145927648700981	0.9232020143625230	T	T	T
0.8848622092868658	0.6413687581064329	0.9403174920327753	T	T	T
0.6966421998089943	0.3630462923810141	0.8887697540684951	T	T	T
0.6807523835186532	0.4946824167895005	0.9261251042117872	T	T	T
0.6897214538444428	0.6279054353618329	0.9576201530664782	T	T	T
0.4870918250595349	0.4542199258822190	0.7174352832059278	T	T	T
0.4883353963548845	0.6335633257227480	0.7097893926041552	T	T	T
0.6386427821259544	0.9342972154823174	0.2653061521925641	T	T	T
0.6840358187982412	0.9634081123149492	0.0847942834035016	T	T	T
0.7985422522513341	0.9608600441233697	0.9836156439290866	T	T	T
0.9066686546409000	0.9349543024260052	0.0928574133063911	T	T	T
0.8934689267573415	0.9334973615107024	0.2904575111288850	T	T	T
0.7687074965624575	0.9429343031516035	0.2316647258379086	T	T	T
0.6370259255148064	0.1730561210040820	0.2373727395397771	T	T	T
0.7005781001887500	0.1349692382532901	0.0736716562471068	T	T	T
0.8145718964868914	0.1518109097501759	0.9748912334495747	T	T	T
0.9209330825091755	0.1630960327637551	0.0889141851572954	T	T	T
0.8980250226606885	0.1645622524835563	0.2847108870552184	T	T	T
0.7701497280132964	0.1623173443638832	0.2347843188807396	T	T	T
0.6930923407889540	0.0534187777329290	0.2318033973817043	T	T	T
0.9146694487654612	0.0486613735049662	0.1937274001007093	T	T	T
0.5682549197584803	0.8735419115349459	0.4077631797458551	T	T	T
0.5908774289755659	0.0033490192803700	0.4209772676217957	T	T	T
0.6079132180272238	0.1353275525272675	0.4229947535844455	T	T	T
0.8018083849543072	0.8572356472664220	0.3760344290017973	T	T	T
0.8035694383627119	0.9891949924727633	0.4109798644352551	T	T	T
0.8072684052069452	0.1226669742472909	0.4178306577586769	T	T	T
0.0108458083240106	0.9552922600689636	0.2130101514406643	T	T	T
0.0176077814576782	0.1326210687361712	0.2136418569204557	T	T	T
0.8591965511293160	0.0722678185892009	0.7696378081141835	T	T	T
0.8199665482591564	0.0526517202813812	0.5829591168412768	T	T	T
0.7030620402940886	0.0553581059430305	0.4913415640652926	T	T	T
0.5887088007293697	0.0705768694234579	0.5901153812361570	T	T	T
0.6047200345915333	0.0739215819772708	0.7852957248631139	T	T	T
0.7306398343829295	0.0599889238547687	0.7278227638344941	T	T	T
0.8591703646587338	0.8324062244803314	0.7401639989573349	T	T	T

Structure files (CONTCAR) involved in this work:

0.8016976473287365	0.8676187424826044	0.5709295347649553	T	T	T
0.6881887843031161	0.8399190766276703	0.4743488548670928	T	T	T
0.5859548354327656	0.8407930589034633	0.6000271260350598	T	T	T
0.5945512124047939	0.8436093221475233	0.7995457269145085	T	T	T
0.7278345470993913	0.8506246295124312	0.7337068758210438	T	T	T
0.8124654784459679	0.9542760306342529	0.7196538833386348	T	T	T
0.5832239135742868	0.9567255624864949	0.6934697973397376	T	T	T
0.9356877248677187	0.1418059893637788	0.8922476904192528	T	T	T
0.9121165207799622	0.0181404897784790	0.9383959996943897	T	T	T
0.9021921805651081	0.8890889015703872	0.9104559508872396	T	T	T
0.6991823605070958	0.1410643638119883	0.8785748833682603	T	T	T
0.6884713211981196	0.0069076583484073	0.8986296452134910	T	T	T
0.6994803605319421	0.8757800656210234	0.9416052989375557	T	T	T
0.4861936156998847	0.0476368429891905	0.7119716703842754	T	T	T
0.4804985394246520	0.8719334751813810	0.7086599347196489	T	T	T
0.3564427817854248	0.4380667958179815	0.7169078764506448	T	T	T
0.2992405056169591	0.4292934021659734	0.8937818662874689	T	T	T
0.2013595614682014	0.4446239835017027	0.0289140856063018	T	T	T
0.1040165002045194	0.4307150661976698	0.8939103805266471	T	T	T
0.1040620324893418	0.4460080053585866	0.6967891577168994	T	T	T
0.2297042515987722	0.4725359434364920	0.7379665217122287	T	T	T
0.3641904466382007	0.6688126004377057	0.7474683487575255	T	T	T
0.3038696682106642	0.6609549083718895	0.9190113553349666	T	T	T
0.1919304989854234	0.6467546943334070	0.0235575045718064	T	T	T
0.0939342659193493	0.6715513083647161	0.8970785733074789	T	T	T
0.1090879436432117	0.6573061534429382	0.7021276130015160	T	T	T
0.2348477579756648	0.6384757205611845	0.7526512326939211	T	T	T
0.3245294956208142	0.5496986930237090	0.8145268189222272	T	T	T
0.0836390872392111	0.5510472851832143	0.8176442223949766	T	T	T
0.4308312383568506	0.3727586697543340	0.5863942898708343	T	T	T
0.4180443528099189	0.5048275839332446	0.5670430758601228	T	T	T
0.3991301149649693	0.6373078454190232	0.5616794942328597	T	T	T
0.1976043769982014	0.3722829939332358	0.6130847741553166	T	T	T
0.1810065681761916	0.4997740716561715	0.5572616482693572	T	T	T
0.1983095241351397	0.6339078888857387	0.5603421977077003	T	T	T
0.9914810296820546	0.4545494591224593	0.7920565180235416	T	T	T
0.9897234959178681	0.6438850195251665	0.7829105737008386	T	T	T
0.1426522368827585	0.5618645514096376	0.2143354303859377	T	T	T
0.1991619970139530	0.5678500643108836	0.3911002730553351	T	T	T
0.2995101090415082	0.5519856469741149	0.5218542015755604	T	T	T
0.4000418722536997	0.5694067280215608	0.3942583241002020	T	T	T
0.3977072286561472	0.5532094638342246	0.1960568669152513	T	T	T
0.2710297641082209	0.5306721119436527	0.2357297416867269	T	T	T
0.1434133215757217	0.3274823953523726	0.2409374754724143	T	T	T
0.1940989371971418	0.3416727026122440	0.4195341600942787	T	T	T
0.3097426283339951	0.3511684407818806	0.5131437521939041	T	T	T
0.4165673556546893	0.3290905187935306	0.4002633335740177	T	T	T
0.3976839026832285	0.3406922292456870	0.2050872429055884	T	T	T
0.2719784726346331	0.3578756671432237	0.2600144084780650	T	T	T
0.1781099776440827	0.4485739576485437	0.3042207953958109	T	T	T
0.4179927521072763	0.4492666867381431	0.3177742287818442	T	T	T
0.0674372369315400	0.6265623952399656	0.0820005120494936	T	T	T
0.0819178083625945	0.4951745709370617	0.0647916098650263	T	T	T

Structure files (CONTCAR) involved in this work:

0.0979018628289562	0.3632816228379266	0.0619979572780130	T	T	T
0.3083290897525227	0.6297193386814010	0.1118292772825564	T	T	T
0.3192913076386555	0.5014085127060453	0.0559885834736636	T	T	T
0.3061947462264816	0.3671526630937871	0.0668137269513544	T	T	T
0.5106987528526953	0.5443164442364401	0.2884598253910303	T	T	T
0.5176892989287298	0.3644048735883574	0.2835195216228587	T	T	T
0.4421010588478500	0.7503183753308770	0.6430140033418821	T	T	T
0.2011868273896585	0.7493402757071265	0.6537520294937458	T	T	T
0.2729110060593962	0.7508592967106975	0.0573101416614327	T	T	T
0.1085540919783779	0.7502916634066945	0.0536354857470901	T	T	T
0.0601673142089348	0.2493022958442165	0.1401913092315517	T	T	T
0.3057185099650421	0.2493961128590227	0.1549145507660383	T	T	T
0.2257693139639111	0.2499761805929676	0.5560508233658534	T	T	T
0.3912957401895292	0.2483377111097740	0.5512677105447716	T	T	T
0.5606180737555291	0.2483811175945808	0.3567476593646535	T	T	T
0.8140388061126956	0.2497236613351530	0.3688309293921513	T	T	T
0.7261501129913618	0.2511369966928957	0.9833321085222057	T	T	T
0.8956028348061951	0.2574751777553643	0.9522578893108996	T	T	T
0.9138869078886157	0.7581304514973273	0.8828866849949596	T	T	T
0.6885926774348977	0.7439416412234029	0.8692890976115151	T	T	T
0.7854401320936187	0.7482368422209675	0.4859524686151190	T	T	T
0.5889650777338242	0.7497335841889052	0.4580630991548089	T	T	T
0.7992522994031619	0.6860225289837104	0.0863620934510675	T	T	T
0.6965087036409915	0.7630609332143513	0.1485157985691357	T	T	T
0.8133397875663186	0.8074994473257602	0.0159470020186140	T	T	T
0.9163859078767838	0.6761725774050130	0.8245700664510882	T	T	T
0.6766627078646372	0.8279217996022858	0.8314353657745569	T	T	T
0.7041393028416679	0.6905457765633708	0.0705909285240311	T	T	T
0.7259457107961939	0.8160697239830734	0.0513278524041375	T	T	T
0.8491591799609041	0.7275164083667182	0.9870997472003349	T	T	T
0.8727135951915758	0.7355061769285697	0.2233275137172630	T	T	T
0.8286733930833251	0.7075630751243148	0.1590436361017156	T	T	T
0.8744318455727068	0.7878146400724261	0.1987253088947752	T	T	T
0.8457960922720086	0.7256478167720811	0.2928132924045062	T	T	T
0.9190718977259237	0.7069445400773456	0.2138406650935762	T	T	T

Figure S6(a) IS as same as Figure S2 Zn/ZSM-5**Figure S6(a) TS**

1.0000000000000000

20.0219993591000005 0.0000000000000000 0.0000000000000000

0.0000000000000000 19.8990001678000006 0.0000000000000000

0.0000000000000000 0.0000000000000000 13.3830003737999998

Si O Al Zn C H

94 193 2 2 1 4

Direct

0.4225501123524456 0.0599165354770691 0.6487164025125568

0.3045902298180718 0.0319330375009994 0.7912812517311634

0.2821855003833723 0.0564048078393069 0.0171540321347230

0.1222744071484424 0.0651111975919456 0.0130796844788433

0.0676452736444824 0.0322368890417532 0.8012397603015055

0.1799768658747939 0.0653477339839530 0.6640496903011389

0.4185521862900739 0.8275660062122404 0.6687357173949088

0.3006571970324857 0.8732440930665611 0.7999478531549719

0.2671780161073094 0.8306180925327087 0.0187305380616644

Structure files (CONTCAR) involved in this work:

0.1112553897150814	0.8268153366370222	0.0117273900185757
0.0655964199667885	0.8749344258208335	0.7981769953658319
0.1786593163325702	0.8290670492937640	0.6640776245485075
0.0760728303845230	0.9418279049634549	0.1482805608733688
0.1950473843230336	0.9699908162304978	0.2899028807517955
0.2164037693259250	0.9439117807753472	0.5158107236905073
0.3766353613348968	0.9357037328916491	0.5136650871046536
0.4330576674041957	0.9682103916074867	0.3012913623230753
0.3199832442607721	0.9349332608415772	0.1640450023975578
0.0815069194936345	0.1739103128069393	0.1679752668191930
0.1990816601734278	0.1286723991583022	0.3001982860893681
0.2318908216358040	0.1701744748621767	0.5179917311738023
0.3881117904820485	0.1740781605330405	0.5093323546334391
0.4357244386401011	0.1266452124905376	0.2957102221138399
0.3201208307782426	0.1722346858407915	0.1655176663790274
0.5755114956132326	0.5554208145186442	0.3581708022934211
0.6886427341209135	0.5270758526037317	0.2018863441926098
0.7122080103426784	0.5692058762983871	0.9888172273289062
0.8728182350665448	0.5720156179150462	0.9875864797043052
0.9263903525651261	0.5309386343841671	0.1944069309136111
0.8104573094815865	0.5526292928325084	0.3376780311854971
0.5722023464250634	0.3287609945460699	0.3327938683943793
0.6922291515542938	0.3727037084265006	0.1924844548770565
0.7292092276932437	0.3272180959317666	0.9800380320353388
0.8839834639691659	0.3267100602508123	0.9924559451953445
0.9397620289578973	0.3761211888041459	0.1924766242808802
0.9182918536508585	0.4452135329721877	0.8574942823633614
0.7994137510816263	0.4741638732551346	0.7168977971565220
0.7733587192752353	0.4379056096999865	0.4912825927277640
0.6153682661677250	0.4290285634366360	0.4915233713234793
0.5682276468161394	0.4696558732275429	0.7041468179803826
0.6759280729538973	0.4477412699894876	0.8566645520955630
0.9200345422335033	0.6778620474657474	0.8326822932507338
0.7691578202191469	0.6693218282086789	0.4646444088963730
0.6140632511845824	0.6734821851460056	0.4880762263438876
0.5604540282350051	0.6279195720077323	0.6985344435781504
0.6727837690182339	0.6749987656363563	0.8257403454373915
0.5775793107771072	0.9452759317054260	0.3588965065277553
0.6980100962750845	0.9736536153139339	0.2159540046380863
0.7194201132208125	0.9381781207454479	0.9939843956780617
0.8793240959672676	0.9346204446303845	0.9953428199004972
0.9315292984694622	0.9705942979156940	0.2048396127274849
0.8224348873753697	0.9469148891823853	0.3554697524866105
0.5783166510315532	0.1736012164884958	0.3300864718133398
0.6975951174446067	0.1313766297419352	0.1939297731559244
0.7320827848373679	0.1711294697566058	0.9732959999973677
0.8868112505630721	0.1738560078385752	0.9862512678374189
0.9362990731839979	0.1283791333132389	0.1988519173441595
0.8198928648112151	0.1720328864368915	0.3306747133249950
0.9230035234880476	0.0552561220879332	0.8575155317772319
0.8024020734136278	0.0264146981639979	0.7111975879340396
0.7807322974877265	0.0657565305952673	0.4931334560628072
0.6205983427915637	0.0699645671021371	0.4906225903052722

Structure files (CONTCAR) involved in this work:

0.5678606446463212	0.0322665109988196	0.6993789183421555
0.6785859758012069	0.0534254505077168	0.8498254303170769
0.9230551994552670	0.8302975219219543	0.8379668834765062
0.8031729822909173	0.8693998491282396	0.6965506095825046
0.7700803764899433	0.8271562769909143	0.4786521794100250
0.6151807080641948	0.8271137520409353	0.4909028870944838
0.5638788040474763	0.8752077882616049	0.6982786884248066
0.6786238033842028	0.8337576429134573	0.8332523820853027
0.4226411714954776	0.4423273936716295	0.6476425676770771
0.3051911151687245	0.4696507790677700	0.7908886180381278
0.2804700529110683	0.4457655732940378	0.0160680452126762
0.1223996946191885	0.4372922779752138	0.0165349869603215
0.0639911682977517	0.4683786618820042	0.8049873016940599
0.1787047668297680	0.4348958462044516	0.6679693553167564
0.4149895429306794	0.6737296015692414	0.6672066411380790
0.2993890193242665	0.6278265341212083	0.7998097563746218
0.2666670270557865	0.6693697613988709	0.0184614250781021
0.1110441787504268	0.6727497433415083	0.0105709032226521
0.0629966759883123	0.6273376515286136	0.7966983155602563
0.1778909777144873	0.6716703915085057	0.6643285063260834
0.0723233094658396	0.5593808353904421	0.1512350436132226
0.1916283591553861	0.5311846302645077	0.2915758611210297
0.2144212247259238	0.5553702717229062	0.5185184301044825
0.3733641353346430	0.5656042034088690	0.5153305122382315
0.4295467509533258	0.5321651139560302	0.3043322923810364
0.3179479576777356	0.5655244245573143	0.1653357994934943
0.0844140099717627	0.3272484555493382	0.1660492789379956
0.1977159775819267	0.3729139588482098	0.3014199246913996
0.2310499081626585	0.3315267852191927	0.5195316306048305
0.3866203160060661	0.3281300637611624	0.5081922854992370
0.4306823869215209	0.3745587817713467	0.2938094763868490
0.3166530204885194	0.3295375003496179	0.1624899600483168
0.3588476748140119	0.0707046656252226	0.7221386347854849
0.3157147848917461	0.0530255173434164	0.9069058386211026
0.2016858092110705	0.0498644235975952	0.0095777338290924
0.0927992065630099	0.0709312861099164	0.9009969744859671
0.1034133796786708	0.0651324009620835	0.7038341765358832
0.2292853461521421	0.0531173884734373	0.7590711657054721
0.3601467767900271	0.8283210684151590	0.7527623870637081
0.3006452578035576	0.8628939047610249	0.9195783278015419
0.1886056055832042	0.8509335808487748	0.0223990041807543
0.0884546050083452	0.8325222592365402	0.8960074893964582
0.1021673348373981	0.8427620458624726	0.7004511840142578
0.2287418946211438	0.8501789223778569	0.7549417410751964
0.3147770609188132	0.9516418501898602	0.7737445407664305
0.0877045320156446	0.9531009650288028	0.8105799969208510
0.4332435876220632	0.1273630528258640	0.5820286056803149
0.4121853435263606	0.9964253829446027	0.5742702074072467
0.3924539095138976	0.8645767818128209	0.5679233029356113
0.1957651099723692	0.1384177907628127	0.6154639204444203
0.1890908792727773	0.0059052908348628	0.5825099922723045
0.1947453297622498	0.8722875568685171	0.5641597228148090
0.9876679673868854	0.0414259052381199	0.7873277452008721

Structure files (CONTCAR) involved in this work:

0.9850361064020582	0.8700959039295318	0.7850181077059240
0.1405477780164461	0.9319827619381134	0.2203980870568563
0.1831711562343563	0.9494623065366627	0.4055887424015107
0.2969580775614009	0.9490761806799259	0.5087082496693603
0.4068290288949982	0.9313806946860975	0.4019433823106308
0.3963226854354863	0.9355606963998749	0.2045583348171564
0.2701214991679570	0.9474559566342245	0.2584231677013995
0.1407421158200815	0.1739786534601867	0.2506726382531626
0.1963011886696621	0.1384909032819404	0.4199620998669725
0.3105424286080418	0.1499013499513427	0.5169771506482806
0.4135560644089579	0.1680127466687882	0.3949067973690256
0.3971296201147471	0.1588035409864590	0.1996025422967143
0.2719118516744788	0.1523891325087385	0.2593831484754578
0.1860275410822784	0.0504149254315474	0.2720257764943428
0.4155201771387302	0.0480199104748175	0.3082342672052606
0.0651946196958610	0.8738691540815864	0.0826912450923524
0.0850239897394432	0.0047984459134242	0.0723982092969601
0.1071821016461373	0.1362689384641287	0.0675709331719302
0.3051080850404607	0.8616917069782779	0.1152423307580584
0.3106820487056062	0.9940731261682517	0.0819859614144333
0.3021939369690171	0.1277246126707235	0.0676999708249304
0.5126602005970952	0.9557370150995914	0.2879260109596091
0.5159901333892047	0.1330570628601535	0.2795112377218744
0.6392028080569299	0.5591108237614403	0.2844228695798482
0.6899203372520331	0.5761977342742244	0.1052050524425261
0.7927968839055077	0.5614171760132546	0.9773966997957667
0.8932625729760238	0.5753152800808222	0.1055301247529873
0.8870561650192309	0.5413610942954955	0.3006007242506180
0.7635688971878279	0.5259286639351249	0.2491504905370167
0.6385534153097607	0.3362901251294300	0.2657761154238070
0.6891523397985047	0.3346522283752777	0.0846367769547072
0.8065952124038879	0.3515662595971149	0.9934192428697997
0.9121589533275355	0.3259404362163518	0.1066051136316040
0.9038000949083966	0.3589565577014904	0.2989603881270392
0.7655698796670307	0.3693451408884456	0.2400373388078628
0.6680045356172789	0.4506271339696930	0.1746000445140510
0.9224363493837258	0.4528362374510917	0.1599644671532494
0.5686893089705092	0.6271428651061440	0.4148956645880403
0.5843943792555926	0.4965973881494727	0.4416240288590597
0.5818566890831656	0.3626019238245159	0.4429720049171759
0.7986344569193680	0.6312454007252991	0.3658079954935495
0.7954229324908556	0.5120167320417973	0.4437602404216630
0.8205759324579470	0.3813801545640657	0.4398579435997380
0.0037165334036563	0.5517995344817357	0.2154899969525251
0.0198067161045390	0.3684134213276729	0.2066470367489338
0.8545249545844179	0.4346124001374667	0.7834827115788517
0.7897495183104456	0.4372021371177983	0.6094286229357185
0.6953453279880774	0.4258500461443982	0.4685792295893949
0.6017368741947983	0.4293088012731124	0.6106181786684176
0.6020301587607406	0.4444079840776309	0.8075336859183545
0.7279916582283525	0.4749791187667303	0.7723978208631808
0.8600277422921854	0.6810034698240206	0.7545087932333937
0.8144804029633830	0.6445737839041270	0.5610899479814403

Structure files (CONTCAR) involved in this work:

0.6917973134126416	0.6477856894867096	0.4848237877578971
0.5855274237409943	0.6687965577147278	0.6005806404666414
0.5942586248008745	0.6614959932012611	0.7969993366646674
0.7191120852285101	0.6503153041931033	0.7342990357787658
0.8249813515244512	0.5506226304309003	0.6946291076308166
0.5813851823655019	0.5493827636414819	0.6874179721327438
0.9279654146392928	0.3775423170105267	0.9239719043046850
0.9092331278947323	0.5091324820557279	0.9318355712037960
0.8974835146016110	0.6416205949132094	0.9371831372995978
0.6950956158239191	0.3728958673361727	0.8937178258426621
0.6765499050548424	0.5009368698495299	0.9482647766038053
0.6881393166483910	0.6353988453626949	0.9297423362493964
0.4892396264387328	0.4531374948077209	0.7141422971460302
0.4796428426390769	0.6328647493293043	0.7081793343728642
0.6434047583241798	0.9393807085686143	0.2892213505894700
0.6987869441420989	0.9330443589152462	0.1108418550856510
0.7997436017850680	0.9467241417383497	0.9809370225755476
0.8984358902559381	0.9288237035483351	0.1127696984539162
0.8975386766106308	0.9490838862721306	0.3100925913909113
0.7713222468818944	0.9683557860927003	0.2667832309693122
0.6412370999552660	0.1735029336709405	0.2542354831863768
0.6954889407102807	0.1571534971980060	0.0792097029500028
0.8098302986224688	0.1475884684114517	0.9821929656118267
0.9140787858558813	0.1701403989235453	0.1000113293018812
0.8968874595311188	0.1557780777167201	0.2964934072595519
0.7710246682215038	0.1430140448304674	0.2421398175572921
0.6787465240948489	0.0519271535575740	0.1980423031180065
0.9195434298511714	0.0496147925512223	0.1811232048048107
0.5694535604106410	0.8757094601068915	0.4217042322767356
0.5819287945750579	0.0076965236328105	0.4371508593419962
0.5996948254127857	0.1397771086216203	0.4360684177665546
0.8083464858416481	0.8709884572619875	0.3945247516235503
0.8164725983136190	0.9986685133188669	0.4486796035747170
0.8052072213494462	0.1325605109201290	0.4352651859169588
0.0105261087536431	0.9540734921612396	0.2166712183640719
0.0162833357269196	0.1377342507812113	0.2161428924198858
0.8570808113104571	0.0571185818143006	0.7876129718794254
0.8013893339498938	0.0718441429305479	0.6103322477766767
0.7002925369829698	0.0570438731059648	0.4811750573612770
0.5984777823186016	0.0758270747050366	0.6070686894912568
0.6035864376062894	0.0523394011294693	0.8039969078542845
0.7290832052065257	0.0279672006075880	0.7626905841715114
0.8593713897344946	0.8331012403318476	0.7638972956462311
0.8051745884434578	0.8342234923514265	0.5872441855415098
0.6927067100715198	0.8519501694195309	0.4858117866633750
0.5893902001958305	0.8289318717969303	0.6057421601114622
0.6027457727553015	0.8532408730770575	0.7997020890244655
0.7296501973747698	0.8596174722263977	0.7461421379611547
0.8204062284117349	0.9487992107327540	0.6848275654982484
0.5794512896159750	0.9533664473356546	0.6725878470450363
0.9319755489651604	0.1276518775577557	0.9125228567900693
0.9183561450800914	0.9972415160450810	0.9431474209085852
0.9028969960113534	0.8648046529281220	0.9437937995462278

Structure files (CONTCAR) involved in this work:

0.6959638715476258	0.1294597445081920	0.8844227227337068
0.6827295738680277	0.0035948391192315	0.9459144113899718
0.6955661605211113	0.8697171432617884	0.9390767949423081
0.4889486558364780	0.0477635589319116	0.7153855166677315
0.4841518195233783	0.8645530198539479	0.7145657775376485
0.3594527702255488	0.4306116888202589	0.7220004252431594
0.3160166146353161	0.4499785490701204	0.9071988200392065
0.2004596726310521	0.4579129312164888	0.0059830341253077
0.0879818329535507	0.4329431689746912	0.9076526760789387
0.1030811484202027	0.4331229946971712	0.7120905578450465
0.2299177547096266	0.4472808369361957	0.7601054164787479
0.3578674377707972	0.6744918570153604	0.7534150581751556
0.3000319845539073	0.6363567785711759	0.9197069004347476
0.1882199874713878	0.6483757645420689	0.0223688515604240
0.0887504799960865	0.6678292698493007	0.8945926273192916
0.1009729696446775	0.6574069216837031	0.6984856719801831
0.2267851044197814	0.6502057968211785	0.7565146203269714
0.3144027909120452	0.5498533312890158	0.7710941380851839
0.0815773071700907	0.5480760871804069	0.8081642678448501
0.4328671213105151	0.3766327234102392	0.5768843942331121
0.4125389844767167	0.5076515836600749	0.5767936286630775
0.3843412519125269	0.6382806028867329	0.5676637521283434
0.1933894825371834	0.3625801492457263	0.6164231241024631
0.1841972196574607	0.4954146478932323	0.5870186584036962
0.1952748046764362	0.6281800282338429	0.5648959638773898
0.9844583283929492	0.4563570343327689	0.7887938946584131
0.9830086218605393	0.6362999908897770	0.7834410040957953
0.1346669651412477	0.5699533160130239	0.2273311734112041
0.1809512244807523	0.5496282598264454	0.4083893686435506
0.2946472429434122	0.5465769528577946	0.5109294521092157
0.4037042091301375	0.5705742984970638	0.4037803831392708
0.3937422915209173	0.5656712501564399	0.2077758616311163
0.2658625060680400	0.5545634063974076	0.2576418923215805
0.1394422242321983	0.3261029253200150	0.2549368856675658
0.1964504817544701	0.3645187655540979	0.4214495857706290
0.3094244811107476	0.3525679100589471	0.5208726076335510
0.4079988891450735	0.3316427829289882	0.3914541555830905
0.3933143077326041	0.3461105495830756	0.1944621042185730
0.2698361213541305	0.3498231567094925	0.2577752456584753
0.1828048436344593	0.4508409786766769	0.2722041121522150
0.4106173416127489	0.4527978037604765	0.3120961217380084
0.0644762857526072	0.6247748894246908	0.0795497434579232
0.0830678753938151	0.4929554350010046	0.0827719320868994
0.1156100205212985	0.3636238885917303	0.0677737842503786
0.3044172568574359	0.6383239420800115	0.1149650749211930
0.3109885747689459	0.5048569642561281	0.0853200841600995
0.2955491740525229	0.3723084063325235	0.0640408348228237
0.5094491254105146	0.5416175339591592	0.2915559973977811
0.5104654890656412	0.3662275244666778	0.2760042636915371
0.4358683766018575	0.7502603514125228	0.6401551874006748
0.1882252223462103	0.7502182943998957	0.6364905101645688
0.2759494866112622	0.7498980193391214	0.0181466081329771
0.1027901290912055	0.7496094888240402	0.0484628906810355

Structure files (CONTCAR) involved in this work:

0.0638215559077371	0.2509664562056972	0.1377866503451182
0.3089269439336483	0.2505147409348939	0.1356650637638143
0.2224727589886043	0.2508990874448402	0.5197469261079852
0.3952790403615618	0.2513561798202752	0.5463658901788357
0.5550985526433280	0.2502599402849676	0.3513220760525113
0.8093697297115107	0.2505433023199428	0.3475374622835160
0.7267532311558510	0.2497905832241847	0.9430527821314012
0.8910207263465467	0.2512668290890641	0.9477380522330981
0.9453169167957609	0.7534668834922083	0.8606543028668810
0.6847102562913552	0.7539091723860989	0.8499990315514308
0.7750181742041248	0.7489634093419412	0.4449098798544729
0.6094606832283267	0.7506080581210075	0.4495175775457302
0.9324835272212352	0.4964119185795688	0.5102655038154775
0.8191936709010879	0.3342227512972671	0.3255709614310127
0.7990588321116586	0.6367553783901694	0.6943556341108061
0.9208284672302245	0.4135843759020982	0.4316709722541550
0.8754306509283309	0.5616720527780301	0.5574936063389548
0.0293299940591187	0.4866359396633148	0.5153497541858633
0.0510783514115237	0.4492169615759816	0.5651041121649856
0.0587125398721619	0.4972941652699361	0.4483948899588184
1.0007741632850993	0.4274795487635984	0.4622426153358342
0.0213809060584297	0.5335404900694823	0.5575082862562359

Figure S6(a) FS

Si O Al Zn C H

1.0000000000000000

20.0219999999999985 0.0000000000000000 0.0000000000000000

0.0000000000000000 19.8990000000000009 0.0000000000000000

0.0000000000000000 0.0000000000000000 13.3829999999999991

94 193 2 2 1 4

Selective dynamics

Direct

0.4227767912639683	0.0598193632324528	0.6486277642447016	T	T	T
0.3046988158611332	0.0320787010825334	0.7911409750519248	T	T	T
0.2822405212913830	0.0567212220297451	0.0171075314156072	T	T	T
0.1222071272148749	0.0655444642867082	0.0131041438856125	T	T	T
0.0677496269245599	0.0323201311821840	0.8011575756822522	T	T	T
0.1800462035445134	0.0657009838242661	0.6640278739485526	T	T	T
0.4186500666737402	0.8275053592123075	0.6685159936424757	T	T	T
0.3005859305674322	0.8733971892007562	0.7994618410072154	T	T	T
0.2671411771229557	0.8307471422669130	0.0182856260636732	T	T	T
0.1111878964279065	0.8270264198731574	0.0117299436089550	T	T	T
0.0657203470544440	0.8750722837282916	0.7980804186919517	T	T	T
0.1786021195980562	0.8291771205361700	0.6636161737687643	T	T	T
0.0759821777126857	0.9420182847588457	0.1482331790225958	T	T	T
0.1949574712462891	0.9699077208346264	0.2896007299813121	T	T	T
0.2163782767615255	0.9442049267013519	0.5157178150004459	T	T	T
0.3766509271910978	0.9356884500213259	0.5135106331075940	T	T	T
0.4329039082373057	0.9683541401254827	0.3010486111987495	T	T	T
0.3198457087952845	0.9348994235574775	0.1638887820450447	T	T	T
0.0811298549680407	0.1741776969843256	0.1682006286880082	T	T	T
0.1990570674822984	0.1284554054162522	0.2994968648226246	T	T	T
0.2316022790332710	0.1700181173707984	0.5173118509512188	T	T	T
0.3878688263917136	0.1739542410391847	0.5095334885785986	T	T	T

Structure files (CONTCAR) involved in this work:

0.4355209290325050	0.1267845543576389	0.2957809654889950	T	T	T
0.3202084048776729	0.1726036752308172	0.1651661976270322	T	T	T
0.5755707480901000	0.5557152761486022	0.3572831217279501	T	T	T
0.6890940951543517	0.5262453315988619	0.2028301900805911	T	T	T
0.7139572471407586	0.5687288512875864	0.9888402785123949	T	T	T
0.8742524822579364	0.5716387077193811	0.9867454052190531	T	T	T
0.9270986025916125	0.5310462252808745	0.1940406821305311	T	T	T
0.8116325154841648	0.5524192853238497	0.3375523471311060	T	T	T
0.5729025253930330	0.3282767563723450	0.3320533835462844	T	T	T
0.6925693586846267	0.3724718755982869	0.1920777575490432	T	T	T
0.7306826685641379	0.3275629420141797	0.9785740031807246	T	T	T
0.8854909696133240	0.3266167545463537	0.9922538545452030	T	T	T
0.9398781602417547	0.3761711998079895	0.1942718394630814	T	T	T
0.9195560275918554	0.4447163319409581	0.8575592655732481	T	T	T
0.8005800920499440	0.4732813209522531	0.7171789694579589	T	T	T
0.7754240814062544	0.4369786824579171	0.4911143020844691	T	T	T
0.6171880115829759	0.4295043901688944	0.4898271590591272	T	T	T
0.5694812707878197	0.4695640940141371	0.7019877520856674	T	T	T
0.6770275185415651	0.4481632868815623	0.8556948624502714	T	T	T
0.9209310278158895	0.6776262711192822	0.8314286325815134	T	T	T
0.7691452608310601	0.6692099964213627	0.4642011346298405	T	T	T
0.6141478305500284	0.6737542150075142	0.4882036860831364	T	T	T
0.5611281992729320	0.6277235403474036	0.6980383615850412	T	T	T
0.6744265199156024	0.6736443312897936	0.8253219662337796	T	T	T
0.5775446906570068	0.9453828303786045	0.3585863911477939	T	T	T
0.6980368106726688	0.9734161469140464	0.2153661230793323	T	T	T
0.7195068739362367	0.9370292068299678	0.9935670267861818	T	T	T
0.8794523431317761	0.9340981323022506	0.9950228750753977	T	T	T
0.9312940772201588	0.9710662668035663	0.2046965540297702	T	T	T
0.8224785305380913	0.9470387485622117	0.3554846725576014	T	T	T
0.5782929527788044	0.1733309306833564	0.3304746052216043	T	T	T
0.6976322169855464	0.1311066504453945	0.1937529849451071	T	T	T
0.7322799777181962	0.1712630536150009	0.9733492718645577	T	T	T
0.8870939109582007	0.1737917018741463	0.9862180268815931	T	T	T
0.9360353717951193	0.1288543093745491	0.1992567297034621	T	T	T
0.8194586113263586	0.1726177664853451	0.3304715521090830	T	T	T
0.9230556382121909	0.0550309360932663	0.8571512747883495	T	T	T
0.8024825234322844	0.0266095997783643	0.7106458515984330	T	T	T
0.7808505211091209	0.0661546502113037	0.4927187493772290	T	T	T
0.6207946647441018	0.0698378257710437	0.4906396977619521	T	T	T
0.5682297076624330	0.0318631120402261	0.6995374147972309	T	T	T
0.6787875124549301	0.0529659723411859	0.8499502265627615	T	T	T
0.9233146422767513	0.8302924022502647	0.8379218823509570	T	T	T
0.8032839375476514	0.8697325618036611	0.6965757324161411	T	T	T
0.7703923497159478	0.8271274921077453	0.4788419301664207	T	T	T
0.6153485808299548	0.8271509703189600	0.4904857215163778	T	T	T
0.5641476710259585	0.8747057323779249	0.6982516761870557	T	T	T
0.6789902261651795	0.8330204586645855	0.8327050526994558	T	T	T
0.4230962035479418	0.4421704189792598	0.6470495223835321	T	T	T
0.3049970932421034	0.4695174222547342	0.7900194595287695	T	T	T
0.2799992694008658	0.4459661155297704	0.0153270319380025	T	T	T
0.1219324810010704	0.4369251600412879	0.0148095373044420	T	T	T
0.0640766994389184	0.4684808595047963	0.8031495462349744	T	T	T

Structure files (CONTCAR) involved in this work:

0.1781161692197595	0.4347523537800683	0.6661054237319689	T	T	T
0.4154353330349992	0.6735723535630650	0.6677019827502191	T	T	T
0.2997133128468344	0.6277693629654710	0.7999204002881671	T	T	T
0.2666244399578558	0.6694684101947881	0.0183346260362283	T	T	T
0.1109732943016529	0.6730054749362647	0.0102999451005930	T	T	T
0.0636930309613277	0.6273258428241585	0.7963362677901722	T	T	T
0.1785208332492418	0.6718610735121403	0.6638160959248361	T	T	T
0.0727419614279323	0.5592826375217291	0.1499377507038636	T	T	T
0.1915792235541852	0.5314019459090904	0.2910973808117350	T	T	T
0.2143525149601093	0.5553545798050004	0.5175842476692110	T	T	T
0.3733105225192730	0.5656003071659200	0.5152918683309213	T	T	T
0.4293028271186244	0.5323461364690779	0.3043583434989893	T	T	T
0.3176062383065232	0.5657541095491969	0.1651534244930267	T	T	T
0.0842418010416653	0.3276775704721847	0.1658895694135770	T	T	T
0.1978502618588604	0.3732154556699769	0.3009372420525005	T	T	T
0.2303571607568727	0.3313385117894148	0.5189455208239142	T	T	T
0.3858984255424248	0.3278809706183379	0.5082911562541478	T	T	T
0.4305340540154919	0.3746063234311502	0.2945072833784557	T	T	T
0.3168745175602665	0.3299837542792304	0.1624980489086175	T	T	T
0.3593143850316555	0.0706844972440378	0.7224464513378651	T	T	T
0.3158418315753370	0.0526643890468178	0.9069485871363659	T	T	T
0.2017145697678839	0.0508458284766352	0.0094733523721477	T	T	T
0.0927568726499361	0.0710091341580867	0.9009618059036578	T	T	T
0.1035246262958984	0.0652222323152064	0.7038481187649624	T	T	T
0.2295591580844539	0.0538341362884087	0.7589518202269916	T	T	T
0.3602353323460978	0.8285326894338731	0.7525155539862576	T	T	T
0.3004299468593727	0.8631614009586989	0.9190996109023660	T	T	T
0.1885595862790620	0.8510781673433836	0.0225050677256888	T	T	T
0.0884844402089398	0.8326445930867695	0.8959447145850453	T	T	T
0.1021448215823345	0.8426700394256290	0.7003804995753855	T	T	T
0.2287598629941109	0.8500917059722927	0.7544558494912867	T	T	T
0.3145034758845779	0.9517719944292808	0.7730206056033483	T	T	T
0.0879406870049291	0.9531714567689928	0.8104261472486396	T	T	T
0.4332781484707631	0.1273035820753783	0.5819957718016565	T	T	T
0.4122047488466363	0.9963969131427917	0.5741018106204432	T	T	T
0.3927260531295627	0.8645392245112399	0.5676340752014007	T	T	T
0.1953980087107706	0.1387248808552245	0.6150490346800990	T	T	T
0.1893789274447100	0.0060990433937716	0.5827881770650040	T	T	T
0.1944414334739600	0.8725655006614869	0.5638038059926148	T	T	T
0.9877701957717743	0.0413029110655704	0.7870585683678728	T	T	T
0.9851172097586400	0.8703088418661777	0.7849566976518301	T	T	T
0.1401617502115667	0.9317161441124953	0.2208134253231286	T	T	T
0.1831166019445310	0.9501638928598595	0.4055942460408236	T	T	T
0.2969666029785269	0.9489199038917032	0.5086708033429880	T	T	T
0.4067533795352380	0.9314936751487376	0.4017257698452853	T	T	T
0.3962159361185105	0.9356544456315670	0.2043149074904033	T	T	T
0.2699066350470302	0.9467409846854267	0.2583688778218252	T	T	T
0.1405565152428693	0.1738056474185825	0.2506015660548883	T	T	T
0.1966509082635717	0.1374471080257110	0.4193981415730320	T	T	T
0.3103242802930188	0.1498308543539774	0.5173456438053989	T	T	T
0.4132508842609473	0.1679796601839669	0.3950582405238869	T	T	T
0.3971663403370532	0.1591719927779071	0.1996785478721360	T	T	T
0.2717500478542766	0.1525408561817416	0.2585817959052329	T	T	T

Structure files (CONTCAR) involved in this work:

0.1863207379313899	0.0502361016806784	0.2704734077153993	T	T	T
0.4152564160540617	0.0481303253669902	0.3078870670661931	T	T	T
0.0650300214687635	0.8740563894055999	0.0825854686598832	T	T	T
0.0854690944196518	0.0048547189956169	0.0723339451375982	T	T	T
0.1065457171109412	0.1365830501979102	0.0675100337430797	T	T	T
0.3053307321395833	0.8617053655562120	0.1146298810134609	T	T	T
0.3102380083464386	0.9943121878030245	0.0823690378109353	T	T	T
0.3027900214297340	0.1280766336256960	0.0670951122830625	T	T	T
0.5125279793189480	0.9558712748063881	0.2878789220766807	T	T	T
0.5158252799055297	0.1330296529707634	0.2799507280663499	T	T	T
0.6390000921069553	0.5601633293444533	0.2829042479178211	T	T	T
0.6935288627051320	0.5751774048469626	0.1060960435097319	T	T	T
0.7943375124268054	0.5605341737375109	0.9752886940523978	T	T	T
0.8941840202096957	0.5754330513243237	0.1047518646640062	T	T	T
0.8880805793974796	0.5443570907427445	0.2998905418162436	T	T	T
0.7630269300812190	0.5226253704126890	0.2539100637672533	T	T	T
0.6379603758189003	0.3345680206624896	0.2620665540739798	T	T	T
0.6908410112096961	0.3359500664335865	0.0830734516231920	T	T	T
0.8080948760209744	0.3517202789852866	0.9916749125146949	T	T	T
0.9133563603295514	0.3265877561442465	0.1061822151975167	T	T	T
0.9044349499024229	0.3579972762790769	0.2992595705422538	T	T	T
0.7651221576388344	0.3701373245961202	0.2421741161158534	T	T	T
0.6671110060702483	0.4503154589066217	0.1753617398012870	T	T	T
0.9218111236237145	0.4529751698733250	0.1612390648776562	T	T	T
0.5690189646563992	0.6269681120278278	0.4154023732693000	T	T	T
0.5848456919814571	0.4962822498103757	0.4397765517472184	T	T	T
0.5854958952530421	0.3622481686060714	0.4415852104376299	T	T	T
0.7972031892186139	0.6306232289623991	0.3649519498838619	T	T	T
0.8009601309049499	0.5117914335453216	0.4464732277208041	T	T	T
0.8222615931847806	0.3800864655383510	0.4416922815075631	T	T	T
0.0045040487987874	0.5514855750865855	0.2150938868693526	T	T	T
0.0203354723334555	0.3696751216940491	0.2065919949497855	T	T	T
0.8548830175065295	0.4341161365465893	0.7849272469186765	T	T	T
0.7920462647990726	0.4360086108494818	0.6094642664914689	T	T	T
0.6974217126499574	0.4290140446805758	0.4666336217387705	T	T	T
0.6041544271849361	0.4294287310345208	0.6090833542576644	T	T	T
0.6033550395246601	0.4450726236636623	0.8058550440595984	T	T	T
0.7289846606929521	0.4764530069853763	0.7713948880699258	T	T	T
0.8610955010948310	0.6803421455286185	0.7528206702441478	T	T	T
0.8155243695207475	0.6428253085844609	0.5588998893800994	T	T	T
0.6919781260423622	0.6480177865403122	0.4859926686646774	T	T	T
0.5858742655322116	0.6696726067308409	0.6008707505795527	T	T	T
0.5959274646595006	0.6596787336802187	0.7968971091937699	T	T	T
0.7210025476348320	0.6475759512509938	0.7347301748543713	T	T	T
0.8275916611878055	0.5490628199186726	0.6907836575511064	T	T	T
0.5817980205771673	0.5493106127297348	0.6841929051554031	T	T	T
0.9298232262313062	0.3769656121179136	0.9231680298921150	T	T	T
0.9109673059948115	0.5086498294552994	0.9319049559686741	T	T	T
0.8984423693399541	0.6412251412593802	0.9357836689817296	T	T	T
0.6970361207218662	0.3732608150679837	0.8914361805080351	T	T	T
0.6774800741700731	0.5008774236116221	0.9479801512884451	T	T	T
0.6895806143303707	0.6353097881334975	0.9306387105839482	T	T	T
0.4906980670095631	0.4523364781061296	0.7116951915617722	T	T	T

Structure files (CONTCAR) involved in this work:

0.4804362785579353	0.6330386576551891	0.7084836795151045	T	T	T
0.6431906458817305	0.9394489491796245	0.2885734038801918	T	T	T
0.6991548156268920	0.9323312234475354	0.1106012859302311	T	T	T
0.7998081255050040	0.9453567943297918	0.9799195091890257	T	T	T
0.8982433713609765	0.9292741364065665	0.1125961817285836	T	T	T
0.8974811958709005	0.9490190621806152	0.3098248865360754	T	T	T
0.7711049412903849	0.9680962967402562	0.2669473014469315	T	T	T
0.6411326980984445	0.1727145217170317	0.2545572428965924	T	T	T
0.6956678498977193	0.1578484008284712	0.0794451875455585	T	T	T
0.8100188808419182	0.1477333012151052	0.9820391204459121	T	T	T
0.9141126747427208	0.1702930544157726	0.1000136257073770	T	T	T
0.8965478835576950	0.1567950448593766	0.2963985126961226	T	T	T
0.7709880949024325	0.1421910386808229	0.2423229336737742	T	T	T
0.6787871808119619	0.0515554401389362	0.1962825542520351	T	T	T
0.9189221414218035	0.0500749777235594	0.1817703327934265	T	T	T
0.5696354881919166	0.8757970987804040	0.4214888275754108	T	T	T
0.5820469126543438	0.0076597245941982	0.4370121914005712	T	T	T
0.5995091194432590	0.1397257649981454	0.4366937477866616	T	T	T
0.8087265384123612	0.8710846545024487	0.3950538029446337	T	T	T
0.8166440941949070	0.9990201137834610	0.4483630473588902	T	T	T
0.8051616122655795	0.1331247511745901	0.4352639955407915	T	T	T
0.0103096022679305	0.9546321820051804	0.2161956099626394	T	T	T
0.0160475555727808	0.1377844327246885	0.2164301197331011	T	T	T
0.8572084675437317	0.0571197179744069	0.7871124619158310	T	T	T
0.8013076573261405	0.0721873116160980	0.6100072517280957	T	T	T
0.7004434489523506	0.0570855020832863	0.4804574458054785	T	T	T
0.5991449072309740	0.0752711052607805	0.6073115524009088	T	T	T
0.6037171287454313	0.0520739445730286	0.8042790858524428	T	T	T
0.7292445584396381	0.0280859424144358	0.7623978829728927	T	T	T
0.8593430324985403	0.8335422726142624	0.7643922493940279	T	T	T
0.8051433588419022	0.8337810276734959	0.5877297803890978	T	T	T
0.6929700970042586	0.8516875600434072	0.4854177843330734	T	T	T
0.5897144969889165	0.8287475293149376	0.6053675731129269	T	T	T
0.6029273284349179	0.8520466021854582	0.7994890503569471	T	T	T
0.7297472249817164	0.8605169310796518	0.7463522405919506	T	T	T
0.8204919174921107	0.9490119612071558	0.6837034775730771	T	T	T
0.5799702655478390	0.9528759500316422	0.6732483227571906	T	T	T
0.9320231474707634	0.1271642409973768	0.9127732547466749	T	T	T
0.9181905906383496	0.9965725948736731	0.9421195300513311	T	T	T
0.9035268213062845	0.8640413128718499	0.9444709478230854	T	T	T
0.6959850903202524	0.1289290521684461	0.8852590179226210	T	T	T
0.6829323375918871	0.0024154424350982	0.9452272723554506	T	T	T
0.6953942390989379	0.8682924737500270	0.9393053843882406	T	T	T
0.4892865653430476	0.0473736023847062	0.7149179931016136	T	T	T
0.4844009379058942	0.8642210687327352	0.7143557722431901	T	T	T
0.3604664360105678	0.4309521454147036	0.7225697446641096	T	T	T
0.3156431227514463	0.4500957268796913	0.9065232440188504	T	T	T
0.2000183311511842	0.4572981956300607	0.0039159575805206	T	T	T
0.0875970006907524	0.4324272918722351	0.9057024701656188	T	T	T
0.1022799329159578	0.4341965952889941	0.7090442940794353	T	T	T
0.2299919912498980	0.4469835331132809	0.7578638030032517	T	T	T
0.3588309883703393	0.6741475057000890	0.7546141044305128	T	T	T
0.2999623664430499	0.6359858798617000	0.9198831647594132	T	T	T

Structure files (CONTCAR) involved in this work:

0.1881254076171883	0.6485891064320163	0.0221655877662037	T	T	T
0.0887413183139087	0.6682395977767438	0.8942123291004437	T	T	T
0.1016755322233541	0.6573043285397497	0.6981240963345794	T	T	T
0.2275160020888223	0.6510153566502218	0.7561181791435962	T	T	T
0.3140429665354461	0.5498232841673670	0.7705040737795984	T	T	T
0.0820337260783089	0.5481246383437243	0.8083986822036604	T	T	T
0.4326216629993141	0.3764156589624289	0.5762728080685394	T	T	T
0.4126960913652337	0.5075791807093661	0.5764019945814535	T	T	T
0.3844804743227446	0.6379959550233479	0.5684810558967738	T	T	T
0.1926040613373294	0.3620186405523633	0.6158824301458465	T	T	T
0.1839001177884569	0.4951662470363893	0.5851030010735150	T	T	T
0.1956880530025855	0.6281540017489418	0.5646146604625085	T	T	T
0.9843845006697446	0.4570306415757808	0.7866741913726987	T	T	T
0.9837488466376664	0.6361785415172515	0.7818761959023418	T	T	T
0.1351251420047614	0.5701194083664071	0.2257636016486560	T	T	T
0.1805632207127734	0.5503039806860555	0.4076458550368032	T	T	T
0.2946445017467738	0.5465142261348336	0.5104100222156388	T	T	T
0.4036036560906746	0.5710837401638874	0.4036680525502144	T	T	T
0.3935222779436497	0.5652675333518270	0.2073053095977063	T	T	T
0.2659649422285242	0.5549568185987908	0.2579645432470952	T	T	T
0.1399999710175660	0.3262766185891309	0.2537854808753486	T	T	T
0.1966191513622488	0.3651617973075734	0.4209322615833799	T	T	T
0.3088353100140643	0.3522656933846368	0.5218669362235152	T	T	T
0.4069929512741459	0.3314247672022958	0.3913981115842217	T	T	T
0.3936307997815572	0.3465297190268742	0.1944956203035612	T	T	T
0.2702014956848611	0.3501844995698448	0.2578984286068011	T	T	T
0.1830412784485915	0.4511294486016024	0.2713508040486309	T	T	T
0.4107621672268609	0.4529458359419127	0.3129991303204555	T	T	T
0.0642734079327267	0.6249430738212663	0.0789035815005859	T	T	T
0.0831192130686243	0.4932145666160850	0.0807076837232428	T	T	T
0.1150706582924229	0.3635546514499491	0.0667583448786912	T	T	T
0.3043474298128314	0.6387693800717416	0.1151504477160241	T	T	T
0.3096901712189034	0.5055077404787801	0.0846362800020778	T	T	T
0.2956981573113123	0.3728750209872093	0.0641567434887743	T	T	T
0.5092202854163266	0.5421626692850129	0.2913410288529246	T	T	T
0.5104646277956806	0.3663481804344171	0.2780864034871895	T	T	T
0.4358676025255761	0.7501365016598933	0.6401097521233127	T	T	T
0.1882846048646595	0.7504034096005013	0.6355383382723727	T	T	T
0.2759166656541787	0.7500054440198989	0.0172855822871380	T	T	T
0.1026593827076220	0.7498022227857326	0.0484197753376960	T	T	T
0.0634255204738921	0.2512708184414718	0.1384068582052129	T	T	T
0.3091238363256480	0.2509517881991819	0.1355402219294935	T	T	T
0.2218538263601589	0.2506941672641797	0.5175498073025876	T	T	T
0.3949789039637577	0.2512085469826735	0.5466381553071062	T	T	T
0.5553102076474054	0.2500663002274881	0.3518028183424676	T	T	T
0.8075735575144670	0.2509984900164726	0.3462866225291480	T	T	T
0.7271450359044926	0.2499280489359756	0.9424592732696591	T	T	T
0.8917990408035259	0.2510959082679153	0.9475035961261923	T	T	T
0.9456658412250565	0.7533123562903090	0.8594130005569892	T	T	T
0.6862439786677956	0.7529475886486482	0.8468669569347693	T	T	T
0.7757607859911473	0.7487675630112598	0.4451802617680581	T	T	T
0.6096799948065972	0.7506539298124956	0.4487883251533419	T	T	T
0.9357218136135529	0.4946217822916743	0.5061740124323181	T	T	T

Structure files (CONTCAR) involved in this work:

0.8207545039124369	0.3345799116090993	0.3250439184709634	T	T	T
0.8007630188210331	0.6356604338680294	0.6926365986984220	T	T	T
0.9260765091569120	0.3923982249113936	0.4624112547167405	T	T	T
0.8710674526980794	0.5556208447969175	0.5524678646971596	T	T	T
0.0064151884993895	0.5103528224499624	0.5080274996454796	T	T	T
0.0333760325600163	0.4704224171756241	0.5480735561993946	T	T	T
0.0254857655540691	0.5138207415092717	0.4309641915680301	T	T	T
0.9841262078075387	0.3499139697127024	0.5021417847355913	T	T	T
0.0159960606596390	0.5585299220945354	0.5457531513854204	T	T	T

Figure S6(b) IS as same as Figure S2 Cu/ZSM-5**Figure S6(b) TS**

Si O Al Cu C H

1.0000000000000000					
20.0219993591000005	0.0000000000000000	0.0000000000000000			
0.0000000000000000	19.8990001678000006	0.0000000000000000			
0.0000000000000000	0.0000000000000000	13.3830003737999998			
94	195	2	3	1	4

Direct

0.4210347115187439	0.0537548747395575	0.6404277718687533
0.3008597917610476	0.0256628267385770	0.7852952023765843
0.2793475603061978	0.0635401776746175	0.0051375829015472
0.1193431682811342	0.0632092348124934	0.0049265688662701
0.0653332705792951	0.0244953330994191	0.7929368683555774
0.1769806234346639	0.0510260505087604	0.6449394912259810
0.4210802135310484	0.8261464063436892	0.6644032710099731
0.3014721039859197	0.8682818462608272	0.8032533720546546
0.2700730876830247	0.8269467614925445	0.0248698282636936
0.1158689985706166	0.8252239443657094	0.0165585023976759
0.0628731532188058	0.8635193907335367	0.8018454560878087
0.1797626951269980	0.8272442744492537	0.6677191278984980
0.0759047369336720	0.9426087963957098	0.1453448742130642
0.1980573524288841	0.9709981953109343	0.2872781880794935
0.2189356942101574	0.9328397436979132	0.5072443710675977
0.3784564342072702	0.9293932822259684	0.5081756582643824
0.4300778738455420	0.9695209241825219	0.2991683208719831
0.3227777526547227	0.9466630162174128	0.1452942957850752
0.0794480532785724	0.1696640127816485	0.1598872104541327
0.1973181113293784	0.1284632205116580	0.3038767104467469
0.2287131550015070	0.1713195966535055	0.5218513966459939
0.3835984178344984	0.1720735572172148	0.5079495622627880
0.4345050823074564	0.1264973749357184	0.2989187573597964
0.3189343662500750	0.1679702357505087	0.1676814213679698
0.5731884837259817	0.5550106017441249	0.3556718591956013
0.6940166773264999	0.5240208497723523	0.2204505299215360
0.7118067034636028	0.5466231797820693	0.9896329296147196
0.8684446571447196	0.5618157669539254	0.9868003726416199
0.9296117677271362	0.5289420913969689	0.1966843368089226
0.8210098529781068	0.5601927456039154	0.3454402178949333
0.5807764286977637	0.3242200069456626	0.3286234194133439
0.6976932552475390	0.3669563736468918	0.1988502587071140
0.7321432379272689	0.3293836010117023	0.9821264297316111
0.8867789018570448	0.3292745448382458	0.9944206030037223
0.9354717586175184	0.3705255399323333	0.2053429127211091

Structure files (CONTCAR) involved in this work:

0.8187696157025953 0.3271772104251625 0.3335336081275156
0.9231620214743013 0.4430315147369013 0.8541238924826758
0.8055354944478007 0.4652097097326003 0.7109085280905756
0.7795335157585629 0.4403442089810249 0.4879498145720919
0.6208662021804346 0.4314207139038672 0.4859648644834044
0.5660263320204397 0.4619180750160260 0.6961300406713565
0.6769735703201663 0.4327091196299628 0.8375630997144601
0.7976294947871860 0.6218576253729694 0.6961946551015573
0.7650626004876233 0.6709306854340392 0.4763019768800783
0.6102950843104268 0.6738340614561177 0.4846090094732901
0.5712873012469518 0.6201925042733125 0.6975425498659528
0.6783577430521592 0.6640427321002923 0.8427744098095190
0.5768588148126534 0.9412478498203611 0.3510777554287898
0.6925737213939887 0.9710352340134197 0.2064402681266684
0.7187399047586149 0.9496603141675145 0.9814071986987175
0.8762311741919685 0.9474659085209109 0.9852276407778479
0.9313747672411670 0.9686010141988362 0.1975350431007494
0.8154714311799037 0.9332874443356304 0.3305421142382365
0.5796593325214617 0.1721583135580788 0.3270467805988397
0.6982832848558078 0.1284584720867467 0.1972433946192347
0.7346428464088020 0.1676404411566325 0.9790841880908436
0.8900792411250137 0.1760089309637060 0.9813460776151004
0.9367585045606162 0.1267750518307379 0.1965721092021016
0.8216108821505269 0.1719340502079748 0.3300319569812642
0.9233891665485708 0.0650070368442049 0.8458816280027804
0.8056624281252762 0.0312933156527999 0.7032736219812182
0.7832076717324041 0.0560456632942223 0.4795882058866887
0.6232208200639887 0.0667172485993066 0.4844946326980258
0.5651394640168197 0.0337395827022005 0.6956879627544376
0.6804128565814638 0.0652324671885983 0.8272249124149735
0.9102445934425416 0.8288332628051491 0.8328865242819470
0.7997252776922174 0.8735560578882879 0.6922879220698299
0.7679958586618783 0.8276865944327915 0.4781573666317456
0.6078220128519619 0.8247346188725149 0.4935468353257665
0.5631423198129323 0.8752425744811910 0.7084987550450538
0.4207737230906930 0.4434178377811739 0.6421753643220712
0.3004644617177530 0.4709607714456449 0.7874921191543101
0.2795116052200843 0.4318729499669996 0.0063550281142133
0.1198969558317636 0.4311542145038660 0.0070146510429985
0.0683470835074300 0.4707814820275862 0.7973854961551375
0.1768752753001344 0.4477733694630414 0.6456445328377252
0.4246156495866262 0.6701395639641402 0.6623988084601329
0.3058218304601061 0.6274880830953399 0.8041482222500765
0.2705822402368008 0.6707919980018333 0.0244019286955467
0.1174502022724325 0.6720715285485157 0.0121642836199618
0.0677774371777956 0.6303068061014562 0.8000922716442356
0.1839861618225847 0.6687293590516444 0.6631758982909808
0.0750321927938459 0.5550074557844851 0.1389653257500712
0.1961413818716587 0.5260036485349243 0.2821651419709559
0.2181954232783735 0.5640540759730690 0.5034585377878886
0.3773851667803088 0.5664016939793702 0.5071971801582623
0.4295847755568826 0.5269424850303929 0.2980082235350800
0.3225057345219760 0.5504385655715782 0.1427886000878652

Structure files (CONTCAR) involved in this work:

0.0783007832070083	0.3249910476522633	0.1632431515029492
0.1969129072421179	0.3682296159608937	0.3024202127866912
0.2298788168604327	0.3276712891978134	0.5218706817410046
0.3849639509385031	0.3246832162740402	0.5098598614700178
0.4361608626171623	0.3699091513134280	0.3004136419886718
0.3200062588206352	0.3277180690869109	0.1687175193856613
0.3549631610848746	0.0583008216036956	0.7098906647394079
0.2995901500946221	0.0693659679814402	0.8879927428995800
0.1992543993595528	0.0525574370597324	0.0177696649045315
0.0985264088401207	0.0632041739878981	0.8879854057355555
0.1019743646595783	0.0470238389798255	0.6902449555302035
0.2276878648603572	0.0284431845596418	0.7335842313181203
0.3563449794529131	0.8282949037867787	0.7374523419823371
0.3019114406268334	0.8366726784480785	0.9146151009041745
0.1924910688277731	0.8519398474981179	0.0252228675029589
0.0931380840769008	0.8283575912674394	0.9009276411091731
0.1024828414580113	0.8363285680412365	0.7036940482662736
0.2277136926437736	0.8592019579074220	0.7539366587097237
0.3196784547928442	0.9478158297986022	0.8089667053512580
0.0713319078293171	0.9442045384887949	0.8115822808382973
0.4286647580575714	0.1228511850265460	0.5767182719574905
0.4176650532990530	0.9909652266404396	0.5625489371232769
0.4018317067750811	0.8583890894598973	0.5562376839718300
0.1915084951295879	0.1271856498860258	0.6072493112018490
0.1828099217039341	0.9999605369412078	0.5506155528255073
0.1910657934423690	0.8656967730475099	0.5619686806479941
0.9875205948415285	0.0451245937803738	0.7786498207377628
0.9850850782202577	0.8424078739781793	0.7916876657079477
0.1408997578682520	0.9388087571810781	0.2165983844302980
0.2016817002881198	0.9269965306945702	0.3891892929094994
0.2988548877443925	0.9400733588959590	0.5256345068030807
0.3961633178875815	0.9271601843348094	0.3899229745992118
0.3971255653190874	0.9492820052099135	0.1927494365465497
0.2696768529190813	0.9680309783227223	0.2313061962245603
0.1437834407484341	0.1658697892189986	0.2326583161671514
0.1924996982183335	0.1618606566852067	0.4140333577683815
0.3061474603106402	0.1467824107105857	0.5119469759015126
0.4101883099299566	0.1715763582666434	0.3933700661304669
0.3962316971617151	0.1520490320463349	0.1982347582739160
0.2717037687756255	0.1387753023553174	0.2571395721119918
0.1801141773383747	0.0488968751796532	0.3117494850554917
0.4169896389210597	0.0485864213061190	0.3225904087060442
0.0678586574661850	0.8714927091396317	0.0862766593902161
0.0812797555754511	0.0026718025261936	0.0633572091529107
0.0963987520359702	0.1346777144926198	0.0528523905910114
0.3106913232270992	0.8705370447748459	0.1067396814089383
0.3176069544112373	0.9987397797361218	0.0520508927963917
0.3014032042703531	0.1323231405492417	0.0616002387916135
0.5090435439819391	0.9535715099442471	0.2879282862139908
0.5145724970304729	0.1338887612738934	0.2818235337910671
0.6383457474985498	0.5640420012049073	0.2844466556645840
0.6855145844487744	0.5454903885360012	0.1039222988051113
0.7915857108625651	0.5350069559175396	0.9807193740872795

Structure files (CONTCAR) involved in this work:

0.8974249793589253	0.5656144786994303	0.0993076283800436
0.8954640406260357	0.5571112430451911	0.2982072273190108
0.7684527718293721	0.5443766291085474	0.2555938028589226
0.6392199276500906	0.3203257862119332	0.2447799575282920
0.6941768099052551	0.3609915777329378	0.0784875538825377
0.8095120365727966	0.3540131939926591	0.9868429104364711
0.9109452147450848	0.3267074005019320	0.1098708620030510
0.8960261113545651	0.3440451209873731	0.3042085246081321
0.7712332682699065	0.3431684695496111	0.2368891173557972
0.6829080356383170	0.4438473860835985	0.2339016197745202
0.9167888160936072	0.4487164096882008	0.1852848346517391
0.5628837005666428	0.6219469686399524	0.4233247204761973
0.5805490515213191	0.4907066303429679	0.4290721901112460
0.6104484915852660	0.3608539127213538	0.4275791524352741
0.8094701860268601	0.6351225157321719	0.3895782806966792
0.8139074634867278	0.5044072097501270	0.4332512747353953
0.7955640995230171	0.3714052994949000	0.4285380919646965
0.0085186628938622	0.5452132921286507	0.2063141821269851
0.0155881869588497	0.3612803770995934	0.2200656082350987
0.8591857434403601	0.4275200019473739	0.7828857001466906
0.8101666338230499	0.4333116082362567	0.5995719938549970
0.6992106867157941	0.4521321194021664	0.4918121464150212
0.5900557519923946	0.4219618324810989	0.5966877689883534
0.6023330146305133	0.4277052015134797	0.7919050629001190
0.7298235224573377	0.4540845196686698	0.7515721197308629
0.8556141366162756	0.6723846629393834	0.7277280775046704
0.7753852525466075	0.6320710760983609	0.5809792119108117
0.6867178620202681	0.6644818487058529	0.4463865447638591
0.6056120369671004	0.6596493900678073	0.6043430419238136
0.6033825760903651	0.6484398346775095	0.8017453327751787
0.7313604944776828	0.6303894721705485	0.7669277910931498
0.8233424638905461	0.5445357863330041	0.7101390789671567
0.5873785658838924	0.5405361508721814	0.6865397626366984
0.9334639578053732	0.3802626093656729	0.9306604083313359
0.9133804335315319	0.5111383608493891	0.9199475105945433
0.8778760889618846	0.6356446206143740	0.9328859107485659
0.6968166758649423	0.3598812676934178	0.8830707728335482
0.6743178715125631	0.4903929538148359	0.9243678638933559
0.6878917996215564	0.6231486418014159	0.9530120450622367
0.4861011584587888	0.4542407347202216	0.7121962434829020
0.4911836356843745	0.6312005075931325	0.7010760934621437
0.6381250371695265	0.9302970876552087	0.2724784352531783
0.6803562398530238	0.9556153965377739	0.0884843693793179
0.7974501288532083	0.9656743965509651	0.9951675195081424
0.9074591260436502	0.9324276798501498	0.0945857980866310
0.8925095019020152	0.9349490765417593	0.2918487794060772
0.7676724324965052	0.9459070423563649	0.2334827699083885
0.6375569456309116	0.1729714995705592	0.2418324345110348
0.6992633780784010	0.1347857024145579	0.0767452737911064
0.8134912750389918	0.1481375002556681	0.9779874663692038
0.9187121187212146	0.1651159897875794	0.0932121954487453
0.8976149230025670	0.1621838436220568	0.2891633959452061
0.7700802525833780	0.1539820317755920	0.2394433335503094

Structure files (CONTCAR) involved in this work:

0.6853503181252810	0.0507812617576745	0.2301279914694250
0.9144292622244322	0.0483253986882968	0.1908841934028692
0.5671853054834437	0.8756874712350777	0.4210730813551410
0.5907748773771898	0.0054237710713684	0.4219825902518042
0.6076756125638000	0.1369233029845794	0.4277387718701761
0.7995195629093864	0.8596214875862709	0.3763847613354270
0.8039069267952877	0.9915852591155224	0.4126976209111406
0.8080872831337867	0.1247004128957803	0.4261691021200499
0.0104400158360630	0.9547795004589126	0.2147226347355130
0.0169019909604299	0.1321480513157140	0.2149039196297977
0.8582490665847873	0.0705976221915339	0.7746205944142938
0.8195166453552328	0.0512345995199258	0.5876330673566414
0.7030640319470775	0.0562019306436747	0.4940604300023018
0.5892277140066741	0.0706087614116733	0.5935839795742688
0.6038354511658843	0.0689529967106636	0.7889540047617303
0.7300148094726505	0.0542740496607860	0.7323337244251102
0.8617000213244526	0.8294742058062151	0.7366100529813632
0.8010845827362064	0.8678768078518464	0.5709932907857492
0.6874611747193631	0.8366355948939871	0.4775610456282674
0.5883301371800700	0.8344142629348726	0.6095035030549580
0.5975348452542683	0.8465723208530000	0.8079427956073444
0.7299435383445777	0.8486631908705323	0.7359723954145250
0.8154884624493633	0.9516274047123784	0.7224268553768887
0.5818724484161778	0.9542854210403064	0.6900006425872933
0.9356854081507979	0.1371438211289000	0.8995200898829929
0.9145228861706118	0.0109529573685986	0.9361283485902674
0.8873911669463123	0.8825302527889586	0.9157736872107317
0.6981763473835617	0.1357880357386440	0.8821132594048376
0.6864234205776957	0.0011260324086766	0.9025686004783300
0.7083043410878617	0.8709662687208836	0.9454413830023277
0.4856907372817089	0.0458664282586047	0.7123297871188404
0.4817515307178992	0.8675957432437154	0.7159580654147458
0.3553781116723709	0.4385809289867169	0.7128694159163430
0.2965997466023792	0.4252527838733300	0.8881283923183123
0.1996064673397279	0.4407022800385316	0.0245127622886200
0.1022906133288007	0.4288818112513988	0.8890398439952661
0.1021109469122214	0.4481062138472613	0.6923475039550113
0.2282347160850582	0.4715479047080374	0.7328799170779876
0.3672424847651503	0.6634661334334484	0.7469615804946144
0.3006474361557641	0.6622901329343405	0.9129565933000132
0.1934627310250407	0.6448249182710442	0.0276704990714681
0.1001645717224632	0.6710663230817828	0.8943503237805063
0.1082642386694253	0.6534762301372774	0.6999284293030338
0.2362972244119322	0.6372721804982869	0.7436869285614762
0.3210586460220047	0.5475813083596576	0.8162071235815189
0.0795185831738676	0.5501508834878948	0.8189145196419708
0.4291845822724630	0.3733316674562959	0.5810915048162556
0.4165652594866689	0.5052938170283698	0.5627823881432321
0.3985404830849855	0.6375787515181819	0.5576834011251656
0.1941180577920313	0.3723081376823236	0.6077821307463617
0.1796178412110570	0.5000417038171293	0.5523521720415029
0.1954687606903559	0.6344684276104221	0.5541985090086651
0.9895923664244567	0.4521060871059147	0.7868326382076610

Structure files (CONTCAR) involved in this work:

0.9904638855571976 0.6480474622956302 0.7895668481395365
0.1390697275971319 0.5594617745914670 0.2124132025610176
0.1992499967741212 0.5678656479758519 0.3859260074523976
0.2979288688556515 0.5531158993312645 0.5199625851370666
0.3969775854921786 0.5695596356147619 0.3895910284968204
0.3963006971318158 0.5462913232650758 0.1917355003595972
0.2682162592114700 0.5303868745263679 0.2277183967512644
0.1429779193130532 0.3276278568800214 0.2356811953640793
0.1930600324029350 0.3388498972972361 0.4150637592176201
0.3077306213153837 0.3505556316918891 0.5110273040861234
0.4137986714319846 0.3258956114569612 0.3967142180930335
0.3971274300185729 0.3422195270099458 0.2017828073918694
0.2713639520402113 0.3571260827150604 0.2562874504303432
0.1782254867041673 0.4476313023919803 0.3031873351216320
0.4174284288753789 0.4478480922830270 0.3218186482795287
0.0670618603044662 0.6246156731696793 0.0762170777192787
0.0810800292004296 0.4932373995205199 0.0602686688266079
0.0946655822926266 0.3613712159594329 0.0572940302847958
0.3128962475308148 0.6268870334966816 0.1039611243776437
0.3171926072594684 0.4981950538654259 0.0497174481634773
0.3050814558799177 0.3641965603397365 0.0624058687914448
0.5083390274482394 0.5442513349296692 0.2854421426428887
0.5163750374562067 0.3635910219823490 0.2828815322837669
0.4420213210051864 0.7485464255072367 0.6443310917848553
0.1971181875602349 0.7486605166219729 0.6513934421821851
0.2751283089440783 0.7488456246535983 0.0577140429474239
0.1096998520201791 0.7481183688887945 0.0550737919695280
0.0601730085687824 0.2474248611561504 0.1388013722640755
0.3073837193144298 0.2479776947676140 0.1541148993374938
0.2244460081574554 0.2495229406155896 0.5554446843567465
0.3895567635242072 0.2481358761161026 0.5511895376113526
0.5592335792030860 0.2483003528266292 0.3571316281983896
0.8112202710097455 0.2490847778446245 0.3652806854166689
0.7256606903234439 0.2484906452566440 0.9799007726183291
0.8929802849616356 0.2542858660435680 0.9493905055240029
0.9061670490336639 0.7541807050006932 0.8865820028970629
0.6903325309288525 0.7414768848680732 0.8701204397476121
0.7881563105103042 0.7487582953483527 0.4831125406113257
0.5856004073412194 0.7494102257873614 0.4603645393742445
0.7956374935521674 0.6661593697124103 0.0776739171234642
0.6939132938355775 0.7543681871125095 0.1520546661584678
0.8142720792175248 0.7934483905937253 0.0616726070980360
0.9130585061461215 0.6744418746843256 0.8226259962734239
0.6794945878409464 0.8259059154301515 0.8342505641121020
0.7068171806049290 0.6850162652155048 0.0728244985282863
0.7205896481573526 0.8126466555678579 0.0578517587165348
0.8451473688935304 0.7173905056284489 0.9942000719089520
0.8943600796688348 0.7703918873183156 0.2036618003519902
0.8640268665416796 0.7368273467155051 0.2497001821573589
0.8492371243033391 0.7881376551948827 0.1368536814605785
0.9073292938673323 0.8185809832786787 0.2372777036534696
0.9354080426780053 0.7459940926526615 0.1637595308423771

Figure S6(b) FS

Structure files (CONTCAR) involved in this work:

Si O Al Cu C H
1.0000000000000000
20.0219993591000005 0.0000000000000000 0.0000000000000000
0.0000000000000000 19.8990001678000006 0.0000000000000000
0.0000000000000000 0.0000000000000000 13.3830003737999998
94 195 2 3 1 4

Selective dynamics

Direct

0.4226207352104502	0.0540114333852369	0.6414247976986076	T	T	T
0.3036030387795936	0.0267454608348812	0.7877543717681890	T	T	T
0.2798777533497522	0.0644159065024425	0.0071673274014108	T	T	T
0.1197803733480570	0.0655279087307216	0.0043368787778144	T	T	T
0.0666372480852738	0.0262357740733715	0.7929197684870757	T	T	T
0.1793934263645356	0.0511963718275662	0.6489125866385356	T	T	T
0.4212059981045660	0.8268779519609830	0.6638411882759813	T	T	T
0.3058662817455842	0.8693630348780681	0.8078432220333184	T	T	T
0.2681633699206990	0.8285991671903813	0.0255749045866730	T	T	T
0.1138112026155822	0.8259781880165620	0.0092978965201642	T	T	T
0.0661580547328507	0.8661493963188371	0.7931065691818043	T	T	T
0.1871783559588940	0.8271212654015516	0.6688365189230951	T	T	T
0.0769221135745005	0.9434361477727078	0.1417784419818672	T	T	T
0.1959204803420110	0.9714966371756889	0.2892080654054037	T	T	T
0.2206502869752046	0.9334766191806309	0.5065779868738076	T	T	T
0.3798178245784126	0.9309571202425929	0.5060853818982223	T	T	T
0.4328252929347214	0.9693382078352197	0.2968948711365582	T	T	T
0.3203781688695062	0.9471016657544020	0.1510884032702048	T	T	T
0.0804454716359394	0.1708141836321048	0.1613335687324310	T	T	T
0.1968183748789786	0.1286169465735079	0.3057367423482477	T	T	T
0.2315213932047546	0.1708830662174893	0.5224620910663733	T	T	T
0.3864254560931538	0.1720469723748445	0.5075447251303864	T	T	T
0.4356387582916927	0.1266731336348700	0.2972505283977509	T	T	T
0.3178952233169176	0.1686577233856232	0.1697773928578862	T	T	T
0.5759357052389208	0.5552872828070653	0.3575053111361029	T	T	T
0.6960435183503836	0.5237555653841127	0.2216979347185317	T	T	T
0.7173712964727276	0.5520138637002897	0.9932730611212367	T	T	T
0.8758204001473482	0.5683546199752679	0.9911895306606056	T	T	T
0.9313039304042013	0.5279913880838861	0.2022576811873683	T	T	T
0.8230054865851739	0.5522232642455732	0.3550525476871761	T	T	T
0.5814669965542786	0.3240589950101318	0.3337703097909552	T	T	T
0.6974802189045504	0.3673094686195452	0.1994884215830240	T	T	T
0.7332093530161130	0.3273522076861773	0.9816591144758203	T	T	T
0.8873020797606626	0.3306803139163683	0.9983891666248221	T	T	T
0.9365175118252860	0.3700697127764293	0.2084715669524102	T	T	T
0.8194003865989450	0.3282867690462194	0.3360370613778573	T	T	T
0.9256338827817019	0.4461794311032734	0.8610800625507409	T	T	T
0.8069989794949316	0.4670308673047933	0.7175128228641162	T	T	T
0.7821825520830302	0.4353724382249623	0.4968283088229152	T	T	T
0.6225468196361702	0.4318351454239399	0.4913486734454625	T	T	T
0.5677422223514073	0.4651561847031669	0.7015156611866912	T	T	T
0.6793843841528463	0.4364573360927628	0.8466343562634389	T	T	T
0.7995024548037181	0.6233207397519750	0.7021456111976200	T	T	T
0.7647790667673848	0.6671735574388209	0.4787369904207938	T	T	T
0.6098539214775524	0.6722188212987590	0.4880456121875558	T	T	T

Structure files (CONTCAR) involved in this work:

0.5650169024929701	0.6231531648883206	0.7007994525973805	T	T	T
0.6777607248698779	0.6634450515102828	0.8366005444891748	T	T	T
0.5789197116643825	0.9397286671840124	0.3429639956074080	T	T	T
0.6949226645904096	0.9717830273645083	0.2002937000611172	T	T	T
0.7204650033273019	0.9471552213000958	0.9732916445802529	T	T	T
0.8799336379938958	0.9506333974136973	0.9784210772783734	T	T	T
0.9322701647233743	0.9687149657764553	0.1939381575041869	T	T	T
0.8172740105303671	0.9333982165105564	0.3274537968690107	T	T	T
0.5806969779719137	0.1717091732431174	0.3235477409328920	T	T	T
0.6980891155422451	0.1289666776670134	0.1907683564544660	T	T	T
0.7373519594456103	0.1662887337451291	0.9737404239522359	T	T	T
0.8926249999416502	0.1774176104323657	0.9765497834967283	T	T	T
0.9385936710463375	0.1267841336297872	0.1915014761601383	T	T	T
0.8213402199692470	0.1721337281241827	0.3215468776748293	T	T	T
0.9239445467033168	0.0669303938373398	0.8430636782080347	T	T	T
0.8073464307210724	0.0298972688332140	0.6959431659411540	T	T	T
0.7845859532268251	0.0564096681462604	0.4747967516972547	T	T	T
0.6244355883692113	0.0639906620532295	0.4799448085996752	T	T	T
0.5668715906088480	0.0330707493018665	0.6924641732816073	T	T	T
0.6828782197191906	0.0632359775874164	0.8212425837121914	T	T	T
0.9185986463599034	0.8334035354856137	0.8235826703874616	T	T	T
0.8014383163048522	0.8705307684915331	0.6865396308354942	T	T	T
0.7678100684208307	0.8269762560657585	0.4706444799461257	T	T	T
0.6109158751648838	0.8264383497931015	0.4857188846874105	T	T	T
0.5647190840305514	0.8744844189060967	0.7021291135315901	T	T	T
0.4227554689897043	0.4422392804791284	0.6484460495236150	T	T	T
0.3035351038801653	0.4720586134363052	0.7928862500699845	T	T	T
0.2811094294201615	0.4351290929501532	0.0143754766331420	T	T	T
0.1214197873519335	0.4328002490341659	0.0119088627763635	T	T	T
0.0704479543809651	0.4698262445949043	0.8002537714149690	T	T	T
0.1800955301912582	0.4456759773284379	0.6527647640458693	T	T	T
0.4210346086801875	0.6720415311287947	0.6659117341931052	T	T	T
0.3059666204788281	0.6289564485590944	0.8101007666038603	T	T	T
0.2688748562275010	0.6715561997002898	0.0283914383536584	T	T	T
0.1150496196934462	0.6727918958517414	0.0114436524535927	T	T	T
0.0665621280880359	0.6292633943257879	0.7975017694499904	T	T	T
0.1861622335278417	0.6685818920046351	0.6703258305702682	T	T	T
0.0762075459948040	0.5563333900164869	0.1430662808764834	T	T	T
0.1958006887291091	0.5269297103826396	0.2888780232529935	T	T	T
0.2199811237821763	0.5619733141049835	0.5086856861631949	T	T	T
0.3794843801821536	0.5646540065905953	0.5108762067801592	T	T	T
0.4331615251808122	0.5279640234547557	0.2999291502553764	T	T	T
0.3218384240006271	0.5541068478855264	0.1536551531460778	T	T	T
0.0797902559086834	0.3255174548700567	0.1676769351590958	T	T	T
0.1974643973709752	0.3689061475016397	0.3075992772582890	T	T	T
0.2328904351407636	0.3276370737997716	0.5257582623985438	T	T	T
0.3878120790304785	0.3249872964809654	0.5127589652598170	T	T	T
0.4380696099798158	0.3701517506278098	0.3012350096706783	T	T	T
0.3199547047775327	0.3280132475946961	0.1736080718166707	T	T	T
0.3564361770107961	0.0600762613734009	0.7107710320091221	T	T	T
0.3039241121252838	0.0691749943770738	0.8915650641539933	T	T	T
0.1995694889766342	0.0537433471000872	0.0142951230728458	T	T	T
0.0971502174962388	0.0664806422426830	0.8883878689700964	T	T	T

Structure files (CONTCAR) involved in this work:

0.1036905872838842	0.0513007680494749	0.6919092910129341	T	T	T
0.2292561517365553	0.0296090813493678	0.7393823721500834	T	T	T
0.3605748689870889	0.8280329027085612	0.7441785168595005	T	T	T
0.3069224090103050	0.8402864829288156	0.9207798680294207	T	T	T
0.1906853890625475	0.8524618665243384	0.0134746938155088	T	T	T
0.0878524080164927	0.8275360691071131	0.8948896888191651	T	T	T
0.1094990442801540	0.8397306623456346	0.6984779473484409	T	T	T
0.2322204243224561	0.8586597890119306	0.7587578879431519	T	T	T
0.3238408165336540	0.9489704388873488	0.8087969280060368	T	T	T
0.0770503597178519	0.9461448228757837	0.8101877177921084	T	T	T
0.4307713261786344	0.1227695436397343	0.5770515288621614	T	T	T
0.4187920983632830	0.9909277034609907	0.5642782303923637	T	T	T
0.3958140590451448	0.8593013956176812	0.5586494111769325	T	T	T
0.1965925954932644	0.1261500065372088	0.6089125161092769	T	T	T
0.1833962181799384	-0.0029543700863472	0.5583568240949845	T	T	T
0.2031890225689549	0.8634825399250303	0.5628985880228569	T	T	T
0.9880030885241264	0.0432810119517297	0.7782793744678915	T	T	T
0.9891733943218225	0.8478792352663824	0.7677322648232727	T	T	T
0.1422753903627191	0.9388385854555442	0.2126139966099437	T	T	T
0.1948831508020325	0.9279164692383022	0.3917541619514271	T	T	T
0.3004589027070147	0.9472463997493711	0.5107831727774348	T	T	T
0.4044211569471526	0.9262321884469087	0.3909037644085455	T	T	T
0.3959117784617843	0.9470578013767312	0.1942970305931104	T	T	T
0.2700979664411471	0.9692131702165693	0.2406645792490704	T	T	T
0.1441277415326436	0.1679031363807058	0.2354581937876415	T	T	T
0.1929683943072044	0.1610222510763919	0.4166048348259964	T	T	T
0.3088715173349086	0.1472592766689182	0.5091310057688183	T	T	T
0.4136736049691606	0.1713426775663841	0.3933697361353627	T	T	T
0.3953599988171957	0.1529725669953520	0.1989110975177972	T	T	T
0.2713814830511090	0.1379858767550233	0.2590650284015693	T	T	T
0.1770156214862309	0.0495198332200731	0.3115669163047389	T	T	T
0.4187057200889808	0.0484157724099685	0.3199865302621460	T	T	T
0.0678999431516992	0.8734584984102123	0.0803257278212118	T	T	T
0.0818010099931568	0.0049536471435708	0.0625123982644260	T	T	T
0.0985877262683408	0.1369116679190576	0.0540574801033217	T	T	T
0.3030261216591660	0.8717780744743373	0.1135536452305731	T	T	T
0.3156860666070087	0.9998699408848010	0.0587384716619937	T	T	T
0.3003056074903561	0.1338332562683626	0.0631992217606283	T	T	T
0.5117061910040936	0.9553091737696513	0.2796293003422904	T	T	T
0.5151787319406740	0.1351211634500349	0.2766310509694886	T	T	T
0.6419901329223401	0.5647347376009469	0.2874797180317634	T	T	T
0.6971435408731590	0.5573582050130647	0.1103692126585908	T	T	T
0.7971869129844444	0.5484689373297342	0.9775868914067867	T	T	T
0.8968037394953178	0.5666424567990789	0.1080190605251659	T	T	T
0.8969286153156819	0.5533571432204153	0.3054430023205821	T	T	T
0.7704619577904642	0.5298411863744561	0.2679804601283161	T	T	T
0.6430662872093272	0.3210931733000108	0.2553921034958919	T	T	T
0.6940972473333733	0.3506247368008553	0.0817372148496933	T	T	T
0.8096868260212484	0.3547587844867255	0.9905216323731686	T	T	T
0.9108735497280385	0.3256267153286991	0.1141437298163926	T	T	T
0.8969391308403452	0.3450129107757399	0.3079422507447093	T	T	T
0.7721244974659224	0.3534667596509217	0.2433774418473111	T	T	T
0.6756398917225545	0.4453197876023882	0.2162666603331790	T	T	T

Structure files (CONTCAR) involved in this work:

0.9188869420063175	0.4482839209411006	0.1860376703417163	T	T	T
0.5622631722148482	0.6233576645789451	0.4214497011346942	T	T	T
0.5844945104804035	0.4929143504377195	0.4346906024521209	T	T	T
0.6064141031324397	0.3615042552128153	0.4350497655158896	T	T	T
0.8064180707560029	0.6276990380119084	0.3925114249685810	T	T	T
0.8204265549365670	0.4990881434823488	0.4464361367754302	T	T	T
0.7995946758889120	0.3663695230274667	0.4386122138761416	T	T	T
0.0099515406451846	0.5456771220337061	0.2112129502978935	T	T	T
0.0165210036579482	0.3612010103474109	0.2237914147128259	T	T	T
0.8605645055097663	0.4316367369570796	0.7919446211170117	T	T	T
0.8087571809688491	0.4284174148855152	0.6106679577945981	T	T	T
0.7020749413547427	0.4484381281514722	0.4917429561321843	T	T	T
0.5953441886791658	0.4244069417636864	0.6047010673504731	T	T	T
0.6045794425782161	0.4371157592599575	0.8013049698015335	T	T	T
0.7316906914247271	0.4602071729606518	0.7615748480093112	T	T	T
0.8505684041385239	0.6734740815975534	0.7535381538179786	T	T	T
0.7904309207702700	0.6426866056343579	0.5860352532718266	T	T	T
0.6862958024961607	0.6481523544459609	0.4681735242744386	T	T	T
0.5925319398533937	0.6661489662780634	0.6062594152215023	T	T	T
0.6007941039090517	0.6503568451914862	0.8026842015235488	T	T	T
0.7263248600877437	0.6257212142050047	0.7578665011468396	T	T	T
0.8260698787907856	0.5457313840757604	0.7070925705238181	T	T	T
0.5835574769338053	0.5444540547620554	0.6848213648085417	T	T	T
0.9340868672257242	0.3841995682820482	0.9394466891439570	T	T	T
0.9188523174687468	0.5160231845160269	0.9245869962354040	T	T	T
0.8910082852924969	0.6442247255717071	0.9499174440127165	T	T	T
0.6971536421447160	0.3615364220488720	0.8856681896187708	T	T	T
0.6815602625354995	0.4889923150760858	0.9408533663722530	T	T	T
0.6870944231513352	0.6239633854424649	0.9487207063890202	T	T	T
0.4884686565293090	0.4525783699350113	0.7177364586836205	T	T	T
0.4848967967314746	0.6318978926895782	0.7121175375654990	T	T	T
0.6404320388152659	0.9300399357388469	0.2646658989437897	T	T	T
0.6856862305317702	0.9572207957291775	0.0822958338433724	T	T	T
0.8000075294892579	0.9631249283526502	0.9799198231480989	T	T	T
0.9066914761318959	0.9326976112232545	0.0908267028811953	T	T	T
0.8940352161116399	0.9344104808274161	0.2879774447561285	T	T	T
0.7699795286405567	0.9476259396104049	0.2304107587630425	T	T	T
0.6380098179608348	0.1737511703199460	0.2371933451754314	T	T	T
0.6984413495445078	0.1355535775127049	0.0701771680932061	T	T	T
0.8164679854251070	0.1482304882505938	0.9791153421801332	T	T	T
0.9253661589305395	0.1633229772245433	0.0851253469998143	T	T	T
0.8974078941746808	0.1642421745474981	0.2802927778544723	T	T	T
0.7704447745879253	0.1546066562486487	0.2303638996237189	T	T	T
0.6860414611832010	0.0513917991870026	0.2246633284735947	T	T	T
0.9154503029441059	0.0484600819303751	0.1880156308905500	T	T	T
0.5677398870096086	0.8720934362690173	0.4084472840240019	T	T	T
0.5936359487323281	0.0012110414638943	0.4188763232305950	T	T	T
0.6085397443177168	0.1334651152076099	0.4216375720321233	T	T	T
0.8014360552441654	0.8589595571637061	0.3704603250393206	T	T	T
0.8062032263819212	0.9899514766185488	0.4124015436394862	T	T	T
0.8082583906364810	0.1236740001490467	0.4164179158779466	T	T	T
0.0112207082658205	0.9547227259660267	0.2109091708949925	T	T	T
0.0182055819982993	0.1318958414803125	0.2149413496223493	T	T	T

Structure files (CONTCAR) involved in this work:

0.8587789940929034	0.0668263532165131	0.7717239929008285	T	T	T
0.8216506427092254	0.0554513554535264	0.5825420664516319	T	T	T
0.7045067875645407	0.0553868222752313	0.4905050631330030	T	T	T
0.5891036853778427	0.0683396810636641	0.5880711750395143	T	T	T
0.6064260151548838	0.0701176147148529	0.7832701576909328	T	T	T
0.7313284647881581	0.0508695903180984	0.7254819382461550	T	T	T
0.8617499504194088	0.8283772724576677	0.7389122684390137	T	T	T
0.8066250662304716	0.8566285385873162	0.5666947641660965	T	T	T
0.6892841435677427	0.8472124863316922	0.4747730181607823	T	T	T
0.5868184411260255	0.8355138817721337	0.5996166347648484	T	T	T
0.5988635415382931	0.8422915583126004	0.7990576922961848	T	T	T
0.7305803178685424	0.8489661679387431	0.7301770763719824	T	T	T
0.8178490519686153	0.9497914830806948	0.7063048206513842	T	T	T
0.5844508707547826	0.9537369323287344	0.6885598927941619	T	T	T
0.9350343415710761	0.1423020094952845	0.8870776728969884	T	T	T
0.9152494607834494	0.0199062610407982	0.9421713054007366	T	T	T
0.9041920681964767	0.8927805663443008	0.9027194795041434	T	T	T
0.7040910402900912	0.1328682004038854	0.8756701876368962	T	T	T
0.6865973847127637	-0.0010324413469067	0.8959939065509263	T	T	T
0.7077509952314144	0.8689314298529959	0.9411121029286745	T	T	T
0.4876517495965589	0.0454060653685329	0.7122651933941924	T	T	T
0.4832360090306036	0.8688477712423596	0.7096485837889369	T	T	T
0.3575028720602049	0.4367065440008962	0.7195335552388076	T	T	T
0.3010232675436926	0.4303715470216520	0.8971462084891307	T	T	T
0.2009277627014217	0.4437876228177933	0.0290418083302796	T	T	T
0.1037454058419503	0.4297370031578672	0.8940726209908605	T	T	T
0.1047597186307631	0.4439296218271677	0.6973117013483617	T	T	T
0.2303169188861790	0.4704758609418795	0.7410154440116387	T	T	T
0.3615706635958573	0.6701986049952698	0.7477296220947198	T	T	T
0.3056779345074174	0.6591379959030104	0.9222355989530151	T	T	T
0.1916670856326843	0.6461226394202986	0.0219440301216307	T	T	T
0.0929924639242660	0.6699517383462107	0.8957714177880380	T	T	T
0.1087341785950228	0.6559670486777159	0.7007237064442937	T	T	T
0.2328665712104408	0.6379071253025745	0.7591459949124091	T	T	T
0.3253520148318033	0.5495728366451855	0.8130042467475144	T	T	T
0.0821654142143673	0.5496877148772447	0.8155790955890065	T	T	T
0.4312785884716055	0.3725190674144235	0.5865713219845771	T	T	T
0.4178592144978097	0.5046080361531196	0.5700846888218568	T	T	T
0.3960517010452081	0.6364344944160307	0.5629435969121641	T	T	T
0.1993353138793225	0.3707014642133691	0.6152435771159340	T	T	T
0.1826845355806555	0.4980966096699390	0.5597829023269048	T	T	T
0.2021157065241972	0.6318699843669390	0.5645813315695855	T	T	T
0.9913996320465547	0.4518001114845960	0.7915985102474570	T	T	T
0.9888301243692050	0.6434999047263416	0.7811211533688005	T	T	T
0.1411582154696805	0.5606471874616051	0.2148341297566397	T	T	T
0.1944234253760189	0.5675605573347889	0.3939309241964737	T	T	T
0.3000582357847679	0.5488425426807834	0.5137659106590600	T	T	T
0.4052342714681217	0.5687475075551451	0.3963272976490542	T	T	T
0.3969980944606293	0.5538864483111023	0.1987920543398929	T	T	T
0.2701696075744661	0.5324689584147989	0.2415717416471573	T	T	T
0.1436917545533851	0.3273165825856781	0.2417775683945964	T	T	T
0.1939418762851910	0.3412626518900215	0.4212413934519472	T	T	T
0.3105158326382331	0.3505134526710529	0.5123524867400727	T	T	T

Structure files (CONTCAR) involved in this work:

0.4175898258310011	0.3284322056938022	0.4004732858751617	T	T	T
0.3976903960942752	0.3399381491423761	0.2056109667168367	T	T	T
0.2721614691908951	0.3576459249347761	0.2621825927833464	T	T	T
0.1777963920383900	0.4481096418330745	0.3056972077289577	T	T	T
0.4186455891239700	0.4485111801476416	0.3173542104544493	T	T	T
0.0673071412044612	0.6262018155765726	0.0814074382028991	T	T	T
0.0815732695789811	0.4948418841795386	0.0637416798679462	T	T	T
0.0972891766353509	0.3629147776928264	0.0629542737381885	T	T	T
0.3064968504466485	0.6296601292053394	0.1153501801051766	T	T	T
0.3176325243966362	0.5007981347445071	0.0617809174316634	T	T	T
0.3053505082474665	0.3663742484093037	0.0686987497035788	T	T	T
0.5126171808477825	0.5414917250320798	0.2849391578496188	T	T	T
0.5181906511517266	0.3627949528637425	0.2829957940258140	T	T	T
0.4414184436272382	0.7490981599917650	0.6418178301631576	T	T	T
0.2021995430460589	0.7477651276650343	0.6557652332621758	T	T	T
0.2721108458539320	0.7503117286881580	0.0578687481111643	T	T	T
0.1082244768449252	0.7496417664668896	0.0512404612000171	T	T	T
0.0608328237711921	0.2485651322684094	0.1409553498907280	T	T	T
0.3054759553785201	0.2486946916055635	0.1577510917338927	T	T	T
0.2273606434374461	0.2490128130173576	0.5562462137467123	T	T	T
0.3924493458318601	0.2479177106399889	0.5515240722232366	T	T	T
0.5611984581977792	0.2472491348469978	0.3591260322981805	T	T	T
0.8091820322511332	0.2489803956704886	0.3571136346020587	T	T	T
0.7290171480491987	0.2470725580160374	0.9686788811004736	T	T	T
0.8942847074265027	0.2567588003191620	0.9498735193370023	T	T	T
0.9216102835564672	0.7610572226810558	0.8832352488400759	T	T	T
0.6939547316675310	0.7399992550973539	0.8622829282434734	T	T	T
0.7770132665926113	0.7463938115837501	0.4618321635632127	T	T	T
0.5992931146184499	0.7488382568014060	0.4521164623037755	T	T	T
0.7860526478278667	0.6972058800413753	0.0781954056498647	T	T	T
0.6698117912854592	0.7669812841811641	0.1246201912607460	T	T	T
0.8282231476993079	0.8205051089709008	0.0399717739294236	T	T	T
0.9183325818680990	0.6780278526759880	0.8309414379803487	T	T	T
0.6810985840613004	0.8249846329648860	0.8301248642909479	T	T	T
0.6871032889503890	0.6921235480373834	0.0575707434839571	T	T	T
0.7355281332233106	0.8131182360046907	0.0659435347550457	T	T	T
0.8575128718496502	0.7326173766469524	0.9966032031400601	T	T	T
0.8052557872444858	0.6890404052657308	0.1816948966676366	T	T	T
0.8024336326420758	0.6359235830364983	0.2014780914808876	T	T	T
0.8554868515850028	0.8367788472266091	0.0957970957254741	T	T	T
0.7725549723112107	0.7190622370399541	0.2302615674696290	T	T	T
0.8571751629845870	0.7057849318859686	0.1925489232699904	T	T	T

Figure S7 IS

Si Al O Zn H C

1.0000000000000000

20.0219999999999985 0.0000000000000000 0.0000000000000000

0.0000000000000000 19.8990000000000009 0.0000000000000000

0.0000000000000000 0.0000000000000000 13.3829999999999991

94 2 192 1 4 1

Selective dynamics

Direct

0.2672864914172786 0.8305765348550681 0.0252984628691927 T T T

0.3032414515251736 0.8708222016185171 0.8070377401990101 T T T

Structure files (CONTCAR) involved in this work:

0.9403878215489508	0.3764418089030842	0.1875623915810386	T	T	T
0.8845390969317602	0.3253360092615060	0.9906629607618088	T	T	T
0.7300858986969530	0.3259548905941331	0.9738867314982400	T	T	T
0.6928842394974486	0.3712615749806225	0.1864304399659497	T	T	T
0.5749112527485208	0.3288240532517340	0.3303676483625494	T	T	T
0.8118736281184681	0.5540786552419451	0.3367187015488080	T	T	T
0.9292678705935761	0.5304680121297517	0.1880409127074907	T	T	T
0.8743919407586723	0.5728981636687013	0.9855730495397955	T	T	T
0.7139745638988022	0.5673326100612226	0.9834682577089647	T	T	T
0.6900044050593092	0.5265372920226233	0.1985875844595339	T	T	T
0.4194989232193601	0.8271294156102524	0.6688500066577001	T	T	T
0.5751399718869854	0.5557043235908785	0.3530497925686141	T	T	T
0.1812049357215470	0.0618421332313605	0.6666294284635540	T	T	T
0.0677520147561329	0.0310219218671451	0.8022791989403892	T	T	T
0.3174650630410257	0.1723282551232476	0.1724314663976133	T	T	T
0.4357776073034109	0.1277626704466576	0.2983040497634440	T	T	T
0.3872626902838867	0.1740414052623095	0.5115451446276241	T	T	T
0.2323376221617760	0.1706662148473498	0.5251465496459309	T	T	T
0.1965662928338476	0.1300045909917377	0.3079042317291873	T	T	T
0.0812461893241840	0.1728302272604626	0.1685439742210966	T	T	T
0.3196311845144914	0.9387871932062529	0.1663970345425826	T	T	T
0.1220681428832018	0.0647939744550611	0.0134339685199886	T	T	T
0.4341097374827175	0.9694096425970592	0.3016715323528076	T	T	T
0.3785341609918014	0.9360954850549349	0.5136024409716182	T	T	T
0.2184583398989051	0.9414594358120280	0.5186180366754157	T	T	T
0.1949576281043445	0.9705879512760915	0.2956597251589019	T	T	T
0.0776217490867915	0.9417376325153213	0.1504995019253253	T	T	T
0.2817545785915488	0.0590044418237362	0.0188424208331623	T	T	T
0.3151163840703689	0.3302525770814342	0.1701086517988810	T	T	T
0.1912777812495238	0.5293636346534497	0.2928526691736035	T	T	T
0.2160465840982700	0.5583419544909289	0.5156855215364433	T	T	T
0.3745094170705290	0.5654023422490220	0.5134596324112091	T	T	T
0.4300489273078500	0.5309987775705610	0.3033822270562543	T	T	T
0.3177870790107008	0.5606399965127445	0.1629521086420973	T	T	T
0.0841221145828434	0.3257345069977604	0.1656175039011340	T	T	T
0.1951411751568509	0.3709543431713379	0.3081537298500150	T	T	T
0.2310793475209003	0.3311152581685374	0.5262265873998039	T	T	T
0.3855681804950736	0.3281504064450823	0.5103234164974443	T	T	T
0.4317024036515762	0.3738155426654447	0.2974635271207914	T	T	T
0.0739750154455695	0.5590423302348548	0.1476995569489198	T	T	T
0.1772700415331327	0.4407566509189151	0.6641593691115827	T	T	T
0.4163776370980420	0.6735833718707974	0.6655068449460686	T	T	T
0.3036220328534867	0.6297015256664388	0.8071568358750016	T	T	T
0.2664972494693075	0.6701164929607236	0.0248869087242337	T	T	T
0.1123869512798662	0.6735317279843839	0.0099097599227739	T	T	T
0.0632643643895285	0.6280235830520219	0.7984069578494817	T	T	T
0.1818569520863669	0.6705656215964159	0.6705457744405785	T	T	T
0.4211859319141900	0.4428748746542586	0.6483482010503675	T	T	T
0.3037456746375822	0.4709907354093154	0.7923203284405609	T	T	T
0.2796633213738559	0.4426830260815505	0.0153703803745697	T	T	T
0.1214539214114845	0.4360722709549270	0.0142165137193178	T	T	T
0.0638022857916086	0.4695123497721819	0.8047503277283181	T	T	T
0.3055545567076736	0.0303399423625197	0.7961867573173915	T	T	T

Structure files (CONTCAR) involved in this work:

0.6138324912663520	0.8269259055809546	0.4885945095101917	T	T	T
0.5642494320492483	0.8742744909758017	0.6975831989260969	T	T	T
0.6812698797891039	0.8315774545575763	0.8290759874190626	T	T	T
0.9229170711274582	0.0530329969230358	0.8555690572760413	T	T	T
0.8029817996957599	0.0242957302581715	0.7066374146774012	T	T	T
0.7806663813289658	0.0658274795082734	0.4907362875164542	T	T	T
0.6203938978556126	0.0696776340494183	0.4900812563812000	T	T	T
0.5673556878040380	0.0316712351982472	0.6987196454805686	T	T	T
0.6799530717845592	0.0519673965429137	0.8457344417075136	T	T	T
0.9231210328424636	0.8295747711792294	0.8332826089531443	T	T	T
0.8042251924122330	0.8669321917652186	0.6886283156169162	T	T	T
0.7681140614457801	0.8268131811332348	0.4714518238564138	T	T	T
0.8802115181764782	0.9328686350206862	0.9940263747637376	T	T	T
0.9330249237507611	0.9683297610019708	0.2021954401233240	T	T	T
0.8210690881033001	0.9476381171487899	0.3493391429105203	T	T	T
0.5788517696250994	0.1739540933533320	0.3292670004854950	T	T	T
0.6965581799670455	0.1307860775919475	0.1903757590911974	T	T	T
0.7327549314557622	0.1697989806849448	0.9705969016053974	T	T	T
0.8875263330358528	0.1723421082852299	0.9846465180364835	T	T	T
0.9368924184284303	0.1252384929865046	0.1957313940601451	T	T	T
0.8201208331034009	0.1697122260218397	0.3266303840441834	T	T	T
0.5780913045844993	0.9453802313347460	0.3569554117411921	T	T	T
0.6970562474335034	0.9733299371427059	0.2112911899473671	T	T	T
0.7203176148106099	0.9367880952502345	0.9914469656897485	T	T	T
0.1815179841772757	0.8285771372468602	0.6715704454771780	T	T	T
0.0659156501123775	0.8744176285233243	0.8000949830395186	T	T	T
0.7689029896694382	0.6712300986157330	0.4613850108444799	T	T	T
0.6140814640285486	0.6728809374904333	0.4800070350787921	T	T	T
0.5625625776852312	0.6273060460771329	0.6935377358482381	T	T	T
0.6758887356930136	0.6731589056244897	0.8200546483047090	T	T	T
0.1126231184524109	0.8273015323070139	0.0127841035014776	T	T	T
0.9186647846315756	0.4449575079679963	0.8599651412340659	T	T	T
0.8025983330048460	0.4759461789462247	0.7174054960769926	T	T	T
0.7756527690751275	0.4392668654729820	0.4954400311361752	T	T	T
0.6154818083121624	0.4324052736961459	0.4915237294188916	T	T	T
0.5658835014449419	0.4690539023877051	0.7039302030303626	T	T	T
0.6773180968348630	0.4451150069761030	0.8488288871014699	T	T	T
0.9202989314000017	0.6781885091296749	0.8289651857597538	T	T	T
0.4224347591743620	0.0597077721108704	0.6502243218380974	T	T	T
0.8182253201083534	0.3328628132166874	0.3226978715471040	T	T	T
0.8032757945986196	0.6349200122154631	0.6864000090021567	T	T	T
0.8088995581537880	0.5068391634666481	0.4386009155951114	T	T	T
0.8027172849125186	0.6316417373252375	0.3635741559152528	T	T	T
0.5913198609248300	0.3639055470936119	0.4375706444839856	T	T	T
0.5827151169309535	0.4978239676314417	0.4386293937418787	T	T	T
0.5666332080184607	0.6280735415245073	0.4068498917904589	T	T	T
0.9261473534280248	0.4530250642303700	0.1510925916370001	T	T	T
0.6703640532921242	0.4497717439094795	0.1723121689270063	T	T	T
0.7661054064510303	0.3670704956629741	0.2349728937665930	T	T	T
0.9020253259243144	0.3671547566294520	0.2959888708561532	T	T	T
0.9107010756042817	0.3243399868865817	0.1069972327641142	T	T	T
0.8074259985954412	0.3504081168533774	0.9892810626487695	T	T	T
0.6897551252728376	0.3346591649012867	0.0779878966623835	T	T	T

Structure files (CONTCAR) involved in this work:

0.6385632823251257	0.3339061253842700	0.2572090424740912	T	T	T
0.7649841560013495	0.5267897014408642	0.2486406752556259	T	T	T
0.8902014692058984	0.5326761139472420	0.3001446593469224	T	T	T
0.8933098809254049	0.5770268238754511	0.1059631577652355	T	T	T
0.7949188237315847	0.5613081547706229	0.9762914599172421	T	T	T
0.6912489385555117	0.5736453739807361	0.1002210422742899	T	T	T
0.6396286639208556	0.5576698400883622	0.2803981677819617	T	T	T
0.5155535882184873	0.1351695605845293	0.2785228170947588	T	T	T
0.5134586879245218	0.9570437153087193	0.2856159574672515	T	T	T
0.2993408569536847	0.1299168878788529	0.0726077799966623	T	T	T
0.3112629940618936	0.9962010772499811	0.0815495731621752	T	T	T
0.3023794067318274	0.8652427290092959	0.1212324154145286	T	T	T
0.1074657286607174	0.1360415324475570	0.0680233521841678	T	T	T
0.0856722463751804	0.0045067551563486	0.0738993827295123	T	T	T
0.0671724671208443	0.8733207251779342	0.0859985042308396	T	T	T
0.4165596557697804	0.0490688311810311	0.3116923581051674	T	T	T
0.1812706458232823	0.0510429043777763	0.2886698650116781	T	T	T
0.2704439445626441	0.1495682519339496	0.2661708136486460	T	T	T
0.3950030746932104	0.1595344298374912	0.2039161025100310	T	T	T
0.4155472380236624	0.1689436741879094	0.3985738992223225	T	T	T
0.3100588435202359	0.1481003944614615	0.5143300137165294	T	T	T
0.1922638319127238	0.1471427963614055	0.4258488782115433	T	T	T
0.1401157506752023	0.1741554787140911	0.2515666341219238	T	T	T
0.2710768155776158	0.9546190834965071	0.2611514149263643	T	T	T
0.3963659407507304	0.9382323263447384	0.2048561278837180	T	T	T
0.4084823897927061	0.9314317198761830	0.4017701514973440	T	T	T
0.2987392219318482	0.9492200194946326	0.5100233648097993	T	T	T
0.1845938373314784	0.9430452082713350	0.4084753084408298	T	T	T
0.1426014146229825	0.9331390539538665	0.2219534098856848	T	T	T
0.9857351300833379	0.8706135905835675	0.7837665424373738	T	T	T
0.9879652598401550	0.0398211834394233	0.7858298720948346	T	T	T
0.1994772781883508	0.8705497051467963	0.5712064958482808	T	T	T
0.1894770441277633	0.0044275854829968	0.5817837686505117	T	T	T
0.1988581155936592	0.1353671587570545	0.6216969306253722	T	T	T
0.3947278893945609	0.8654552560528822	0.5684700452115508	T	T	T
0.6076796042872018	0.7508802370221924	0.4460945691578472	T	T	T
0.7709384347941636	0.7502347954661742	0.4311019153702318	T	T	T
0.6865152105444186	0.7520459160072358	0.8478005687873611	T	T	T
0.9464728761757903	0.7535339464257276	0.8581985614544897	T	T	T
0.8925624345630316	0.2499841022307637	0.9466160881998672	T	T	T
0.7282320590913544	0.2481999976716356	0.9389755210478127	T	T	T
0.8144324650773672	0.2491107725471596	0.3410315197417722	T	T	T
0.5573371567251869	0.2509121299391472	0.3526036252863290	T	T	T
0.3910745119281964	0.2513744027582026	0.5495884124127673	T	T	T
0.4138249759867998	0.9974675378801499	0.5730638714698773	T	T	T
0.2259200322757967	0.2509435385075943	0.5404956501876639	T	T	T
0.3047443899018143	0.2510894015495745	0.1471433541911533	T	T	T
0.0626456138072820	0.2497841464604890	0.1380424419809703	T	T	T
0.1074795673623396	0.7499515801476089	0.0507544104270422	T	T	T
0.2720333032352462	0.7502022672570505	0.0390570879972408	T	T	T
0.1922525621014009	0.7495827198209588	0.6465538985317705	T	T	T
0.4362560408932344	0.7502009705016821	0.6375766299655865	T	T	T
0.5113932502573362	0.3661993762034366	0.2780526858664837	T	T	T

Structure files (CONTCAR) involved in this work:

0.5095628422520498	0.5402879489398793	0.2860331769740018	T	T	T
0.2942364257798796	0.3714713502656667	0.0701786274742471	T	T	T
0.4319404819530178	0.1285130326215738	0.5863376330493911	T	T	T
0.3133879295201243	0.5047787065426514	0.0749764621351933	T	T	T
0.3006546455406242	0.6349421389822569	0.1212190244650961	T	T	T
0.1127034949751254	0.3630028691023030	0.0666683893902431	T	T	T
0.0808999945820167	0.4927817342386650	0.0775213288221668	T	T	T
0.0656492221178605	0.6257299125227208	0.0795527740373094	T	T	T
0.4116782349956566	0.4518443666501775	0.3167186298792195	T	T	T
0.1751836088660758	0.4492013484273145	0.2895022924691175	T	T	T
0.2690571249012955	0.3541771639252509	0.2647138726278380	T	T	T
0.3925088334052046	0.3453990879409652	0.1995352192343317	T	T	T
0.4103449392976832	0.3304061217437670	0.3951138656975721	T	T	T
0.0885067293809362	0.9523217621669560	0.8141868069626654	T	T	T
0.3085794104308615	0.3547331097562588	0.5174335801410499	T	T	T
0.1915175343320212	0.3548076058975190	0.4262974517402406	T	T	T
0.1399259963243917	0.3245407381734138	0.2529715650189198	T	T	T
0.2667529892925350	0.5418446415738992	0.2536312076519018	T	T	T
0.3933295467079286	0.5616154615553641	0.2056279428618252	T	T	T
0.4050949880820751	0.5713092719008517	0.4019223310479706	T	T	T
0.2958182988044244	0.5454129899420447	0.5087392318068352	T	T	T
0.1832739637585084	0.5594342262684140	0.4046651049160173	T	T	T
0.1370329679606189	0.5672377573366850	0.2224041435228646	T	T	T
0.3186613877306856	0.9499290228176605	0.7887331801140742	T	T	T
0.2296467517610393	0.8511845101704182	0.7641060291105840	T	T	T
0.9840852831858065	0.6371022995490655	0.7804654429409186	T	T	T
0.9843299595164379	0.4559584511718963	0.7892518803531721	T	T	T
0.2006360765585179	0.6295555410347480	0.5693346904808319	T	T	T
0.1815570051237735	0.4964744805313705	0.5758025914796379	T	T	T
0.1953087066442480	0.3667266426779117	0.6213190269594746	T	T	T
0.3841110514666878	0.6377135837344107	0.5672601686956594	T	T	T
0.4136253507769075	0.5071351450598003	0.5744961990032892	T	T	T
0.4316407000263816	0.3757382335264593	0.5806194558117151	T	T	T
0.0804429140364382	0.5488411514747522	0.8169389604887206	T	T	T
0.1042719142792614	0.8423473851516601	0.7037815586566143	T	T	T
0.3204986250839027	0.5507459105426511	0.7891466538655063	T	T	T
0.2299089659854951	0.6473642358246742	0.7628106030639659	T	T	T
0.1047133978278716	0.6545779964176962	0.7010867414538721	T	T	T
0.0876117859625856	0.6706659285715337	0.8951934404916025	T	T	T
0.1888691950810526	0.6462356191737181	0.0173506211001397	T	T	T
0.3055830783636796	0.6460302880429809	0.9253130244649135	T	T	T
0.3606112693706847	0.6744661364935668	0.7536505683817039	T	T	T
0.2269993809753586	0.4596321158933376	0.7558371870565898	T	T	T
0.1005780169043905	0.4398702482914752	0.7052082888306916	T	T	T
0.0905999889874825	0.4300847101940155	0.9029625685642785	T	T	T
0.0866138550381911	0.8317545361278131	0.8986882871677734	T	T	T
0.1996568087291330	0.4565173115460254	0.0100973540586339	T	T	T
0.3112354567586788	0.4401010815034461	0.9038790927740408	T	T	T
0.3554855357681664	0.4327595757053649	0.7184083338823970	T	T	T
0.1895361124218972	0.8537213981936289	0.0181250285808303	T	T	T
0.4847984690196593	0.8630436757593849	0.7174864665204508	T	T	T
0.4886964986573940	0.0476802285534167	0.7171839060014888	T	T	T
0.6996139276244812	0.8683879165246625	0.9340257421162800	T	T	T

Structure files (CONTCAR) involved in this work:

0.6845475165220969	0.0019152605382953	0.9411854784949538	T	T	T
0.6983460419304158	0.1277046085737835	0.8808851545567080	T	T	T
0.3062663288391147	0.8541382733164347	0.9251788888130154	T	T	T
0.9001364620306272	0.8636435654506456	0.9382032542775963	T	T	T
0.9192776370239888	0.9956512017571899	0.9420760708442133	T	T	T
0.9312703650282474	0.1260165993347348	0.9094586363889375	T	T	T
0.5783229510981495	0.9527947476490747	0.6716518274031545	T	T	T
0.8197553505325937	0.9469891078438508	0.6778003643348481	T	T	T
0.7314205177493071	0.8562043350148603	0.7401489610139997	T	T	T
0.6053413507552932	0.8524638328944341	0.7969565730929050	T	T	T
0.5873917867533803	0.8285314085261438	0.6031802409022323	T	T	T
0.6911406622874269	0.8522594676752131	0.4847104343051433	T	T	T
0.8057580997503067	0.8329427733821433	0.5785312175397925	T	T	T
0.3601250927740592	0.8270973002877313	0.7513058349295658	T	T	T
0.8618349848705038	0.8322706791438931	0.7550709317981098	T	T	T
0.7291734330313476	0.0269053564263012	0.7567004876700448	T	T	T
0.6043954533758963	0.0518730923931137	0.8021771029197354	T	T	T
0.5967007048890312	0.0755451851589970	0.6057420977448231	T	T	T
0.7001331973448709	0.0568788110297998	0.4831269969493399	T	T	T
0.8040729243267366	0.0711094424344362	0.6068982248540796	T	T	T
0.8570298606931392	0.0534383070802714	0.7856381567817181	T	T	T
0.2293962870194941	0.0463706376842555	0.7617745959545117	T	T	T
0.0163899369030967	0.1358673878923616	0.2162248171887802	T	T	T
0.1043675200062234	0.0629520094281177	0.7049582155862864	T	T	T
0.0120301034321061	0.9534364732617142	0.2190796952220220	T	T	T
0.8031232810252875	0.1335474399086785	0.4328239705720898	T	T	T
0.8155730318468224	0.9999079688381046	0.4419055684512667	T	T	T
0.8046105947810407	0.8723773405784464	0.3874119178512793	T	T	T
0.6002985780400417	0.1394334503171220	0.4345802255592400	T	T	T
0.5824240584516546	0.0075470799930072	0.4355964908162139	T	T	T
0.5684831971598563	0.8759292365191204	0.4191740584545073	T	T	T
0.9211247219676195	0.0468455253358950	0.1740110827100774	T	T	T
0.6770287173012647	0.0515482086663309	0.1933786601677106	T	T	T
0.7701558939369818	0.1423540287877547	0.2385852653655064	T	T	T
0.0916346971813816	0.0707636315913379	0.9019901002257322	T	T	T
0.8963718231966714	0.1499676468565684	0.2938587205840112	T	T	T
0.9157688858306789	0.1687894513656782	0.0980109507107885	T	T	T
0.8104196429499515	0.1467731459642866	0.9828176715346596	T	T	T
0.6946631153554187	0.1569682547653435	0.0757530505365309	T	T	T
0.6409979867081201	0.1732145842879308	0.2518800323399369	T	T	T
0.7715510304703758	0.9698904120231940	0.2588119096061791	T	T	T
0.8968794035389164	0.9485938110697597	0.3063969931250191	T	T	T
0.9028508905462503	0.9246479702576001	0.1098994010622456	T	T	T
0.8007237925246133	0.9472900354323106	0.9857652570791501	T	T	T
0.6958360976915235	0.9318238623612384	0.1069028483964485	T	T	T
0.2015540858838863	0.0502471533683737	0.0094396260518912	T	T	T
0.6442285333136835	0.9394049715917288	0.2878248829890167	T	T	T
0.3158876309827706	0.0582377622208247	0.9089041144870554	T	T	T
0.4817307095099206	0.6331642889404938	0.7038411288876982	T	T	T
0.4865492096827559	0.4539417169688154	0.7176684792966294	T	T	T
0.6885804294412409	0.6329028556012987	0.9250681143797782	T	T	T
0.6817152120152306	0.4979134025587342	0.9410029702117059	T	T	T
0.6959647773196328	0.3700787986545434	0.8864472511896774	T	T	T

Structure files (CONTCAR) involved in this work:

0.9002469465752451	0.6416193505174030	0.9353974593234863	T	T	T
0.9121898796439837	0.5085285084023558	0.9358749215684643	T	T	T
0.3579557004764052	0.0679641645137686	0.7227618192414240	T	T	T
0.9302356610156267	0.3770710975085858	0.9263996680969071	T	T	T
0.5810768848293523	0.5479435480417896	0.6850816110550049	T	T	T
0.8267780353544142	0.5511493584898033	0.7055712055705645	T	T	T
0.7223467770630181	0.6485647658845132	0.7303893639779816	T	T	T
0.5968206875886545	0.6612842877859626	0.7908708939475748	T	T	T
0.5877830811656348	0.6656616036423540	0.5935862699782615	T	T	T
0.6906940264658771	0.6464588050777534	0.4678923719770653	T	T	T
0.8093137591619515	0.6527379111830397	0.5592521270655479	T	T	T
0.8598603147123770	0.6827105497727685	0.7533345860756875	T	T	T
0.7268035564815583	0.4681924573179432	0.7593153164535932	T	T	T
0.6015686904887313	0.4430812135829659	0.8054928698111845	T	T	T
0.5952191588859631	0.4278186653077899	0.6079488128495392	T	T	T
0.6966465515809757	0.4384444274927554	0.4797649213064522	T	T	T
0.8023483270845025	0.4372051809113945	0.6082277515021239	T	T	T
0.8538103344059549	0.4335947233848268	0.7893948809102479	T	T	T
0.0192816136982645	0.3665090362066909	0.2084627993694982	T	T	T
0.0054726252963266	0.5515972849610347	0.2142244289749846	T	T	T
0.8162807070719229	0.3801745836216334	0.4363681244679679	T	T	T
0.8962856921283112	0.4427938389592743	0.3908928847993571	T	T	T
0.9250739055951519	0.4385901580943235	0.5400729034773510	T	T	T
0.9980381260882756	0.4575172699324511	0.4541379407196626	T	T	T
0.9993557896981485	0.4685489751452894	0.5825987844305909	T	T	T
0.9493485375926797	0.5258475094952099	0.5123318703194161	T	T	T
0.9659643378651249	0.4734433378581671	0.5175059888693688	T	T	T

Figure S7 TS

Si Al O Zn H C

1.0000000000000000

20.0219999999999985 0.0000000000000000 0.0000000000000000

0.0000000000000000 19.8990000000000009 0.0000000000000000

0.0000000000000000 0.0000000000000000 13.3829999999999991

94 2 192 1 4 1

Selective dynamics

Direct

0.2677371500926237	0.8303223110210548	0.0253084666495777	T	T	T
0.3034298628266957	0.8707385704054085	0.8067548414403418	T	T	T
0.9383333324784685	0.3782722614175511	0.1848899998263258	T	T	T
0.8842452732482665	0.3265201657951673	0.9877336465116826	T	T	T
0.7304382669049128	0.3265161489047016	0.9820872638334806	T	T	T
0.6953620436813289	0.3737387370474100	0.1976468035083913	T	T	T
0.5723099676494643	0.3297175085768559	0.3322429499533529	T	T	T
0.8116844159011100	0.5538002618834162	0.3317802826607105	T	T	T
0.9297843706972778	0.5322842837597956	0.1821678744058157	T	T	T
0.8719415465098621	0.5729540705187910	0.9816826835987651	T	T	T
0.7118828651831931	0.5697836713531033	0.9831807594331781	T	T	T
0.6901815885098069	0.5283174788559902	0.1957056188482378	T	T	T
0.4195236702078444	0.8273156362927444	0.6682449088942976	T	T	T
0.5766462067856812	0.5547194455187299	0.3542529236097122	T	T	T
0.1811113156869831	0.0618848190110680	0.6661920186857836	T	T	T
0.0679274436266765	0.0310426688928899	0.8022766920066428	T	T	T
0.3173775743769675	0.1722395179805719	0.1716471332703548	T	T	T

Structure files (CONTCAR) involved in this work:

0.4356252963214672	0.1278157948758425	0.2976505276696790	T	T	T
0.3869972912414126	0.1738979249925836	0.5108569002866237	T	T	T
0.2321245779535673	0.1703977287261802	0.5243824254584964	T	T	T
0.1965134922590818	0.1302033851278199	0.3070877227466838	T	T	T
0.0816789563015808	0.1734557125625566	0.1676005065559564	T	T	T
0.3200732976240997	0.9386628080564903	0.1659414768208395	T	T	T
0.1223259367881862	0.0647806230976688	0.0132268875583000	T	T	T
0.4342230865848496	0.9695183391673200	0.3017348974200265	T	T	T
0.3784227460951417	0.9359830285403770	0.5135618952598274	T	T	T
0.2184427702951766	0.9417753769951609	0.5180362135248114	T	T	T
0.1952160550179418	0.9709109264407914	0.2947380007709407	T	T	T
0.0777690629763416	0.9419003942780338	0.1502262263652122	T	T	T
0.2818600609740031	0.0585330491883419	0.0182525770735627	T	T	T
0.3139404254762042	0.3301573214971235	0.1679652072378909	T	T	T
0.1918586663007129	0.5298641889946176	0.2921244884428709	T	T	T
0.2163697811540957	0.5586105251697440	0.5148012039893111	T	T	T
0.3748389634967309	0.5662795121173417	0.5125295132419301	T	T	T
0.4306657531393444	0.5303710081973864	0.3042125375170009	T	T	T
0.3190556060276227	0.5601806379334684	0.1627861963015387	T	T	T
0.0831881623760045	0.3265384774329595	0.1637297790349839	T	T	T
0.1940147387861025	0.3712137725089892	0.3072643870634334	T	T	T
0.2305652180014990	0.3309411359132966	0.5253338816658453	T	T	T
0.3847853142664620	0.3277889921063231	0.5089575456282228	T	T	T
0.4297395625027448	0.3738451711991006	0.2968205010458776	T	T	T
0.0749361922541358	0.5592902300082561	0.1460988460559769	T	T	T
0.1779971991490128	0.4406307574669452	0.6631596205011664	T	T	T
0.4169024554553033	0.6737884680277209	0.6654898864937221	T	T	T
0.3039211671760380	0.6298200368617758	0.8061960199842407	T	T	T
0.2672981862139170	0.6698074760502077	0.0246152666412101	T	T	T
0.1131944429988399	0.6738654812281017	0.0092739179720579	T	T	T
0.0637186056428240	0.6286503638580440	0.7980544652912569	T	T	T
0.1819731098841565	0.6708591744221212	0.6698772735559151	T	T	T
0.4218142903689759	0.4429330664751524	0.6456082787515931	T	T	T
0.3049286674301234	0.4711662428273826	0.7908671894493330	T	T	T
0.2801393696484172	0.4428638078942437	0.0139334629050586	T	T	T
0.1222065232997089	0.4364335776530396	0.0126315002037248	T	T	T
0.0646055775352763	0.4702501098557618	0.8033113671535552	T	T	T
0.3056024936728739	0.0302713351549658	0.7956400996828787	T	T	T
0.6143505211225934	0.8268339717017991	0.4889396076469065	T	T	T
0.5641018705943881	0.8756823693486753	0.6967140495327581	T	T	T
0.6798417754777655	0.8346170688757023	0.8307281807256914	T	T	T
0.9230494634749757	0.0533911912129636	0.8557671856678521	T	T	T
0.8030277995610092	0.0254266768561398	0.7061867518666468	T	T	T
0.7811380044698272	0.0672090781193084	0.4903235634732158	T	T	T
0.6206803384232837	0.0707523983478572	0.4899648506204178	T	T	T
0.5676501688494633	0.0326976511932129	0.6983215539935437	T	T	T
0.6801672594383105	0.0541708347848625	0.8455993544655367	T	T	T
0.9233617270800565	0.8302819597922845	0.8348640083017086	T	T	T
0.8035886465113257	0.8680261785702039	0.6907178179018857	T	T	T
0.7693150392320933	0.8258265813733980	0.4738299699365160	T	T	T
0.8805803504999039	0.9334904997699387	0.9951729715563128	T	T	T
0.9333767299267083	0.9688182412467813	0.2034852923570709	T	T	T
0.8220584445531223	0.9472764088870758	0.3512115285962428	T	T	T

Structure files (CONTCAR) involved in this work:

0.5783338618778617	0.1746615510699578	0.3288085600513147	T	T	T
0.6972976946598305	0.1327888049591258	0.1922284560916648	T	T	T
0.7323521490191265	0.1706512707299833	0.9714776449780501	T	T	T
0.8873271888474241	0.1729162303620490	0.9842539546890208	T	T	T
0.9371908788192933	0.1259510057606948	0.1956096954445194	T	T	T
0.8216180208836252	0.1724688682142299	0.3276772976544823	T	T	T
0.5784001937534361	0.9459047530380236	0.3578553799524544	T	T	T
0.6979046055194117	0.9743498500493609	0.2136052141111902	T	T	T
0.7204796479745342	0.9394263581279263	0.9924542218834547	T	T	T
0.1817355278357952	0.8287126757446721	0.6708746833382909	T	T	T
0.0663432731210681	0.8743990067479509	0.8000701124058293	T	T	T
0.7693914357389677	0.6693359217371230	0.4620617970570288	T	T	T
0.6139126025590086	0.6727366671968013	0.4797783694959672	T	T	T
0.5629378386909755	0.6275260245916487	0.6942724015812468	T	T	T
0.6752076488425124	0.6771188161662394	0.8200170871186179	T	T	T
0.1130239254295260	0.8274155243415564	0.0128650853531075	T	T	T
0.9192347454362126	0.4452954647762483	0.8571512638740226	T	T	T
0.8000127818395765	0.4780901105216776	0.7238701254320293	T	T	T
0.7759539674541155	0.4398627729428323	0.4952439890454427	T	T	T
0.6170325643166825	0.4304736034537044	0.4919118998030552	T	T	T
0.5673438151893828	0.4690442112635225	0.7039172683174053	T	T	T
0.6734697847631695	0.4444773163253436	0.8564230582433944	T	T	T
0.9196946044842965	0.6792992533960648	0.8256971311356284	T	T	T
0.4225565910760837	0.0596529920276601	0.6498907721759511	T	T	T
0.8224750974605501	0.3363717727879473	0.3334950336538791	T	T	T
0.8021443588862259	0.6371805608887058	0.6883189185976987	T	T	T
0.8065679731688307	0.5024485216648846	0.4274935705027790	T	T	T
0.8028341583729004	0.6305766096178244	0.3634165618314404	T	T	T
0.5854038700659611	0.3639761021363088	0.4411587756961498	T	T	T
0.5874904124634702	0.4981425540165721	0.4409625103779461	T	T	T
0.5667725680967378	0.6274942628477267	0.4064987380407209	T	T	T
0.9254395160794044	0.4547720297890603	0.1459721887097835	T	T	T
0.6729943450437533	0.4506944581036307	0.1693375236671706	T	T	T
0.7637450345640222	0.3750062822196000	0.2604740829798853	T	T	T
0.9015897581641302	0.3731953916813874	0.2950145207417464	T	T	T
0.9069117510166970	0.3260608539451955	0.1059106995634303	T	T	T
0.8077307850189253	0.3530347088944873	0.9810639620416282	T	T	T
0.7019302434994615	0.3306424548707866	0.0950451645998614	T	T	T
0.6369202537600211	0.3378562788728149	0.2619869971654729	T	T	T
0.7669811556290617	0.5311129411638991	0.2387444369700313	T	T	T
0.8915496993745082	0.5353658963646862	0.2957306186237253	T	T	T
0.8943351716866079	0.5794053148311702	0.1008572752256782	T	T	T
0.7925326320040020	0.5590011512966943	0.9793442752087621	T	T	T
0.6872656939538625	0.5768614004851058	0.0990066269536033	T	T	T
0.6409895329189150	0.5569378501561039	0.2811391219847591	T	T	T
0.5154593932925888	0.1352156640967561	0.2779861917368705	T	T	T
0.5137018719744696	0.9574580302194681	0.2865892704299435	T	T	T
0.2991306317774196	0.1293629787658522	0.0723804692775732	T	T	T
0.3117682603262034	0.9956647271153324	0.0804182744359924	T	T	T
0.3030074284619552	0.8649490634241719	0.1211808037017546	T	T	T
0.1083167803108364	0.1362090603879412	0.0676785351981035	T	T	T
0.0855072045031664	0.0047310891425665	0.0736510276383594	T	T	T
0.0673115198512714	0.8734624233355681	0.0857291496796306	T	T	T

Structure files (CONTCAR) involved in this work:

0.4164329142777491	0.0491425737848413	0.3112815814565429	T	T	T
0.1812299492354443	0.0513216279170554	0.2868269294050189	T	T	T
0.2704547337715097	0.1499780683226000	0.2657965855744772	T	T	T
0.3949272748568720	0.1595056377254973	0.2031503567070662	T	T	T
0.4152718901466286	0.1689802765100074	0.3978623815447480	T	T	T
0.3098500285349141	0.1478260822600237	0.5136721150156986	T	T	T
0.1920520059753152	0.1464477890168507	0.4252864086383281	T	T	T
0.1402994959907767	0.1749707231172030	0.2510986696476979	T	T	T
0.2713788654280794	0.9549296338802790	0.2604077169583695	T	T	T
0.3967627674539506	0.9382028823470057	0.2047504213344065	T	T	T
0.4084170738917474	0.9315824415772885	0.4017405128576979	T	T	T
0.2987360317655186	0.9497736066934714	0.5099468772407381	T	T	T
0.1848950496898105	0.9435732289283536	0.4076777983081419	T	T	T
0.1429476002343578	0.9331696947170787	0.2212364010413136	T	T	T
0.9861059029396276	0.8705070024847077	0.7842445921870708	T	T	T
0.9881117705430712	0.0397998948136230	0.7862590320090830	T	T	T
0.1994677387468698	0.8708362560380271	0.5705222142113671	T	T	T
0.1891353508755954	0.0045999961080384	0.5811437062701663	T	T	T
0.1987253637674384	0.1354280918756964	0.6212758398819611	T	T	T
0.3938394867305868	0.8648542602468290	0.5676546346292799	T	T	T
0.6069270344185957	0.7508328569954525	0.4465525883386541	T	T	T
0.7735817518950805	0.7489134966658409	0.4349107029338538	T	T	T
0.6839126280660934	0.7553908804644073	0.8516170400151197	T	T	T
0.9459523215078791	0.7538773262640193	0.8590821029838798	T	T	T
0.8924231989321181	0.2505740468474384	0.9461738401308927	T	T	T
0.7273988784180572	0.2496230858399578	0.9434093329942119	T	T	T
0.8187558786262563	0.2519515419769527	0.3441135325179557	T	T	T
0.5558898612485613	0.2513222517287986	0.3520279352128245	T	T	T
0.3907628410980670	0.2512235888070068	0.5490902198176352	T	T	T
0.4142378717810369	0.9967464913775960	0.5737903455973651	T	T	T
0.2256059873660161	0.2506985839891424	0.5388891854113912	T	T	T
0.3047737166497722	0.2508245617386659	0.1452366181497748	T	T	T
0.0627827544675053	0.2502192593990449	0.1362506739044024	T	T	T
0.1079254413392921	0.7500737133883228	0.0508519021205082	T	T	T
0.2728240499782949	0.7499245679864037	0.0388801683008783	T	T	T
0.1926521389971511	0.7498093979785534	0.6455151341336455	T	T	T
0.4372539623625236	0.7503916602406955	0.6380284100111392	T	T	T
0.5093827470182091	0.3663021286355200	0.2774377693806435	T	T	T
0.5107555351598334	0.5370222611416108	0.2889693821586169	T	T	T
0.2932619766297787	0.3709359989571887	0.0675776263812054	T	T	T
0.4317553326800896	0.1281811130892734	0.5852573513347264	T	T	T
0.3143683040719989	0.5038479235349993	0.0754758148808467	T	T	T
0.3021805893617768	0.6343607080963006	0.1201756640296188	T	T	T
0.1137408659304453	0.3634790394538230	0.0657715371335048	T	T	T
0.0817120690065895	0.4929709538199626	0.0763276101049343	T	T	T
0.0660586354349979	0.6258622304470181	0.0779783586940414	T	T	T
0.4101139478289288	0.4517575722418754	0.3185724124086994	T	T	T
0.1755472756947324	0.4497975975910364	0.2887489880887672	T	T	T
0.2671648815732290	0.3532746418333729	0.2620871698653286	T	T	T
0.3909638595891153	0.3467323694275286	0.1978226533760489	T	T	T
0.4080553893653102	0.3291149637159106	0.3929575220234623	T	T	T
0.0888036431471192	0.9523718253027347	0.8140856797608289	T	T	T
0.3080504687488461	0.3546623595121799	0.5174004326241937	T	T	T

Structure files (CONTCAR) involved in this work:

0.1912968735939614	0.3548663357764528	0.4253447744846781	T	T	T
0.1372271863207704	0.3259872328836790	0.2535364093232651	T	T	T
0.2674908222172632	0.5422417216887427	0.2532431580687866	T	T	T
0.3947433231644741	0.5608377264002883	0.2054937439660684	T	T	T
0.4059008545201851	0.5723910443107446	0.4012488521557759	T	T	T
0.2962280150113272	0.5464853935948570	0.5072000561226991	T	T	T
0.1836008091162985	0.5600488805741706	0.4037749348495295	T	T	T
0.1375950188440956	0.5676405963895654	0.2213772771744422	T	T	T
0.3188156563720432	0.9498703371409495	0.7885533930777571	T	T	T
0.2299369770520079	0.8511991681137813	0.7633967406322703	T	T	T
0.9843802109205414	0.6375333640998803	0.7816746884624736	T	T	T
0.9851937998479918	0.4571282794170420	0.7881327408385292	T	T	T
0.2004531520348505	0.6295344703675585	0.5689051093811235	T	T	T
0.1829649361009750	0.4961097983676894	0.5745809369193894	T	T	T
0.1948709619348043	0.3661975885905634	0.6206207575995253	T	T	T
0.3845102626426565	0.6383355392784666	0.5669964347373603	T	T	T
0.4137349171380913	0.5076006107656731	0.5728546619513983	T	T	T
0.4315351990807371	0.3760014651787765	0.5772292257462970	T	T	T
0.0813378865102127	0.5495588445740902	0.8163221463034982	T	T	T
0.1045470915877334	0.8424003079687087	0.7035539173270088	T	T	T
0.3211260877997797	0.5510498397923558	0.7870067673394798	T	T	T
0.2301941567167889	0.6476345532886448	0.7619997683883600	T	T	T
0.1047291921210799	0.6555326545343254	0.7005330002261911	T	T	T
0.0888139016842334	0.6713935422273917	0.8944165564745956	T	T	T
0.1895206382903825	0.6462794202191822	0.0179077354577017	T	T	T
0.3057403966931768	0.6456018699481018	0.9245298217403619	T	T	T
0.3609945864150462	0.6749275357419707	0.7534250914720625	T	T	T
0.2283979024075630	0.4590421589504094	0.7542825570353014	T	T	T
0.1017138321763333	0.4402870500618430	0.7047482199111502	T	T	T
0.0908977871562295	0.4305251316059833	0.9018078496704457	T	T	T
0.0873637849714997	0.8318415088248091	0.8985989569051530	T	T	T
0.2002694359345344	0.4575244993945494	0.0078782713791940	T	T	T
0.3124132180012034	0.4409492722236754	0.9028833287129205	T	T	T
0.3571213152276507	0.4328717381584331	0.7176903084709237	T	T	T
0.1899900588990249	0.8535897180875470	0.0187367607914041	T	T	T
0.4845759604366592	0.8644236734693456	0.7154672936013660	T	T	T
0.4889816008973527	0.0486077066245580	0.7168766511288313	T	T	T
0.6980568712743527	0.8716777265364467	0.9352459515521280	T	T	T
0.6861214252959613	0.0052470286501498	0.9421349923422319	T	T	T
0.6976114629865608	0.1303566276006449	0.8800622603440850	T	T	T
0.3063045704759569	0.8539740815625471	0.9248762620568366	T	T	T
0.9015847202664835	0.8642210420386756	0.9404387261022910	T	T	T
0.9192362577726574	0.9963958930858259	0.9428146606120504	T	T	T
0.9311376078271559	0.1266131411020819	0.9090802220358893	T	T	T
0.5783557394119444	0.9540048588174407	0.6698224420913128	T	T	T
0.8187020615521717	0.9479775734760164	0.6767957954073083	T	T	T
0.7306494033385691	0.8581545027488148	0.7420992943142035	T	T	T
0.6041708717205037	0.8553528510095814	0.7975856892571345	T	T	T
0.5884065687653166	0.8290708808006280	0.6038535484718983	T	T	T
0.6920016082486536	0.8509800542857319	0.4840139870031848	T	T	T
0.8053406720219479	0.8321036112445906	0.5820590084724553	T	T	T
0.3604982683494157	0.8270979646536365	0.7512580420447267	T	T	T
0.8611584991982386	0.8347111991037633	0.7585673403176615	T	T	T

Structure files (CONTCAR) involved in this work:

0.7293602664491777	0.0292304491189172	0.7564980849157393	T	T	T
0.6045626101526793	0.0524053356910669	0.8021838048454548	T	T	T
0.5972513213516898	0.0768429153016460	0.6057740525515449	T	T	T
0.7005555581777642	0.0587197742017239	0.4826530015246574	T	T	T
0.8046010896398816	0.0723208450570203	0.6065188048234903	T	T	T
0.8574212074950007	0.0536546621280979	0.7853430096215793	T	T	T
0.2294551079387198	0.0462232360198401	0.7610878762176355	T	T	T
0.0167778931029032	0.1364749496891973	0.2150934656171107	T	T	T
0.1043394200774967	0.0630231349772348	0.7048242347521448	T	T	T
0.0124424280616992	0.9537692238902612	0.2192781506703964	T	T	T
0.8037449476939736	0.1351173027529308	0.4326933136935899	T	T	T
0.8158548114712827	1.0011427952318621	0.4416849132402502	T	T	T
0.8066494969472430	0.8722465994346155	0.3915344666279612	T	T	T
0.6000450318231796	0.1402002706903401	0.4340443556717962	T	T	T
0.5829606389544401	0.0081584534837314	0.4363069251420015	T	T	T
0.5691707743734946	0.8764225151791525	0.4201271672354081	T	T	T
0.9212108372548364	0.0473935957640247	0.1757908299930757	T	T	T
0.6795996040694613	0.0533238585379455	0.2000787569294082	T	T	T
0.7706055665725753	0.1478350278989150	0.2392523648633720	T	T	T
0.0918518797804454	0.0709277910100517	0.9018275757471205	T	T	T
0.8972486149050799	0.1514397372860458	0.2938046370706701	T	T	T
0.9155427349299559	0.1690114194121420	0.0976082656266454	T	T	T
0.8101383453079166	0.1475606163950466	0.9820630698340873	T	T	T
0.6945796643032278	0.1556351095148840	0.0761614314837798	T	T	T
0.6406560158886491	0.1751352511745544	0.2517049706330309	T	T	T
0.7724269009540118	0.9678450726958254	0.2600382719301477	T	T	T
0.8978128655530431	0.9486402083578748	0.3079737093922220	T	T	T
0.9027736701487796	0.9255065770449173	0.1112214966020067	T	T	T
0.8010813424385685	0.9476075911587180	0.9864107199881501	T	T	T
0.6955961915389089	0.9349956769696530	0.1076022280747687	T	T	T
0.2016723858216151	0.0494941494382026	0.0091016442941542	T	T	T
0.6444795919637223	0.9400052252574516	0.2886714610553002	T	T	T
0.3158827953234423	0.0583260523536336	0.9082598624416427	T	T	T
0.4819869801026117	0.6327205982671541	0.7035713707356025	T	T	T
0.4880035174690542	0.4535615019953541	0.7128350024977133	T	T	T
0.6910382180357237	0.6361673171736898	0.9232895972251094	T	T	T
0.6758379820968393	0.5025502741907272	0.9409116234296427	T	T	T
0.6869525019406416	0.3716602772836001	0.9061824529668883	T	T	T
0.8946085459614680	0.6417734311960006	0.9288760748056760	T	T	T
0.9102123715170297	0.5087012754150871	0.9327323502461835	T	T	T
0.3580183945420309	0.0679331379860684	0.7222816627081389	T	T	T
0.9312272247021512	0.3775784752586210	0.9243191324036663	T	T	T
0.5825634738590063	0.5482780866928486	0.6881341388837656	T	T	T
0.8203259169532671	0.5548231134044760	0.7257680097627205	T	T	T
0.7215911108668263	0.6569033419646184	0.7279730145525547	T	T	T
0.5964502700436926	0.6627730098070861	0.7913403171715928	T	T	T
0.5879292536629190	0.6649350546468726	0.5934160266076729	T	T	T
0.6905232820941979	0.6468313948497847	0.4666294851937812	T	T	T
0.8084592101923957	0.6462821917999753	0.5591176716652856	T	T	T
0.8622752999795760	0.6865031505603514	0.7451780175034657	T	T	T
0.7269795915893870	0.4608374490229519	0.7692505390819702	T	T	T
0.5995456534460436	0.4417140100555798	0.8071181046025230	T	T	T
0.6006569702905107	0.4288490749194839	0.6098155136931580	T	T	T

Structure files (CONTCAR) involved in this work:

0.6982399880061119	0.4285820202272165	0.4734845205847985	T	T	T
0.7969816161933434	0.4493801756502549	0.6089151942014093	T	T	T
0.8561407797626026	0.4329729665370475	0.7831303296447555	T	T	T
0.0172960929178620	0.3669803872110726	0.2035001206198907	T	T	T
0.0058707676185562	0.5517424460962439	0.2115087345894001	T	T	T
0.8238017976346086	0.3758729138655817	0.4571766225622770	T	T	T
0.9148097667744116	0.4552315378574924	0.3836312184712480	T	T	T
0.8824810963675030	0.3961771000492287	0.4869550672738833	T	T	T
0.9885527606894333	0.3924996521599062	0.5125801292702682	T	T	T
0.9189385466523680	0.4117038030058940	0.5907512240126755	T	T	T
0.9622593266282572	0.4770566726270494	0.5409870611253149	T	T	T
0.9453316805385841	0.4257775834545196	0.5212725177189236	T	T	T

Figure S7 FS

Si Al O Zn H C

1.0000000000000000

20.0219999999999985 0.0000000000000000 0.0000000000000000

0.0000000000000000 19.8990000000000009 0.0000000000000000

0.0000000000000000 0.0000000000000000 13.3829999999999991

94 2 192 1 4 1

Selective dynamics

Direct

0.2678638866464722	0.8305388386462660	0.0257600659575473	T	T	T
0.3039590917776484	0.8705760730082084	0.8077266444552818	T	T	T
0.9376805821667640	0.3787388330945742	0.1886307857791885	T	T	T
0.8845824322826932	0.3257686364600815	0.9914447335792087	T	T	T
0.7307901488611240	0.3263209203979411	0.9697748841912782	T	T	T
0.6893694551107648	0.3710201984326352	0.1832203699706478	T	T	T
0.5763507742046705	0.3278055950357886	0.3289303570526497	T	T	T
0.8139715621527732	0.5477133488559464	0.3281399562517196	T	T	T
0.9322792464548585	0.5322194178578613	0.1820873549465034	T	T	T
0.8757882377146035	0.5729615273740293	0.9808149065841354	T	T	T
0.7155183651390804	0.5648561534724048	0.9792624444955229	T	T	T
0.6889361026608869	0.5257053049786181	0.1955258535412697	T	T	T
0.4204195855912112	0.8266102773843267	0.6694222051069382	T	T	T
0.5760837500688575	0.5563427394134016	0.3491881540908850	T	T	T
0.1820022719019516	0.0617270948160459	0.6677502526399657	T	T	T
0.0679362769853697	0.0314429350831259	0.8023555606812997	T	T	T
0.3176020541853738	0.1718992760064508	0.1736113572364076	T	T	T
0.4359291146612400	0.1275637486402480	0.2997452925701726	T	T	T
0.3875884872086532	0.1736508454849168	0.5128473542904798	T	T	T
0.2327806287287316	0.1703647955650701	0.5258765751428507	T	T	T
0.1966192188304593	0.1296802646960042	0.3089605645620840	T	T	T
0.0815179652811064	0.1726033446700289	0.1694644051143263	T	T	T
0.3194473730644211	0.9388093184629741	0.1673856042377114	T	T	T
0.1221553904707130	0.0650937915594569	0.0136839882599359	T	T	T
0.4342314376846677	0.9691677987838510	0.3023896156233808	T	T	T
0.3788510463564794	0.9351863990536390	0.5139582352496681	T	T	T
0.2187390346712572	0.9409115273476948	0.5196362978558787	T	T	T
0.1951553290320621	0.9703827511635629	0.2968800860078146	T	T	T
0.0784383636563932	0.9416479766292229	0.1510275102490628	T	T	T
0.2817259469676466	0.0590606095353866	0.0193701561458685	T	T	T
0.3156093949924340	0.3298476378369757	0.1720123042139916	T	T	T
0.1919012699938733	0.5298904660432651	0.2953769213994752	T	T	T

Structure files (CONTCAR) involved in this work:

0.2181467507016782	0.5581448889824721	0.5168788310357698	T	T	T
0.3763879839124123	0.5655273608833149	0.5124119466022833	T	T	T
0.4315930718165162	0.5313763633211120	0.3026844847293066	T	T	T
0.3173558726163726	0.5609743498380383	0.1658174335387038	T	T	T
0.0817063367489229	0.3259461677222276	0.1690589512941483	T	T	T
0.1945315265259930	0.3713162952570390	0.3094136994057535	T	T	T
0.2313825674414486	0.3309969206692914	0.5275036314035210	T	T	T
0.3856821894099256	0.3276953036497983	0.5130183265873438	T	T	T
0.4317974420267093	0.3740740622366822	0.3006454518258134	T	T	T
0.0766492712854309	0.5598494212614541	0.1474049616637782	T	T	T
0.1793169369332302	0.4400117822517909	0.6667018907386765	T	T	T
0.4173012603252753	0.6730289062622961	0.6667298004966333	T	T	T
0.3046146412711880	0.6297011644321838	0.8088401994681277	T	T	T
0.2674461059332714	0.6700666529942189	0.0254732978457456	T	T	T
0.1134920664599584	0.6737406630182461	0.0082943062101832	T	T	T
0.0640040548921391	0.6270766859684407	0.7977850707944693	T	T	T
0.1833393946328094	0.6699964918101728	0.6720890243491203	T	T	T
0.4214494632113281	0.4428052799358618	0.6490910518362704	T	T	T
0.3050288375108535	0.4708739482060068	0.7948622281525091	T	T	T
0.2804405317783542	0.4419494469646711	0.0171376737040051	T	T	T
0.1215099315121059	0.4350361711967556	0.0146799428679635	T	T	T
0.0646495673326389	0.4686388733020235	0.8048003036680035	T	T	T
0.3058344726364228	0.0301181681560326	0.7973082590303108	T	T	T
0.6144582450182150	0.8258449000897036	0.4870685634209525	T	T	T
0.5653953059201627	0.8737583380580372	0.6969491898719914	T	T	T
0.6827661625805261	0.8302882201286274	0.8266038694182672	T	T	T
0.9230106812946666	0.0530683610022136	0.8539937944156863	T	T	T
0.8040898419292590	0.0240380447152038	0.7031909282065734	T	T	T
0.7812314910460336	0.0644719253126432	0.4876368470514910	T	T	T
0.6206357706223122	0.0690968801343851	0.4898539641600674	T	T	T
0.5669307722536731	0.0312587981985606	0.6982518548246734	T	T	T
0.6810224270227960	0.0528728904529706	0.8415038354675654	T	T	T
0.9232318147020894	0.8295054809795313	0.8308125396436826	T	T	T
0.8048477020130587	0.8655705185175302	0.6849027808940763	T	T	T
0.7695037820418710	0.8229497010044153	0.4679707738110789	T	T	T
0.8807789135601644	0.9324864706731606	0.9926329114433207	T	T	T
0.9339646352783070	0.9671894385446876	0.2007140718084823	T	T	T
0.8203697645220704	0.9445005586472076	0.3446978649372552	T	T	T
0.5791555225547367	0.1737717430469929	0.3298342247065891	T	T	T
0.6966049390736737	0.1307940933246975	0.1898262871201458	T	T	T
0.7330868087637987	0.1693073691050870	0.9705564591638054	T	T	T
0.8877900353369189	0.1721419373373604	0.9849696356698052	T	T	T
0.9377586906039896	0.1238290216982320	0.1949263412459024	T	T	T
0.8212060538517455	0.1695236015346144	0.3247201707478369	T	T	T
0.5786208036104388	0.9446867982850921	0.3553778087859422	T	T	T
0.6965412044638641	0.9720616375354684	0.2078657180713003	T	T	T
0.7210318968402963	0.9367813157091939	0.9883860972725624	T	T	T
0.1819189561791585	0.8281848587986237	0.6727763851505397	T	T	T
0.0661180002970847	0.8748599850421183	0.8004834447187414	T	T	T
0.7682196032172846	0.6661077128014007	0.4599353640364460	T	T	T
0.6127072214537286	0.6724428096750723	0.4794793890080961	T	T	T
0.5628553623501324	0.6267101752923989	0.6929011874116333	T	T	T
0.6773063400812184	0.6721614853021346	0.8182679166323095	T	T	T

Structure files (CONTCAR) involved in this work:

0.1133287750676407	0.8275122649457157	0.0128151352953240	T	T	T
0.9204112382687849	0.4434082625188817	0.8589106657029156	T	T	T
0.8061646980713283	0.4733943037020716	0.7155025935119372	T	T	T
0.7776627254741532	0.4390700572525387	0.4955268172978491	T	T	T
0.6175321606267550	0.4337378311612907	0.4888389428063573	T	T	T
0.5657816525268753	0.4688383437928518	0.7001921545710589	T	T	T
0.6795509508130614	0.4424327866830981	0.8404039707134067	T	T	T
0.9209560465715086	0.6784301455261493	0.8231377474886025	T	T	T
0.4222638239593522	0.0589709330883669	0.6507998684751862	T	T	T
0.8185976016003418	0.3331044329029841	0.3150417810498451	T	T	T
0.8045231788495742	0.6328969957774327	0.6847687491253526	T	T	T
0.8154487618561234	0.4909138788897452	0.4200411834194269	T	T	T
0.7986991012213709	0.6226244602265073	0.3641548524407890	T	T	T
0.6021291562394165	0.3639099066225140	0.4314795087800286	T	T	T
0.5838553991977931	0.4968304145178021	0.4323416987114777	T	T	T
0.5657128216648739	0.6272993667773199	0.4061958426661287	T	T	T
0.9288581133272507	0.4544560156220433	0.1450640897748025	T	T	T
0.6646849832250000	0.4491122405792637	0.1764235236266435	T	T	T
0.7612426666881842	0.3671331318416259	0.2366791777848096	T	T	T
0.8963134265509687	0.3754190070789293	0.2958003404221125	T	T	T
0.9067579720997399	0.3255026303116446	0.1098571223490417	T	T	T
0.8077445251175643	0.3514055396701571	0.9851508926269826	T	T	T
0.6899250180198354	0.3385576808297650	0.0722990045100732	T	T	T
0.6348149521779413	0.3285791651526874	0.2463507141004113	T	T	T
0.7655348347871247	0.5237872144516569	0.2393591825885422	T	T	T
0.8923342417200679	0.5364886482806809	0.2909945340250082	T	T	T
0.8988045855904510	0.5793726386210045	0.0987020058606973	T	T	T
0.7963711135940840	0.5595475801882450	0.9784888529901664	T	T	T
0.6884303002114492	0.5693304079564616	0.0939612643624800	T	T	T
0.6415163405148839	0.5608849186553566	0.2781859111930055	T	T	T
0.5156363782518377	0.1354136280778052	0.2793585290458299	T	T	T
0.5134823418045896	0.9566621449617141	0.2853901491369342	T	T	T
0.2992265540950969	0.1298242023774474	0.0735680754528520	T	T	T
0.3104079207281504	0.9961779489852243	0.0826719044391494	T	T	T
0.3024691201907813	0.8652475590640146	0.1221448564976407	T	T	T
0.1079874499220116	0.1364063012412557	0.0685138193798049	T	T	T
0.0863884540255938	0.0046121709994749	0.0746766781651419	T	T	T
0.0679898614586001	0.8731860164580343	0.0867221569233303	T	T	T
0.4172042275552367	0.0488386248978628	0.3141358534605944	T	T	T
0.1812455288172506	0.0507695282923800	0.2893872570325701	T	T	T
0.2705270536053978	0.1491915882235443	0.2673001481985433	T	T	T
0.3950646051201960	0.1586436616154210	0.2050689264260312	T	T	T
0.4159921601177734	0.1690815196968310	0.3998139706845150	T	T	T
0.3104653930470033	0.1475828684971718	0.5149571104458806	T	T	T
0.1924296448428967	0.1464363871017212	0.4270129338560800	T	T	T
0.1402133943967458	0.1739688960579099	0.2527599144812800	T	T	T
0.2713884507807975	0.9544478420316256	0.2627905176701754	T	T	T
0.3963298999032898	0.9387906352628372	0.2052236515025634	T	T	T
0.4089273648769500	0.9305900709017189	0.4021433418252711	T	T	T
0.2990445289472830	0.9478481425183517	0.5101734978680939	T	T	T
0.1845304501180593	0.9429564997356968	0.4097050835880756	T	T	T
0.1432828852954415	0.9328302681201410	0.2226025193071330	T	T	T
0.9859576151804851	0.8715762384816468	0.7837075714627011	T	T	T

Structure files (CONTCAR) involved in this work:

0.9882819665832822	0.0406160528412675	0.7845161495526060	T	T	T
0.1995085923434890	0.8701281800929092	0.5722011035904621	T	T	T
0.1907014228715981	0.0041880476612823	0.5831477061846547	T	T	T
0.1997961256909311	0.1352398633148594	0.6229521729082799	T	T	T
0.3956112934889114	0.8646687457617829	0.5688148715024502	T	T	T
0.6060508781442536	0.7501199349007486	0.4444260226017623	T	T	T
0.7735514815336078	0.7455322715938048	0.4303724327832016	T	T	T
0.6872277009781675	0.7509294049131695	0.8473592622645670	T	T	T
0.9468720836296823	0.7534999582306742	0.8548516127539718	T	T	T
0.8928050179992896	0.2500911955430546	0.9484490996557806	T	T	T
0.7291056374091369	0.2477661328318783	0.9398370325712553	T	T	T
0.8185000356500644	0.2495606661161997	0.3404544658358791	T	T	T
0.5582231943722097	0.2506475459873062	0.3556712795715577	T	T	T
0.3914066219915915	0.2507949879255765	0.5517136357617678	T	T	T
0.4136576330412846	0.9968833449844351	0.5733840746525433	T	T	T
0.2264076454441584	0.2506434121988330	0.5402419299861186	T	T	T
0.3055410501966729	0.2507050706953633	0.1486598515708927	T	T	T
0.0619115714816004	0.2495068206030469	0.1407694927910371	T	T	T
0.1088518015660290	0.7500398708529151	0.0497848332756739	T	T	T
0.2727960918471503	0.7502135897898252	0.0397700875831580	T	T	T
0.1925973896656755	0.7492144522040030	0.6481408046958606	T	T	T
0.4374206944097614	0.7496184828577933	0.6389096783993228	T	T	T
0.5117207013087299	0.3667464748754365	0.2835755335956968	T	T	T
0.5109012858232532	0.5403990394592803	0.2814999096984951	T	T	T
0.2964789408046182	0.3708995367215140	0.0713274138871963	T	T	T
0.4323107669412762	0.1278362538964940	0.5872299175349853	T	T	T
0.3111229300946104	0.5046350608188079	0.0789193389436331	T	T	T
0.2999794978631266	0.6350377223475037	0.1232064555493433	T	T	T
0.1096997539937701	0.3632862821559842	0.0698498780120402	T	T	T
0.0838436350325842	0.4939482551060569	0.0769587190420027	T	T	T
0.0674668414965649	0.6263669134125537	0.0792288487982195	T	T	T
0.4126076839291131	0.4524670260505476	0.3181047492590993	T	T	T
0.1760716890997455	0.4497476321659695	0.2897018270984720	T	T	T
0.2679986151531605	0.3532948240527570	0.2649551164739174	T	T	T
0.3928096434732845	0.3450575023336928	0.2030104509979036	T	T	T
0.4101770312525643	0.3305532149666994	0.3977941610808681	T	T	T
0.0886704292402488	0.9527862363305107	0.8144417254248291	T	T	T
0.3089761062509197	0.3545460078726806	0.5199010145708941	T	T	T
0.1922060052853136	0.3554528914894592	0.4277235496792504	T	T	T
0.1378719011013732	0.3256944286189696	0.2559904106669093	T	T	T
0.2679939337745919	0.5431418418710872	0.2588634780865042	T	T	T
0.3935752318682933	0.5617313558538904	0.2059225271152559	T	T	T
0.4092281348713082	0.5721019367772147	0.4022776118891800	T	T	T
0.2977961405706803	0.5463719294106657	0.5039516867604602	T	T	T
0.1825134396030989	0.5587447950492749	0.4076858193968999	T	T	T
0.1392592906818484	0.5684034823003765	0.2229226979902734	T	T	T
0.3190404831030256	0.9497586181503980	0.7894266745858191	T	T	T
0.2303006032640059	0.8509139582038520	0.7650184257295481	T	T	T
0.9851892195962986	0.6369529619180192	0.7777485243747859	T	T	T
0.9855939446685591	0.4538187871803536	0.7880164827801758	T	T	T
0.2041509007270392	0.6293022728843702	0.5715631310993198	T	T	T
0.1866654242451417	0.4960162764887641	0.5793961149926922	T	T	T
0.1962470112154255	0.3657605729228054	0.6234976810418471	T	T	T

Structure files (CONTCAR) involved in this work:

0.3857962420525414	0.6372684738151323	0.5679561597189919	T	T	T
0.4138685415654811	0.5062958868241152	0.5738778568937187	T	T	T
0.4322380935139440	0.3749416340468570	0.5830657573961766	T	T	T
0.0803004379877408	0.5481146488562137	0.8191447018559778	T	T	T
0.1047299020125656	0.8423469715084528	0.7048349156558564	T	T	T
0.3209487409600489	0.5507823237574787	0.7898193572392611	T	T	T
0.2307263631303782	0.6480664647698565	0.7659244627623865	T	T	T
0.1063228265135990	0.6525442137879247	0.7007319650734001	T	T	T
0.0877480830830476	0.6708164287559301	0.8940973541800011	T	T	T
0.1899966087955410	0.6464150049778676	0.0146762300280226	T	T	T
0.3079757834388934	0.6458300362780635	0.9271362792252467	T	T	T
0.3612403981214927	0.6743634229374260	0.7542594986013714	T	T	T
0.2284420921377152	0.4575795404762386	0.7599070968136498	T	T	T
0.1028972935889114	0.4397658173281822	0.7067754349928552	T	T	T
0.0903081655485385	0.4290282301797644	0.9038287088868926	T	T	T
0.0864685992598009	0.8324012727269671	0.8992892620774242	T	T	T
0.2002870645003897	0.4525866945381306	0.0090257172366664	T	T	T
0.3140973202463690	0.4412517415820578	0.9069194931541121	T	T	T
0.3564668599587066	0.4328553880559171	0.7202270133125034	T	T	T
0.1902331744683307	0.8540822643133535	0.0176334529682542	T	T	T
0.4860137741690497	0.8624963803648531	0.7172498173597767	T	T	T
0.4882801566151032	0.0462899634219925	0.7181534616351150	T	T	T
0.7030587551498210	0.8680266296424635	0.9300335725364880	T	T	T
0.6867128888592599	0.0012695607805447	0.9346637364363031	T	T	T
0.6994149313976342	0.1279849029875791	0.8795126977981704	T	T	T
0.3072862525303816	0.8539438281417386	0.9258896660090131	T	T	T
0.8981706699134075	0.8632810189138115	0.9349653384505704	T	T	T
0.9193627853085253	0.9952256310100189	0.9397195750819315	T	T	T
0.9306231850822714	0.1260165561770685	0.9083641497686967	T	T	T
0.5791747692339032	0.9524865838527682	0.6719850510928186	T	T	T
0.8190635530589792	0.9460634284594081	0.6766529588189309	T	T	T
0.7320145711579311	0.8531443629052297	0.7355338025900047	T	T	T
0.6067200795661908	0.8517958604304630	0.7960607327119975	T	T	T
0.5889114851342780	0.8286518007333074	0.6020898341469778	T	T	T
0.6924833312900990	0.8483528784426660	0.4811721648468086	T	T	T
0.8073614573577956	0.8321203487637456	0.5744773620321714	T	T	T
0.3610554361419843	0.8271448935461122	0.7518962384269445	T	T	T
0.8628977674463904	0.8317017285827564	0.7510401988262684	T	T	T
0.7294600060794280	0.0302376858651056	0.7499833626281441	T	T	T
0.6049369153683024	0.0530809666206162	0.8001935466604351	T	T	T
0.5945868877799163	0.0750297331453913	0.6041649209993032	T	T	T
0.7005511080731518	0.0571033336490184	0.4865139589300549	T	T	T
0.8085595202817566	0.0692465485905547	0.6019163504430065	T	T	T
0.8572944791948723	0.0531059873056202	0.7835288070954753	T	T	T
0.2295517005935174	0.0462593974667752	0.7636210852808587	T	T	T
0.0171112737207060	0.1340425773147373	0.2161582620266401	T	T	T
0.1050090445771980	0.0631882945276743	0.7053375260957605	T	T	T
0.0129144869183133	0.9534810626371673	0.2198275157357399	T	T	T
0.8026455358045290	0.1330861611064830	0.4301852109605131	T	T	T
0.8129463232571257	0.9981662166974351	0.4354491472523160	T	T	T
0.8048765482624280	0.8690430253071124	0.3831574823396156	T	T	T
0.6014296614360192	0.1390024467514931	0.4343855971413154	T	T	T
0.5842378811097413	0.0069625556439420	0.4334875123145804	T	T	T

Structure files (CONTCAR) involved in this work:

0.5695055023913794	0.8756293358543764	0.4184124187783796	T	T	T
0.9211314624727363	0.0456872936928345	0.1727714374423923	T	T	T
0.6786967621440610	0.0513041852290432	0.1948995470498061	T	T	T
0.7704251776264154	0.1447159543217923	0.2364281210740432	T	T	T
0.0908175381016686	0.0710461143338700	0.9027343699832219	T	T	T
0.8970402694069708	0.1485113688725556	0.2930218944365973	T	T	T
0.9168717742596151	0.1680447825318893	0.0978090439183180	T	T	T
0.8106639375896585	0.1464842382256097	0.9843022823835871	T	T	T
0.6938714984037035	0.1560411073411730	0.0747610113359476	T	T	T
0.6409323221865729	0.1727912192203983	0.2516521089132493	T	T	T
0.7716167445430629	0.9651255827415482	0.2523816237039780	T	T	T
0.8965933860449319	0.9466442434316390	0.3035890886928878	T	T	T
0.9061645643662356	0.9233573198973456	0.1070316173709081	T	T	T
0.8013445446516941	0.9481423097490668	0.9896239028042881	T	T	T
0.6922488669478216	0.9328539919792924	0.1017634579680907	T	T	T
0.2016096369442913	0.0507282791200230	0.0081533354097537	T	T	T
0.6440021326482592	0.9381701317667215	0.2847850428084504	T	T	T
0.3166813631490192	0.0579719594365879	0.9099599194212264	T	T	T
0.4822285368640871	0.6322378917108756	0.7061498501308093	T	T	T
0.4868500242326420	0.4546976759423263	0.7180809132071511	T	T	T
0.6910431813448192	0.6311868864845966	0.9221183699850124	T	T	T
0.6863063824646939	0.4956592883622111	0.9314574411235347	T	T	T
0.6968058467868643	0.3672339636303668	0.8789047101348091	T	T	T
0.8978739280068918	0.6417711178697887	0.9276908528239112	T	T	T
0.9131208577924208	0.5085520906117849	0.9311083658802787	T	T	T
0.3578073660676347	0.0677240262550610	0.7231739961203619	T	T	T
0.9318275987736454	0.3768087951177445	0.9286160128858160	T	T	T
0.5818931980470644	0.5475416510813472	0.6811178771078298	T	T	T
0.8273276929008616	0.5496883087201611	0.7110011029999049	T	T	T
0.7237094579650368	0.6484943572210575	0.7280449615954990	T	T	T
0.5982397707330418	0.6596986004593351	0.7899533891433200	T	T	T
0.5861447927204088	0.6663184231401725	0.5930574286981454	T	T	T
0.6890780801539098	0.6457238943873681	0.4688014236029444	T	T	T
0.8088464485925630	0.6452252327058733	0.5564126242413912	T	T	T
0.8620130999477090	0.6835687492479776	0.7447461051693695	T	T	T
0.7286046626135161	0.4617559508447510	0.7480882669372733	T	T	T
0.6033517120188584	0.4418457435695870	0.7994423579196385	T	T	T
0.5917610768339200	0.4270074428617650	0.6024173835822203	T	T	T
0.6987317131776715	0.4462502981187885	0.4884718205357969	T	T	T
0.8110795522494744	0.4368590522169162	0.6035589430150869	T	T	T
0.8553277264468181	0.4300705509777102	0.7888172389482561	T	T	T
0.0156018048015060	0.3643668177078381	0.2126696687311359	T	T	T
0.0080635033447529	0.5518529467441158	0.2126567341121904	T	T	T
0.8006070628084730	0.3627869454329894	0.4465156052866049	T	T	T
0.9296412101227898	0.4527989821579350	0.3923048691391073	T	T	T
0.8065698466675463	0.3267187298704992	0.4952912776373388	T	T	T
1.0191274342925307	0.3952725913351541	0.4908233009437600	T	T	T
0.9788522689204128	0.4575622952489921	0.5667751190753040	T	T	T
0.0393978187900907	0.4823767766418523	0.4751065717862865	T	T	T
0.9991806005957479	0.4467107404045900	0.4923479758381175	T	T	T

Figure 2(a) Zn-IS

1.0000000000000000

20.0219993591000005 0.0000000000000000 0.0000000000000000

Structure files (CONTCAR) involved in this work:

0.0000000000000000 19.8990001678000006 0.0000000000000000
0.0000000000000000 0.0000000000000000 13.3830003737999998
93 3 194 2 5 1

Selective dynamics

Direct

0.4247171342385609	0.0567724569997377	0.6465395174485217	T	T	T
0.3054056157095704	0.0256479993467039	0.7911183933717073	T	T	T
0.2825575388532212	0.0594281293448225	0.0125672329076761	T	T	T
0.1229298077557921	0.0639051383725257	0.0113757860173090	T	T	T
0.0704269480429186	0.0297499681934660	0.7993441709580587	T	T	T
0.1810333105536111	0.0550014032957023	0.6551700533223683	T	T	T
0.4202160073502469	0.8260675734208204	0.6671810717978207	T	T	T
0.3049370330367807	0.8672810577753711	0.8095066190231408	T	T	T
0.2664271640313789	0.8269406217032967	0.0268223286225902	T	T	T
0.1120832714365616	0.8254746289974899	0.0088339740683553	T	T	T
0.0665513808223774	0.8725820867121192	0.7954119358023127	T	T	T
0.1843259051127119	0.8278179176710542	0.6697275836377192	T	T	T
0.0772433284238064	0.9414081207150388	0.1455846523768564	T	T	T
0.1958543119862939	0.9711274099500958	0.2901174903736755	T	T	T
0.2200855818926548	0.9376039143020319	0.5115059204639297	T	T	T
0.3795409924432102	0.9349870013027706	0.5110839110884396	T	T	T
0.4328066934997769	0.9679604377279782	0.2988947746936491	T	T	T
0.3208038455941585	0.9419410232975277	0.1560286896668877	T	T	T
0.0813036366382971	0.1725549875185322	0.1651634905321259	T	T	T
0.1959782859522301	0.1290830107619653	0.3073684505755517	T	T	T
0.2344833063876027	0.1702177932698493	0.5243217395146986	T	T	T
0.3891698862612279	0.1728808539403271	0.5101530752001732	T	T	T
0.4370895886230983	0.1261481864515873	0.2972271902094843	T	T	T
0.3177907052053255	0.1690314747324751	0.1712168334801231	T	T	T
0.5774695079203310	0.5550401976591585	0.3487433109361096	T	T	T
0.6942513778003400	0.5239783184100122	0.1974229504565240	T	T	T
0.7153213938939325	0.5675284994894120	0.9813677180220582	T	T	T
0.8729418373569175	0.5721647880354931	0.9823740465415013	T	T	T
0.8059904167009651	0.5526750758433479	0.3451704711194151	T	T	T
0.5746982696335777	0.3267727396932692	0.3266049073365770	T	T	T
0.6950961586496751	0.3698693957919627	0.1857373714636337	T	T	T
0.7305388439979142	0.3257350757707426	0.9735518745832760	T	T	T
0.8853355644995539	0.3254788786115747	0.9940218674077882	T	T	T
0.9386039888765318	0.3742962383295530	0.1944625706611994	T	T	T
0.9210725124804187	0.4442264743230695	0.8599811664698928	T	T	T
0.8017511998731007	0.4700096414752803	0.7161688124825336	T	T	T
0.7734628192552591	0.4348319556823328	0.4920011019173611	T	T	T
0.6140157219201723	0.4295674684309677	0.4869301910409994	T	T	T
0.5654429550584773	0.4687721739339824	0.7004894351665518	T	T	T
0.6765898632135527	0.4475795008851300	0.8508606865923780	T	T	T
0.9204614867869840	0.6763989610915874	0.8245428349889501	T	T	T
0.7628989085594879	0.6702416332427633	0.4652455519252536	T	T	T
0.6093233048212816	0.6730500719665417	0.4839406754386558	T	T	T
0.5587547867971671	0.6271710411271330	0.6959184644365070	T	T	T
0.6785677947714023	0.6700926868159225	0.8181625059783604	T	T	T
0.5778628853718111	0.9438166026501229	0.3534352861653730	T	T	T
0.6984161655578817	0.9704151886370278	0.2089016122133351	T	T	T
0.7220494774854593	0.9322045460941529	0.9886398849860631	T	T	T

Structure files (CONTCAR) involved in this work:

0.8823772543335086	0.9325791749660619	0.9909505806235058	T	T	T
0.9328568674985930	0.9682445004493657	0.2022189270336920	T	T	T
0.8221504719818002	0.9446120952826380	0.3504891769564931	T	T	T
0.5803478930394822	0.1711436576510538	0.3278270239208045	T	T	T
0.6989694737406649	0.1278046432477817	0.1888533169585535	T	T	T
0.7335087455853557	0.1700796999409229	0.9694927027803466	T	T	T
0.8886325146039386	0.1729814233085715	0.9831103018753348	T	T	T
0.9372952151412800	0.1263196247352028	0.1964202231599441	T	T	T
0.8200494791032222	0.1688765484795901	0.3259945725124209	T	T	T
0.9249197740042867	0.0545757420431001	0.8543120251090703	T	T	T
0.8050899883835557	0.0250421755138305	0.7062037048062544	T	T	T
0.7824028549854706	0.0635621006762404	0.4892025782100007	T	T	T
0.6220893894107495	0.0674464984376032	0.4878193413010221	T	T	T
0.5696206583929472	0.0293084102123652	0.6979035071125336	T	T	T
0.6813963346867808	0.0500042689674112	0.8463208603401291	T	T	T
0.9248203115150319	0.8289068314449589	0.8307816901566363	T	T	T
0.8042419214289357	0.8688090098566870	0.6905309267172403	T	T	T
0.7672050135211820	0.8265281727307099	0.4743750250938311	T	T	T
0.6131251585679343	0.8265100305896175	0.4873493232061323	T	T	T
0.5646771815077258	0.8719519082365186	0.6976102639606526	T	T	T
0.6821979005947990	0.8296178532892498	0.8263236987704263	T	T	T
0.4218600672697581	0.4428594745741565	0.6422532517493957	T	T	T
0.3023815810768439	0.4710795941764033	0.7871461185153289	T	T	T
0.2794960018307587	0.4361368994777986	0.0071571690508919	T	T	T
0.1210758262272978	0.4353227385950149	0.0095687763226293	T	T	T
0.0655821563761374	0.4685660705909834	0.7972707980131939	T	T	T
0.1772408602549032	0.4434256643432415	0.6526090812384817	T	T	T
0.4171584629976953	0.6724063500921379	0.6616504207232955	T	T	T
0.3010181428986393	0.6289943416042413	0.8030132696604170	T	T	T
0.2663418600407753	0.6698009787393954	0.0210506058094316	T	T	T
0.1119588506753801	0.6715630132946289	0.0055902266619962	T	T	T
0.0629506639909866	0.6272199821663320	0.7931308753588396	T	T	T
0.1806027127135584	0.6690159889357474	0.6665810861657810	T	T	T
0.0743169688059861	0.5568958370471374	0.1462261378653315	T	T	T
0.1954150374865059	0.5267434347404100	0.2858612004059520	T	T	T
0.2180436831057422	0.5607940752265314	0.5089758852872419	T	T	T
0.3778371158474995	0.5651626756234402	0.5074383348697211	T	T	T
0.4309637982198767	0.5280242972710666	0.2958567279399001	T	T	T
0.3209589831276441	0.5526805163251067	0.1496106336770554	T	T	T
0.0826095343661553	0.3260697714455097	0.1605266494021362	T	T	T
0.1952541183487938	0.3688347356119925	0.3055783728545713	T	T	T
0.2327523021859648	0.3283029358294360	0.5232099935203453	T	T	T
0.3871554351697333	0.3266041082100658	0.5052837837663218	T	T	T
0.4329796494751405	0.3700854597337335	0.2906534893222277	T	T	T
0.3141420771503757	0.3276315370308841	0.1662209590995440	T	T	T
0.9267579678700392	0.5336631235330935	0.1916212030522492	T	T	T
0.8183314465279993	0.3300622069728247	0.3229065511286150	T	T	T
0.8041464014101688	0.6323877597057190	0.6815103167294519	T	T	T
0.3592724223849054	0.0607428536143631	0.7175291921292679	T	T	T
0.3074060361029530	0.0645239127535042	0.8975503095287242	T	T	T
0.2022747818921116	0.0481817080956233	0.0185311097470922	T	T	T
0.0990511584555513	0.0695621138647680	0.8962226381344234	T	T	T
0.1055439153680130	0.0587388652848329	0.6989300989756114	T	T	T

Structure files (CONTCAR) involved in this work:

0.2307864367896636	0.0314368430254384	0.7445356889818495	T	T	T
0.3607564932293035	0.8251319983152806	0.7490855161347618	T	T	T
0.3066853989899491	0.8420675465795167	0.9242346995466258	T	T	T
0.1893018239784626	0.8511403217773869	0.0131811587797800	T	T	T
0.0855464639538066	0.8299776516614331	0.8947806019605111	T	T	T
0.1067017114922778	0.8421165284883259	0.6996539389326850	T	T	T
0.2313359004042921	0.8534610497628587	0.7616401318585778	T	T	T
0.3235733075765084	0.9466011485856497	0.8041167894985081	T	T	T
0.0876448120293254	0.9504114338899770	0.8128871955053095	T	T	T
0.4326309887837916	0.1273246943311020	0.5866447067385605	T	T	T
0.4191678841095836	0.9958323628190447	0.5659366785105058	T	T	T
0.3955168221075978	0.8643820370200118	0.5665627114677317	T	T	T
0.2014720869586568	0.1291869737893767	0.6162180430383309	T	T	T
0.1827821070157936	0.0007739945340931	0.5643792843175641	T	T	T
0.2025745382082396	0.8672248190307854	0.5670308029966015	T	T	T
0.9906664090941404	0.0408582371583258	0.7866857318102705	T	T	T
0.9867122556197406	0.8668792430728152	0.7744201559322765	T	T	T
0.1430884867018426	0.9348025531977388	0.2156936162486558	T	T	T
0.1937332971643372	0.9326387787922904	0.3970624824641202	T	T	T
0.3000809340470066	0.9510640189630656	0.5153258007233109	T	T	T
0.4046287150102814	0.9284976155150703	0.3965671834562517	T	T	T
0.3962767756821047	0.9390499506295928	0.1996050603099213	T	T	T
0.2709312834883942	0.9661434354537455	0.2450054915021893	T	T	T
0.1415304697425265	0.1726885629208444	0.2460599713554243	T	T	T
0.1939302641211844	0.1541424167272426	0.4222703022961526	T	T	T
0.3119033943467996	0.1471623858797168	0.5104236158153730	T	T	T
0.4187745904623210	0.1675055168790978	0.3979973465856483	T	T	T
0.3954727027915759	0.1580296714742083	0.2038326839599064	T	T	T
0.2703340756086495	0.1411038889106804	0.2612795756585488	T	T	T
0.1760121391088159	0.0499718778679532	0.3017601747331509	T	T	T
0.4170989829832186	0.0477055540147293	0.3118103508463721	T	T	T
0.0674849233284789	0.8722235851733495	0.0825506961633793	T	T	T
0.0830236952175947	0.0037487561262719	0.0675065815465043	T	T	T
0.1056370840372647	0.1352149831334230	0.0636959711217108	T	T	T
0.3004509154268375	0.8673763280127036	0.1184784338470491	T	T	T
0.3186782620111060	0.9949443317850352	0.0637174792224024	T	T	T
0.3028216760500014	0.1288182350744729	0.0681911113774786	T	T	T
0.5122116864821505	0.9549259220781390	0.2845078543670834	T	T	T
0.5169189100593546	0.1328725614086474	0.2762084959329477	T	T	T
0.6416736911554726	0.5571157496497529	0.2751124143020574	T	T	T
0.7010741863196500	0.5726624978259794	0.1010129836476486	T	T	T
0.7942429620444396	0.5573668676108620	0.9573077263673243	T	T	T
0.8862377411960192	0.5781875908531287	0.0998568207435658	T	T	T
0.8872291774244868	0.5536491751144962	0.3144268452120978	T	T	T
0.7672476526127466	0.5189546837796699	0.2533560645604458	T	T	T
0.6415543019086152	0.3348684103559545	0.2607591772864998	T	T	T
0.6895908658476159	0.3324960701863171	0.0775704838083050	T	T	T
0.8077844133270919	0.3495486175817283	0.9895764145197856	T	T	T
0.9104699183079655	0.3227280589937267	0.1098816148977564	T	T	T
0.9066768670078567	0.3514511988818633	0.3050040533501044	T	T	T
0.7688617919525181	0.3648632781862978	0.2319080816425957	T	T	T
0.6726110671127647	0.4482856467008123	0.1681136061034677	T	T	T
0.9149430634357539	0.4491433385715648	0.1733286460734408	T	T	T

Structure files (CONTCAR) involved in this work:

0.5696146586385816	0.6274658880851012	0.4028806801082769	T	T	T
0.5870400409881886	0.4977760506339162	0.4345335739708294	T	T	T
0.5823387397224742	0.3636766397594294	0.4348705169746753	T	T	T
0.7854544624581410	0.6298814897105688	0.3637747757773709	T	T	T
0.7980648048676552	0.5093007765697887	0.4493682404499476	T	T	T
0.8175645251011255	0.3782807898340133	0.4356172272991224	T	T	T
0.0094572341736011	0.5523915310141374	0.2162181179504202	T	T	T
0.0190692518990447	0.3668037148480359	0.2059796891909661	T	T	T
0.8560507377677398	0.4329503823779932	0.7866593236645304	T	T	T
0.7947517137325566	0.4303617702138378	0.6095818029252312	T	T	T
0.6949886864888107	0.4258898897586042	0.4737065045837231	T	T	T
0.5956052343429756	0.4288883525217456	0.6042672232126715	T	T	T
0.6033659798026387	0.4423388354843724	0.8001606745674561	T	T	T
0.7295432458915730	0.4761578809652971	0.7668828871791926	T	T	T
0.8620401533555931	0.6789272064076081	0.7440111897996772	T	T	T
0.8135280686962982	0.6494266801678449	0.5536997686836945	T	T	T
0.6868334430291074	0.6481838440310702	0.4925737003450968	T	T	T
0.5748281920999736	0.6664238670572981	0.5923402935194214	T	T	T
0.5997388165497984	0.6611579268960576	0.7873155900319826	T	T	T
0.7254764760803473	0.6370464444384790	0.7333170408923374	T	T	T
0.8349594010344582	0.5439690866675631	0.6821263931694963	T	T	T
0.5786854309712859	0.5484031846607927	0.6842801647626738	T	T	T
0.9304890289932884	0.3774545837353843	0.9285472812991491	T	T	T
0.9138869510253471	0.5095421000770810	0.9306542803132841	T	T	T
0.8972588116651942	0.6409076654169222	0.9282793926437101	T	T	T
0.6981732026474056	0.3731465933044754	0.8873109565935978	T	T	T
0.6751049393492455	0.5011380171799089	0.9418181244187307	T	T	T
0.6884776774970472	0.6351442342961808	0.9278057099373775	T	T	T
0.4865167920350861	0.4524737934333854	0.7142477061257099	T	T	T
0.4787750837754582	0.6335728608545084	0.7165456843822745	T	T	T
0.6428434591102904	0.9371967937551835	0.2818814672142281	T	T	T
0.7007319913776270	0.9278877740993058	0.1054342307214704	T	T	T
0.8023824129365954	0.9409538670488948	0.9765796547240241	T	T	T
0.9016352818591842	0.9267964658032773	0.1083363971359669	T	T	T
0.8974927161738797	0.9446403983667769	0.3055889531872527	T	T	T
0.7712044081984868	0.9667449555620363	0.2619760747864746	T	T	T
0.6433631562304847	0.1686358065400630	0.2523052536949216	T	T	T
0.6973820523089306	0.1578695762352982	0.0763157553470547	T	T	T
0.8114534925110147	0.1474732298245160	0.9787123778803586	T	T	T
0.9161204483046640	0.1670946767840555	0.0963611528492203	T	T	T
0.8976678000842727	0.1559887200425529	0.2924125351164475	T	T	T
0.7725247239741949	0.1370884485879532	0.2380310225851414	T	T	T
0.6795099774954935	0.0484059543416076	0.1867704320010542	T	T	T
0.9197455652357290	0.0474385184693371	0.1814477787304520	T	T	T
0.5681480492271397	0.8747614474779040	0.4168204504756375	T	T	T
0.5843790694654390	0.0056561783364537	0.4321172951966271	T	T	T
0.6003325192168204	0.1373718655872817	0.4344359114254486	T	T	T
0.8062488409180139	0.8692085846314558	0.3897496015491797	T	T	T
0.8173579003306934	0.9963431261336457	0.4438524774513357	T	T	T
0.8071446150027342	0.1299954863779588	0.4311631824525061	T	T	T
0.0120591990576713	0.9526706826458083	0.2155541373157565	T	T	T
0.0171472432225738	0.1352114838710958	0.2147956414811420	T	T	T
0.8598840768600977	0.0553739941026225	0.7826526985121403	T	T	T

Structure files (CONTCAR) involved in this work:

0.8042059523850669	0.0707033333305085	0.6056828532938877	T	T	T
0.7019052900007292	0.0555420068305908	0.4786068006290684	T	T	T
0.5997198814579667	0.0718351291165609	0.6041956773684203	T	T	T
0.6061161426953187	0.0499880942372697	0.8015633355425973	T	T	T
0.7317865172731306	0.0268613220639412	0.7576605995195962	T	T	T
0.8596740304559911	0.8326207010784104	0.7594957886133323	T	T	T
0.8046150367290893	0.8324099024121751	0.5817616988168389	T	T	T
0.6904015747897811	0.8526273132471154	0.4842529701874061	T	T	T
0.5869655196996133	0.8270606776976949	0.6018623334130716	T	T	T
0.6050565668254195	0.8467995039856235	0.7961629284988314	T	T	T
0.7305445665557856	0.8619347103899795	0.7405488419123722	T	T	T
0.8230863295318945	0.9477759396745158	0.6775029962992711	T	T	T
0.5813202332571591	0.9501044288579661	0.6737473342839368	T	T	T
0.9332216667002466	0.1275386605531338	0.9077015267143531	T	T	T
0.9189016644329330	0.9974867238655322	0.9409903478245186	T	T	T
0.9086532740760302	0.8644809201560754	0.9373976579829228	T	T	T
0.6979492228310107	0.1257209981898833	0.8832893505774754	T	T	T
0.6861348216721143	-0.0023115177738859	0.9393288529021115	T	T	T
0.6985113018219911	0.8630996910965687	0.9345094750073047	T	T	T
0.4908328088730761	0.0454517593265694	0.7143163374244060	T	T	T
0.4849837965874103	0.8627317604679087	0.7164263717974118	T	T	T
0.3551495345152666	0.4368339664324226	0.7104739782878335	T	T	T
0.3050047642330417	0.4303627664181177	0.8922810011890203	T	T	T
0.2001739486032394	0.4538151914453849	0.0116365012400196	T	T	T
0.0945160644466235	0.4306720871037673	0.8953958328539641	T	T	T
0.1015849402465671	0.4401469658386920	0.6969205760327724	T	T	T
0.2272359586757985	0.4664329191874015	0.7420768382757517	T	T	T
0.3532882407328883	0.6710935031755398	0.7357570998914065	T	T	T
0.3045950633988562	0.6585162959079145	0.9154961318101128	T	T	T
0.1891566673395157	0.6458397340893079	0.0089304991912792	T	T	T
0.0857039041251395	0.6692118141045633	0.8911175713134589	T	T	T
0.1024267871179808	0.6567812794930072	0.6957356704442640	T	T	T
0.2261546408216270	0.6388351167803988	0.7572269528528889	T	T	T
0.3212245721586433	0.5498461740949947	0.8033891795980511	T	T	T
0.0808475255539201	0.5483209376700654	0.8082256685916375	T	T	T
0.4318618403563994	0.3748474299001296	0.5766077576150170	T	T	T
0.4182094994577794	0.5061375022929959	0.5655527600065829	T	T	T
0.3970456724250203	0.6372126831725432	0.5561821446003294	T	T	T
0.1975018636936723	0.3691138154773160	0.6135765479281136	T	T	T
0.1805536826434102	0.4973558247749709	0.5613271160705181	T	T	T
0.1969152250367379	0.6311065374674342	0.5619070740168545	T	T	T
0.9854699277203786	0.4540347611603212	0.7864660111366500	T	T	T
0.9833138325156801	0.6348431192306379	0.7745865172348843	T	T	T
0.1420569504683148	0.5636362409933063	0.2135064896346066	T	T	T
0.1950208384688755	0.5649693725799921	0.3930860897834629	T	T	T
0.2983765401920662	0.5499921831542111	0.5180798507306258	T	T	T
0.4004625002083470	0.5678970994710157	0.3914388028540811	T	T	T
0.3961637143140320	0.5559288217528949	0.1946724746609364	T	T	T
0.2699833160323705	0.5308454113356696	0.2385031271826002	T	T	T
0.1407511237573994	0.3253925085709432	0.2444143916769679	T	T	T
0.1927897370118735	0.3432175937867614	0.4201939705860710	T	T	T
0.3099376139672010	0.3524703839977008	0.5099286376460962	T	T	T
0.4129596038244667	0.3279877393781236	0.3904017302515089	T	T	T

Structure files (CONTCAR) involved in this work:

0.3918758221874523	0.3424126102431072	0.1942324429605073	T	T	T
0.2691819864804607	0.3559475896380704	0.2588384745432337	T	T	T
0.1755920462771897	0.4479452409880191	0.2996218204067483	T	T	T
0.4155999925140840	0.4485259769618052	0.3106966007413337	T	T	T
0.0672849428659301	0.6238814697074316	0.0766315259008550	T	T	T
0.0800666399018848	0.4918685344618855	0.0715766303598225	T	T	T
0.1092079548529333	0.3616064144964595	0.0588389585158894	T	T	T
0.3022154430791627	0.6266104386127653	0.1080871358738202	T	T	T
0.3198261879731455	0.4972648718162905	0.0604161343897952	T	T	T
0.2940786106434420	0.3649700556940262	0.0625171101759367	T	T	T
0.5107723299057541	0.5400957583417029	0.2842370823629431	T	T	T
0.5120150202445153	0.3601835102068696	0.2668288423551011	T	T	T
0.4380940504119782	0.7493052965405671	0.6371602397081328	T	T	T
0.1954059832450513	0.7482650926732300	0.6498060336637004	T	T	T
0.2701470550392434	0.7478920560867577	0.0540329923468061	T	T	T
0.1063165892011850	0.7482429243130452	0.0464426744865814	T	T	T
0.0620322045028387	0.2491986317516057	0.1353119461917418	T	T	T
0.3025409308148541	0.2477992103247715	0.1507203217916934	T	T	T
0.2294367736597127	0.2493263734054249	0.5510452044715790	T	T	T
0.3933510895794000	0.2503808479960129	0.5470370911869946	T	T	T
0.5602279528749504	0.2484493408505623	0.3495536244322755	T	T	T
0.8058629984841348	0.2468486480452422	0.3429266802292085	T	T	T
0.7273719224199384	0.2483112205338114	0.9357722814722778	T	T	T
0.8937185170415689	0.2507935979797633	0.9469345500843800	T	T	T
0.9456182758976800	0.7518655219730247	0.8530177502048227	T	T	T
0.6941879439381089	0.7496778020130339	0.8332863432459597	T	T	T
0.7685367632477421	0.7490486315193325	0.4371678617169596	T	T	T
0.6068758243701395	0.7502454172707222	0.4455396920606699	T	T	T
0.9550899684958660	0.4726034284773477	0.5026186425443518	T	T	T
0.9428482019211549	0.6327293023630104	0.4332867086327201	T	T	T
0.9198891608987342	0.4106903689346336	0.4189073176846362	T	T	T
0.9004505948338024	0.5175069836462628	0.5841660800504547	T	T	T
0.9143086275118524	0.5868831949258102	0.3637573971912240	T	T	T
0.0212785263671792	0.6455728948074314	0.3363743763129970	T	T	T
0.0290445536407693	0.6916780367223941	0.4512322576689278	T	T	T
0.9722189672911370	0.7200124457039265	0.3547938510412234	T	T	T
0.9095788354044090	0.6588313278925555	0.4707182019439903	T	T	T
0.9946682888129916	0.6761022354933681	0.3916647818010092	T	T	T

Figure 2(a) Zn-TS

1.0000000000000000

20.0219993591000005 0.0000000000000000 0.0000000000000000

0.0000000000000000 19.8990001678000006 0.0000000000000000

0.0000000000000000 0.0000000000000000 13.3830003737999998

93 3 194 2 5 1

Selective dynamics

Direct

0.4248002841479378	0.0561787980228706	0.6445286540159375	T	T	T
0.3037717690835264	0.0249286850886851	0.7880209903831334	T	T	T
0.2827624913990209	0.0604132097444172	0.0091430336020337	T	T	T
0.1236261204619822	0.0619263950848340	0.0088326711899738	T	T	T
0.0715791046536861	0.0282913195497205	0.7971190062031218	T	T	T
0.1798042473865757	0.0537444538305901	0.6489302708362397	T	T	T
0.4210580746670016	0.8266028093578505	0.6643412783243604	T	T	T

Structure files (CONTCAR) involved in this work:

0.3039229220954947	0.8668552225458508	0.8070594929168727	T	T	T
0.2660089902017638	0.8260961329926996	0.0246354240026420	T	T	T
0.1115428339754841	0.8245005376523651	0.0095869187503773	T	T	T
0.0659754889004069	0.8715323803284448	0.7959950914782086	T	T	T
0.1827221030298663	0.8276722062168598	0.6676460030124193	T	T	T
0.0768118218007509	0.9409298097976933	0.1440838965750843	T	T	T
0.1971294032518538	0.9710562092174979	0.2873034497923145	T	T	T
0.2196420413362499	0.9365800922395223	0.5085859935138171	T	T	T
0.3790964423692761	0.9350204851523090	0.5091941092869150	T	T	T
0.4314691379732871	0.9686639741983158	0.2970716235445233	T	T	T
0.3217837488826313	0.9433852294182863	0.1495323345533656	T	T	T
0.0810133808998040	0.1699629178799179	0.1624693956903639	T	T	T
0.1966682290662097	0.1282665794871274	0.3060428625212615	T	T	T
0.2339594373693336	0.1710603458549811	0.5228951581668716	T	T	T
0.3886701932195338	0.1732700737021242	0.5105490076825304	T	T	T
0.4365368932680915	0.1269529795626248	0.2968544497085397	T	T	T
0.3178037728032618	0.1687684860664948	0.1692475260601216	T	T	T
0.5748863435336365	0.5555884947733098	0.3504267721661996	T	T	T
0.6899445314124126	0.5260088022193057	0.2015643898840244	T	T	T
0.7158008483420046	0.5682888547597037	0.9838252913223118	T	T	T
0.8732339402247005	0.5733578257240861	0.9858347409118013	T	T	T
0.8100355500942845	0.5485331947791066	0.3504927759117116	T	T	T
0.5739978144113767	0.3277454529489571	0.3274149966915316	T	T	T
0.6943037268533971	0.3718441712686838	0.1882601691425537	T	T	T
0.7312774021873103	0.3266615696520597	0.9759930424278140	T	T	T
0.8861746463124079	0.3245718762495398	0.9947161901805568	T	T	T
0.9428391268618200	0.3745990145832317	0.1884350431080372	T	T	T
0.9205194159998749	0.4445979509080119	0.8636101793065429	T	T	T
0.8017116768440342	0.4694813111118658	0.7185928562915841	T	T	T
0.7749183452918514	0.4345144949543713	0.4968158452639476	T	T	T
0.6161924029854575	0.4293728038446171	0.4877343076100344	T	T	T
0.5666295743339551	0.4692762172211949	0.7014791835860195	T	T	T
0.6769803143712237	0.4475210425518250	0.8525754007307310	T	T	T
0.9204559833557417	0.6761648871483514	0.8290710300228922	T	T	T
0.7689753710114122	0.6694913053080624	0.4628818014906259	T	T	T
0.6137456012834779	0.6720567895461744	0.4804917856991476	T	T	T
0.5625827319601260	0.6276841864775181	0.6942731035647447	T	T	T
0.6753141437917360	0.6702590832983237	0.8242809830732090	T	T	T
0.5772365440659420	0.9439795895964165	0.3540300453727424	T	T	T
0.6978943515953143	0.9716247017409650	0.2094938097312782	T	T	T
0.7206096589847603	0.9339298113420191	0.9889399319502566	T	T	T
0.8807240920668782	0.9326423646381758	0.9904748852048093	T	T	T
0.9321823504408112	0.9684326557443325	0.2002910035668777	T	T	T
0.8224188043739505	0.9461078552756356	0.3499654939812925	T	T	T
0.5793508905423814	0.1724216974869030	0.3280850602403387	T	T	T
0.6990171187358436	0.1298859586336433	0.1907078623077205	T	T	T
0.7332914564248960	0.1706551445174485	0.9704724418556394	T	T	T
0.8881509118902567	0.1725771890742443	0.9827050578271112	T	T	T
0.9365830425635732	0.1258444182902451	0.1955983678544210	T	T	T
0.8213648311529729	0.1721407896433446	0.3271455121913741	T	T	T
0.9251973420045171	0.0539001099796024	0.8537165484466617	T	T	T
0.8046120146265208	0.0251120467594978	0.7054926065949666	T	T	T
0.7819738889390084	0.0661240517366742	0.4877648583363594	T	T	T

Structure files (CONTCAR) involved in this work:

0.6218082108234647	0.0680458316114708	0.4867529721982677	T	T	T
0.5700858411596521	0.0291809986844243	0.6967585843815960	T	T	T
0.6807291447769004	0.0513866214652818	0.8466734860725280	T	T	T
0.9236588145084103	0.8289083159004544	0.8308530109309588	T	T	T
0.8035635539681942	0.8681308132178206	0.6895821995467698	T	T	T
0.7685968927837419	0.8256575687022052	0.4727613217360693	T	T	T
0.6141718614480908	0.8257680396491242	0.4863184486597666	T	T	T
0.5654593635229830	0.8717164441227864	0.6966591741973738	T	T	T
0.6817554915829439	0.8294136273614627	0.8276837971555284	T	T	T
0.4217667297318859	0.4435467822206581	0.6434631316515448	T	T	T
0.3011203833823127	0.4712923767094320	0.7866312454186741	T	T	T
0.2778616988315387	0.4357119957604074	0.0075394638372603	T	T	T
0.1199866185885443	0.4350288530837534	0.0119124115098028	T	T	T
0.0648408357640200	0.4692585181859352	0.7985216926612043	T	T	T
0.1751250391410209	0.4439229524431194	0.6514339195131065	T	T	T
0.4179211212396088	0.6724135319996808	0.6583728930400242	T	T	T
0.3021733780906251	0.6288579144686027	0.8017813668954590	T	T	T
0.2654815752554169	0.6696569037760807	0.0206256208455051	T	T	T
0.1113211090009436	0.6707354184587884	0.0061912479495835	T	T	T
0.0621416269035298	0.6279063240628869	0.7928287286169855	T	T	T
0.1802767419695073	0.6692877956627690	0.6642699172597684	T	T	T
0.0722404837613220	0.5561042053792472	0.1465144321394194	T	T	T
0.1945029949980496	0.5247002359751447	0.2843582342359692	T	T	T
0.2144812955968319	0.5603492731549270	0.5088719813584734	T	T	T
0.3734892719222958	0.5649891542884597	0.5094467996011564	T	T	T
0.4260221196877475	0.5260866544139786	0.2992352446279898	T	T	T
0.3205792390757057	0.5518122033711145	0.1471781954804477	T	T	T
0.0845596131465363	0.3229820706058666	0.1595308806307613	T	T	T
0.1963052729292860	0.3672996370756045	0.3042766069777066	T	T	T
0.2322650384564455	0.3283532190730337	0.5230320831618952	T	T	T
0.3866958142648203	0.3268109692041107	0.5061871043958365	T	T	T
0.4316920196287065	0.3690693427032218	0.2913162133295608	T	T	T
0.3143744249439344	0.3271595152011533	0.1658911613749636	T	T	T
0.9231421483011636	0.5288138712892024	0.1921004420680839	T	T	T
0.8218443279663199	0.3354914709188146	0.3227612789376088	T	T	T
0.8003231741877257	0.6323572156476983	0.6888588687427945	T	T	T
0.3595569881856892	0.0581415025179262	0.7160128232274543	T	T	T
0.3026347794071608	0.0667913994074033	0.8920836023357352	T	T	T
0.2029614722083448	0.0479191836645844	0.0221322077221724	T	T	T
0.1032382476372799	0.0677755269250196	0.8921972617930597	T	T	T
0.1048465683235550	0.0563748347600027	0.6947165341757889	T	T	T
0.2307680865649056	0.0285863733356038	0.7357273089014533	T	T	T
0.3601425799396942	0.8271328199410130	0.7439873810454729	T	T	T
0.3047682753562149	0.8376367010378957	0.9197546780658234	T	T	T
0.1887174841956286	0.8504608541508809	0.0131561023567673	T	T	T
0.0847923645737065	0.8291926958205751	0.8957474029140328	T	T	T
0.1050947230673707	0.8391925232884068	0.7002337492385513	T	T	T
0.2305524011411504	0.8541319523908499	0.7575587000889143	T	T	T
0.3212619101873498	0.9464450010768777	0.8085966152840117	T	T	T
0.0890684040054038	0.9489366919870820	0.8106266810134277	T	T	T
0.4321210606698760	0.1276366716762570	0.5869375913159183	T	T	T
0.4190372465464497	0.9966555299180346	0.5614742533111048	T	T	T
0.3988027324263357	0.8646392528808238	0.5623359112475164	T	T	T

Structure files (CONTCAR) involved in this work:

0.1991753719157159	0.1285921134101805	0.6118034917739225	T	T	T
0.1809071862568785	0.0009601740406029	0.5558578239055647	T	T	T
0.1977499501660660	0.8672013326507866	0.5639152646007083	T	T	T
0.9918547497105824	0.0401075919964845	0.7879862298677467	T	T	T
0.9859946822282403	0.8677246963836853	0.7765060716984838	T	T	T
0.1422859306108780	0.9358036386299801	0.2151915133345528	T	T	T
0.1988726152312693	0.9293620543979210	0.3918300577303486	T	T	T
0.2994149380899140	0.9485835414237024	0.5212173671039314	T	T	T
0.3997194214040740	0.9294398338881220	0.3926456913629733	T	T	T
0.3965088584545144	0.9406099988100250	0.1958713182453706	T	T	T
0.2703858510879593	0.9687522756772301	0.2358387564547862	T	T	T
0.1418474040805744	0.1692266327243653	0.2420546631529759	T	T	T
0.1950933985870180	0.1578782387728172	0.4185269331894708	T	T	T
0.3113641876411711	0.1474975011906118	0.5110723987106380	T	T	T
0.4177555104613806	0.1677277245176144	0.3980862202172507	T	T	T
0.3953551758828431	0.1591161694203846	0.2031629214753519	T	T	T
0.2706211701726847	0.1384076135417310	0.2578277289478791	T	T	T
0.1770510487830689	0.0489481616635155	0.3074395047652208	T	T	T
0.4164350077393418	0.0484618640913225	0.3103390449036159	T	T	T
0.0670769626039406	0.8702166837166111	0.0847612347484616	T	T	T
0.0832605781057651	0.0007130422857737	0.0618932841414043	T	T	T
0.1034157422421563	0.1324286252247630	0.0603983946456020	T	T	T
0.3017577538302967	0.8684463885636355	0.1127701059731594	T	T	T
0.3212511116479034	0.9956958583769580	0.0561283509492238	T	T	T
0.3044289113071563	0.1295246032119291	0.0647009579027229	T	T	T
0.5108223422818151	0.9544420356175412	0.2863628655545055	T	T	T
0.5162847720156412	0.1336705703709225	0.2761200142966118	T	T	T
0.6312587367707483	0.5625100677386566	0.2647386004581807	T	T	T
0.7049835986044043	0.5716174188168687	0.1039170039679775	T	T	T
0.7946484616482993	0.5637878354541440	0.9547120332086199	T	T	T
0.8831208087920956	0.5776706051040130	0.1045089988089627	T	T	T
0.8837907676556603	0.5263948447550645	0.3114569707263382	T	T	T
0.7559862659974289	0.5218808014781768	0.2713070480658715	T	T	T
0.6405872241966921	0.3344689307383259	0.2608580777920984	T	T	T
0.6901539829564883	0.3349566391423917	0.0794306845726894	T	T	T
0.8087995352530479	0.3495503798038614	0.9923293678832732	T	T	T
0.9126392678648058	0.3196119251922124	0.1099985483834826	T	T	T
0.9067510958140869	0.3644249445599381	0.2989661838663547	T	T	T
0.7679097090472272	0.3677327145291733	0.2347876102393731	T	T	T
0.6693834459007100	0.4496547991361534	0.1726260703024494	T	T	T
0.9297629038074295	0.4481875454746907	0.1469971719339940	T	T	T
0.5663896580445404	0.6267555830874139	0.4083821955168424	T	T	T
0.5934025925058880	0.4981834105305322	0.4325839274683116	T	T	T
0.5821075946377545	0.3646663594025129	0.4354499496134749	T	T	T
0.8042553506975850	0.6289040054509196	0.3696470493931839	T	T	T
0.7965648983378699	0.5114832893881494	0.4608102684803727	T	T	T
0.8215338278404822	0.3830506938787758	0.4353509448114172	T	T	T
0.0067771440541488	0.5550474933361653	0.2188889226148590	T	T	T
0.0218167601156837	0.3611851232244807	0.2103577999221995	T	T	T
0.8553695177424979	0.4336084405800690	0.7912955100861404	T	T	T
0.7962194775108127	0.4275654617629499	0.6140946665319743	T	T	T
0.6968567686137361	0.4217247754490264	0.4782010023417970	T	T	T
0.5956496001840236	0.4296191583857192	0.6044627495071609	T	T	T

Structure files (CONTCAR) involved in this work:

0.6033413195108640	0.4425004050081033	0.8021976923262677	T	T	T
0.7288812492355495	0.4756395824198711	0.7675411223051247	T	T	T
0.8580502883220704	0.6765755038664438	0.7560294873115649	T	T	T
0.8089404796066366	0.6524008012577158	0.5634387150731146	T	T	T
0.6906696363487708	0.6460300133373130	0.4712286326224240	T	T	T
0.5877302707485828	0.6665223562820559	0.5945965881253185	T	T	T
0.5965671251652012	0.6623114522540674	0.7915953446845500	T	T	T
0.7215091013907644	0.6361210600456343	0.7399417709262677	T	T	T
0.8317072672934005	0.5444558117068010	0.6849453679272108	T	T	T
0.5817046064792951	0.5485867331346952	0.6860550819605483	T	T	T
0.9312122866922794	0.3768385087591228	0.9296440929100621	T	T	T
0.9127169569358030	0.5096809727514496	0.9345197874703711	T	T	T
0.9041971425499554	0.6411906104346342	0.9361513476748932	T	T	T
0.6988213016326538	0.3730495120698850	0.8886332387234672	T	T	T
0.6775178123528813	0.5006387331195584	0.9442629462838666	T	T	T
0.6838153917568340	0.6350799848103138	0.9339314902500644	T	T	T
0.4871147378489378	0.4540694876100894	0.7135000512169803	T	T	T
0.4817120380904353	0.6331024420414800	0.7045465347069404	T	T	T
0.6418882346631424	0.9385307277748641	0.2817826406844726	T	T	T
0.6989228110769520	0.9296885656962921	0.1054907094787317	T	T	T
0.8009663707035659	0.9434725094843499	0.9776508586906164	T	T	T
0.9010013787622710	0.9260054433749466	0.1074444282585146	T	T	T
0.8977149511734591	0.9454818847382342	0.3045059036347770	T	T	T
0.7709742304200216	0.9660016178057000	0.2611045755884815	T	T	T
0.6424153775618604	0.1703599027853466	0.2527628746443234	T	T	T
0.6973489250243008	0.1581712746220098	0.0772868507103479	T	T	T
0.8110205130140528	0.1468513723904550	0.9780855338946203	T	T	T
0.9152176330118381	0.1674049014567629	0.0963989883479762	T	T	T
0.8979077034370796	0.1535866391732451	0.2934396760159818	T	T	T
0.7720394920159981	0.1416396481865208	0.2401697551337164	T	T	T
0.6805488773836423	0.0502215914204587	0.1900414612127020	T	T	T
0.9187805779016661	0.0472233498048247	0.1777560682319602	T	T	T
0.5687953826078688	0.8745925797214549	0.4169466097295221	T	T	T
0.5834922061090634	0.0060083389668014	0.4324473900155236	T	T	T
0.5990340937359161	0.1379905104437552	0.4344062389799382	T	T	T
0.8076720390856184	0.8711252130377835	0.3913537202392520	T	T	T
0.8183924097397093	1.0003128284101837	0.4402204912969660	T	T	T
0.8056715803509529	0.1344354500396851	0.4329865215680538	T	T	T
0.0116199449145516	0.9533568695137646	0.2133309944486042	T	T	T
0.0166614976584443	0.1340235053221737	0.2134675338842613	T	T	T
0.8612345423658758	0.0546322295071210	0.7798904963290948	T	T	T
0.8026980552684246	0.0708311535414832	0.6050125975654589	T	T	T
0.7016180050549183	0.0565782188663957	0.4753641516863874	T	T	T
0.6005994775425417	0.0719214893529785	0.6036532150302414	T	T	T
0.6058238223794536	0.0509140020247663	0.8004365866003467	T	T	T
0.7322519355086324	0.0279218843146625	0.7596715457127466	T	T	T
0.8600335043357406	0.8322553740891434	0.7569883160350913	T	T	T
0.8046650256467680	0.8317552807299632	0.5811171198304961	T	T	T
0.6915391063081602	0.8513000540096209	0.4821020131697289	T	T	T
0.5880621275544853	0.8268868761718361	0.6010564513200770	T	T	T
0.6049144691598597	0.8467354789242827	0.7960150524708363	T	T	T
0.7304496153733698	0.8598311083844257	0.7408333720555730	T	T	T
0.8210881619182320	0.9474716653511994	0.6766086987509022	T	T	T

Structure files (CONTCAR) involved in this work:

0.5822222089162241	0.9499419956923894	0.6732937789481195	T	T	T
0.9329424766561976	0.1265949678722572	0.9080321090760261	T	T	T
0.9186587506892940	0.9963626888854903	0.9396583797607859	T	T	T
0.9049541084275051	0.8637841957006286	0.9369505271240148	T	T	T
0.6967529037870493	0.1271194845299759	0.8840357666226822	T	T	T
0.6842032561062847	0.9990932563171842	0.9397744862784035	T	T	T
0.6980455225558150	0.8647145302871762	0.9345384563404986	T	T	T
0.4909369009015541	0.0443184856368064	0.7117853199715224	T	T	T
0.4855876024462975	0.8624345077934850	0.7152598083822677	T	T	T
0.3558140777719588	0.4366548563267027	0.7135257903652312	T	T	T
0.2991781408294373	0.4295350448707459	0.8909308474401143	T	T	T
0.1988872697155471	0.4543599221458339	0.0188610386382354	T	T	T
0.0957019257102816	0.4331439658771772	0.8968944285414127	T	T	T
0.1006869671087788	0.4391474983891201	0.6991119092596287	T	T	T
0.2273081843908502	0.4692646059202400	0.7365335710427865	T	T	T
0.3573977582838230	0.6699159572837180	0.7387612383696622	T	T	T
0.3016433229666629	0.6601164213694684	0.9132587118214061	T	T	T
0.1883249156341813	0.6445857273232343	0.0111638625484474	T	T	T
0.0854218174446352	0.6687147783823328	0.8918415052296592	T	T	T
0.1026713248709780	0.6586324508825194	0.6970165182338670	T	T	T
0.2289311966785355	0.6380220987950176	0.7495872441301525	T	T	T
0.3210903518715288	0.5495160478286576	0.8063256236435861	T	T	T
0.0807455185470955	0.5491610824601955	0.8061692169281696	T	T	T
0.4311899295835470	0.3758161193383444	0.5767993612435984	T	T	T
0.4154906531755501	0.5070654982573699	0.5671999163066139	T	T	T
0.3927568830404179	0.6381290683079572	0.5544450780533079	T	T	T
0.1961864398189982	0.3701371288361290	0.6116156026352880	T	T	T
0.1747366722604662	0.4979863388010594	0.5596947105567375	T	T	T
0.1906713845179968	0.6320430712410621	0.5565011272631815	T	T	T
0.9850284701669069	0.4549962659785584	0.7903482911363953	T	T	T
0.9828317177185097	0.6365040827596139	0.7735797680237498	T	T	T
0.1388187092468904	0.5628118648300010	0.2165775943364770	T	T	T
0.1947600099260228	0.5638332889346707	0.3912562158184293	T	T	T
0.2941230510858313	0.5498541052526594	0.5251907230447136	T	T	T
0.3916444733986830	0.5659362882538662	0.3918741446266595	T	T	T
0.3946272727669793	0.5546156306926029	0.1957319209928285	T	T	T
0.2675499953991521	0.5298410865101142	0.2335918781785279	T	T	T
0.1450480672671019	0.3221886410673104	0.2398722523932122	T	T	T
0.1930508988699097	0.3419056506384932	0.4188435199059041	T	T	T
0.3094207126840207	0.3528104283653437	0.5106693936285819	T	T	T
0.4123241595434398	0.3267085060762949	0.3911888769537368	T	T	T
0.3924163767921749	0.3402657326261779	0.1936596434768001	T	T	T
0.2710611687414785	0.3572769847553206	0.2592268304511938	T	T	T
0.1744800116388558	0.4461913855630650	0.2985805290328533	T	T	T
0.4101152993263325	0.4465386993511385	0.3114085617872292	T	T	T
0.0661859788712030	0.6231010770071936	0.0773564622689135	T	T	T
0.0773989741882452	0.4902060921327185	0.0753464591608135	T	T	T
0.1080010386231182	0.3605467864570749	0.0575505111384607	T	T	T
0.3029632918098553	0.6259715972283511	0.1054668434622989	T	T	T
0.3202551894111582	0.4967816782812850	0.0575005409134459	T	T	T
0.2940619253381359	0.3646523454126309	0.0622629007765583	T	T	T
0.5055131301744874	0.5376278805867994	0.2951418080240383	T	T	T
0.5110446540241388	0.3618709733827591	0.2686684992889399	T	T	T

Structure files (CONTCAR) involved in this work:

0.4378432385291454	0.7495576530287945	0.6346046456956341	T	T	T
0.1953295440060376	0.7483546401206136	0.6457766986915767	T	T	T
0.2689089778771777	0.7474528761720476	0.0554904527867670	T	T	T
0.1058510654467418	0.7472257492063715	0.0476216220991187	T	T	T
0.0640553022777535	0.2467476338957348	0.1315849729102327	T	T	T
0.3007500259394937	0.2475404844904917	0.1512310812691883	T	T	T
0.2289703814166693	0.2496938857787190	0.5528938892772512	T	T	T
0.3927090065293078	0.2506315643663423	0.5483905660193455	T	T	T
0.5583170159036450	0.2494639410950990	0.3502593810288915	T	T	T
0.8133149548871710	0.2511494104592790	0.3411658101618461	T	T	T
0.7278643932907718	0.2491240915039653	0.9386436527999126	T	T	T
0.8932805914920227	0.2501779767991640	0.9457234039492741	T	T	T
0.9457263204718592	0.7523651309843011	0.8532323672871978	T	T	T
0.6925742883301956	0.7496108291775898	0.8390880711734924	T	T	T
0.7725156073563257	0.7487967996782204	0.4336526594987289	T	T	T
0.6080772691656146	0.7496812928567287	0.4441854998716140	T	T	T
0.9554735105115931	0.4903737428009997	0.4986315829819721	T	T	T
0.0261469867479520	0.6817572420732462	0.4529285133096245	T	T	T
0.9176500079937617	0.4346501831824298	0.4034032781595074	T	T	T
0.8942809985389916	0.5267432897747800	0.5794446758658176	T	T	T
1.0013941556819830	0.7237536650742833	0.4436034704851584	T	T	T
0.9924768329534840	0.5844534386951211	0.3882584627719892	T	T	T
0.0700841112416045	0.6198952971924009	0.3299265757486196	T	T	T
0.9872163546547906	0.6575607068507082	0.2986325076257161	T	T	T
0.0732411178598793	0.6935761183856500	0.4630366898034560	T	T	T
0.0168402404003668	0.6238211744461514	0.3446790108889859	T	T	T

Figure 2(a) Zn-FS

1.0000000000000000

20.0219993591000005 0.0000000000000000 0.0000000000000000

0.0000000000000000 19.8990001678000006 0.0000000000000000

0.0000000000000000 0.0000000000000000 13.3830003737999998

93 3 194 2 5 1

Selective dynamics

Direct

0.4256349182715002	0.0563075356499563	0.6462980909082828	T	T	T
0.3059397887765535	0.0254359932631752	0.7904319946452001	T	T	T
0.2837623299542656	0.0588175020639684	0.0118760698892173	T	T	T
0.1252900964723646	0.0611642242372865	0.0105941992133784	T	T	T
0.0713775364093794	0.0283711822670707	0.7994723369587584	T	T	T
0.1811316441010575	0.0537775518413645	0.6539204934748887	T	T	T
0.4203327813279186	0.8256574397627918	0.6651247648187715	T	T	T
0.3058782931071126	0.8675146758175672	0.8089961854728045	T	T	T
0.2665627811684778	0.8270283326561613	0.0259337134995573	T	T	T
0.1124639421430015	0.8256169895460611	0.0081756523644501	T	T	T
0.0673013638565493	0.8710321563904280	0.7942246101863167	T	T	T
0.1859459446244480	0.8279797827868379	0.6687868556041261	T	T	T
0.0779631527681485	0.9406771131621221	0.1453340079084921	T	T	T
0.1976383938642930	0.9705935169725002	0.2885100721628346	T	T	T
0.2208233596205163	0.9375492024561952	0.5102019647465247	T	T	T
0.3797010717918908	0.9348047845650598	0.51111117690684845	T	T	T
0.4338720906717891	0.9675924743712011	0.2992238447380337	T	T	T
0.3231913212497846	0.9423054220694115	0.1539044706540351	T	T	T
0.0839577275565902	0.1703281997078557	0.1633965111521439	T	T	T

Structure files (CONTCAR) involved in this work:

0.1971158856600642	0.1282208427320468	0.3084978023339427	T	T	T
0.2349812937541088	0.1697922390487842	0.5251909019690322	T	T	T
0.3897015285556801	0.1724283220471727	0.5092337623007850	T	T	T
0.4373135962737393	0.1257921179082951	0.2959462270184722	T	T	T
0.3176246342498342	0.1685843159548959	0.1713485901533714	T	T	T
0.5740657633737644	0.5543718492540504	0.3558890757611249	T	T	T
0.6862946951801052	0.5256509956113573	0.1977226023153639	T	T	T
0.7132317092699939	0.5684794388926326	0.9842126304780795	T	T	T
0.8723731234235418	0.5726266323134123	0.9836930026955345	T	T	T
0.8069698214749713	0.5484066359626679	0.3408605499473812	T	T	T
0.5734871729881557	0.3267779854767010	0.3287839896801228	T	T	T
0.6937709968674751	0.3717335145852085	0.1900753544050204	T	T	T
0.7311247720447482	0.3266030016192543	0.9794827560163404	T	T	T
0.8858764103291749	0.3259590327330784	0.9981374493479399	T	T	T
0.9450762220153182	0.3753776709902935	0.1927635862881387	T	T	T
0.9195923750393122	0.4440586419165853	0.8609829622521581	T	T	T
0.8016758548814511	0.4713179162937522	0.7179815226909526	T	T	T
0.7716180082146499	0.4352620578702130	0.4947330348208843	T	T	T
0.6133464846028964	0.4266194288781791	0.4900742769786372	T	T	T
0.5659586284114125	0.4678070705677859	0.7033784046457342	T	T	T
0.6763763958337043	0.4474425736489195	0.8535947364445221	T	T	T
0.9180832996566262	0.6780424656939432	0.8250293215265861	T	T	T
0.7719993625202952	0.6665205738426521	0.4623446085200070	T	T	T
0.6162801744168583	0.6716430904426973	0.4865408923560897	T	T	T
0.5625308666089897	0.6263149137559418	0.6974044110767286	T	T	T
0.6761473338131434	0.6727250104539438	0.8213360802865497	T	T	T
0.5799458592772092	0.9435982495106869	0.3554638179384894	T	T	T
0.7009052679098634	0.9716015691634036	0.2113443601637521	T	T	T
0.7228951172358620	0.9341671846208633	0.9894519504532816	T	T	T
0.8835178218183369	0.9334199346031288	0.9931252733767545	T	T	T
0.9340972344375394	0.9680422240330118	0.2040242705961032	T	T	T
0.8246637766786556	0.9451254746247847	0.3536781812928877	T	T	T
0.5798367789389169	0.1713237699397001	0.3268694518569978	T	T	T
0.7009798483818501	0.1305025004084772	0.1908771683115689	T	T	T
0.7337768021411737	0.1709703455431074	0.9702495675485575	T	T	T
0.8884998053900164	0.1733098682114566	0.9837395035517239	T	T	T
0.9386110857581753	0.1258554529917926	0.1963166550000999	T	T	T
0.8236093687669769	0.1735267408226948	0.3264642424851555	T	T	T
0.9252376169688821	0.0554761972642862	0.8555827555983819	T	T	T
0.8058002950001342	0.0270634740296343	0.7050406819759510	T	T	T
0.7836983204819812	0.0674005114814720	0.4881065650990078	T	T	T
0.6231047796164425	0.0684726020659865	0.4881030683151077	T	T	T
0.5706720421070755	0.0301278251914208	0.6974547450105344	T	T	T
0.6824640647365399	0.0522258683824249	0.8460469408346514	T	T	T
0.9256149446199633	0.8301757696939313	0.8333543973724219	T	T	T
0.8039035483466513	0.8705381324648582	0.6943000325366055	T	T	T
0.7727070997213583	0.8244526440563086	0.4786761378829480	T	T	T
0.6172586545798514	0.8249723908690515	0.4879134141493133	T	T	T
0.5652485083346092	0.8731099100765283	0.6953021087304183	T	T	T
0.6802591156640611	0.8323135987411594	0.8282928870933662	T	T	T
0.4213697623529561	0.4424311914542788	0.6464239758555442	T	T	T
0.3010100180557986	0.4707892880971487	0.7897170218868690	T	T	T
0.2772532484716327	0.4368069939906898	0.0113412603286596	T	T	T

Structure files (CONTCAR) involved in this work:

0.1190924922090969	0.4375382373074431	0.0161313640441051	T	T	T
0.0643291622066691	0.4691964064469107	0.7991625324181776	T	T	T
0.1757054958275859	0.4423154950580126	0.6545695081003414	T	T	T
0.4178458421802353	0.6715551621952303	0.6606375024221085	T	T	T
0.3019785816202513	0.6283595873476504	0.8047358530185611	T	T	T
0.2653279026096718	0.6699576868346063	0.0222648896910338	T	T	T
0.1112501935804020	0.6718967045076051	0.0086354710152295	T	T	T
0.0606659546404467	0.6283320837947457	0.7938329758113767	T	T	T
0.1806502431001156	0.6701501687978707	0.6685071784363448	T	T	T
0.0770851788402685	0.5591167206057263	0.1510971795037163	T	T	T
0.1970052709075486	0.5241808788233796	0.2902913293360939	T	T	T
0.2148312192605320	0.5594789357058730	0.5150285076009664	T	T	T
0.3729969733273603	0.5635314582234404	0.5131753700410688	T	T	T
0.4252502951648446	0.5275380810788548	0.3012942577783955	T	T	T
0.3205674120010080	0.5529371794989352	0.1498821267225761	T	T	T
0.0855865126994016	0.3226830705097429	0.1619381518868865	T	T	T
0.1976520399122773	0.3667593735760910	0.3069058126443259	T	T	T
0.2331225530706105	0.3273276380820044	0.5247201985736482	T	T	T
0.3876609999499773	0.3263125533703948	0.5070538773113308	T	T	T
0.4326512606759793	0.3698426197933536	0.2916224272850127	T	T	T
0.3149969111640465	0.3271238819140379	0.1684981307103734	T	T	T
0.9226186848804077	0.5288500619925693	0.1908787774933856	T	T	T
0.8219465217443906	0.3372308928275707	0.3235272872910733	T	T	T
0.8009750287438779	0.6328265516563564	0.6888290196252186	T	T	T
0.3600870889336462	0.0604399497974262	0.7171966874186388	T	T	T
0.3066879111749351	0.0655378602060663	0.8960895462527110	T	T	T
0.2041580380239089	0.0432737594282544	0.0192975253148339	T	T	T
0.1023259919931198	0.0677439674097570	0.8951590027505499	T	T	T
0.1057521585093750	0.0571053203220146	0.6982918909467223	T	T	T
0.2316715306647767	0.0293573381475808	0.7419415734890881	T	T	T
0.3615339612616282	0.8253294957796051	0.7482764170756405	T	T	T
0.3066687748793389	0.8403085369168857	0.9227620367707459	T	T	T
0.1895172504578002	0.8516825506280614	0.0124095410671645	T	T	T
0.0863568819827350	0.8282932062443703	0.8936852713837907	T	T	T
0.1075525056587256	0.8403166103341613	0.6982604787239345	T	T	T
0.2320954696746486	0.8556608880614142	0.7602858596242598	T	T	T
0.3250830369660134	0.9467787950412885	0.8063591533442697	T	T	T
0.0881666968928533	0.9487789692794958	0.8117946963602694	T	T	T
0.4332300141911385	0.1261920861028006	0.5846422752261269	T	T	T
0.4204690870795609	0.9943164717633441	0.5672906936210220	T	T	T
0.3944213756262697	0.8632364074896889	0.5646091300789425	T	T	T
0.2016166437671232	0.1281953403958211	0.6161767273474323	T	T	T
0.1820758191262724	0.0003981633709668	0.5617659098589738	T	T	T
0.2028719278460922	0.8672145059947134	0.5656108747245641	T	T	T
0.9915897783427278	0.0399261414844102	0.7899797601659154	T	T	T
0.9877075381042454	0.8646217312535094	0.7721522654995242	T	T	T
0.1443012850286834	0.9344635504101076	0.2146283047393029	T	T	T
0.1966366283602595	0.9311823641656543	0.3948477284071724	T	T	T
0.3005040877373397	0.9521926980425462	0.5168772975188333	T	T	T
0.4040073811280288	0.9287139374717491	0.3962644255913189	T	T	T
0.3982099890445363	0.9382938532081662	0.1992470228245053	T	T	T
0.2722076504748971	0.9670058395909704	0.2412908042167732	T	T	T
0.1426052131770627	0.1712111831373938	0.2466801796541227	T	T	T

Structure files (CONTCAR) involved in this work:

0.1946111499657313	0.1545621870598606	0.4227159626143858	T	T	T
0.3123577969372359	0.1468692822365520	0.5106010814935240	T	T	T
0.4186036532495294	0.1673330922716040	0.3965592975680773	T	T	T
0.3955908040249020	0.1573905126747805	0.2022760108654973	T	T	T
0.2714775558886090	0.1400153304071798	0.2624332168323797	T	T	T
0.1773854595936259	0.0490304799679890	0.3035767551177487	T	T	T
0.4175546498201756	0.0473033102181752	0.3108735896984676	T	T	T
0.0675627183102317	0.8716325305305076	0.0821154140833502	T	T	T
0.0831883849651475	0.0022257876156343	0.0658936336346579	T	T	T
0.1099206598900425	0.1324726983568502	0.0635162860409602	T	T	T
0.3018231648701705	0.8680734816431642	0.1158015660072750	T	T	T
0.3230336095658608	0.9956548000438401	0.0617796930862996	T	T	T
0.3012573962720633	0.1288211320983854	0.0682243575315784	T	T	T
0.5133936620956212	0.9542233515208944	0.2880322330755018	T	T	T
0.5171075169968347	0.1320720170583554	0.2746835134957287	T	T	T
0.6321662490063098	0.5584125230058835	0.2727039389449223	T	T	T
0.6928487027722195	0.5745154449445493	0.1014422988859048	T	T	T
0.7929239824277116	0.5567687703252673	0.9689753799157841	T	T	T
0.8913769473643934	0.5800979355692488	0.1000364549529202	T	T	T
0.8822338647261685	0.5281455721143908	0.3071812357356810	T	T	T
0.7581214382667051	0.5236902436920613	0.2537955975047030	T	T	T
0.6414302209113082	0.3353003950233553	0.2657431233448620	T	T	T
0.6898703932940843	0.3321599393898787	0.0833773898545341	T	T	T
0.8082784244009179	0.3501425311463633	0.9974669804693291	T	T	T
0.9130496562427527	0.3221016748260203	0.1134072392755278	T	T	T
0.9061601919006496	0.3691632939849602	0.3015551781384633	T	T	T
0.7676105243046002	0.3700505301300998	0.2363721610373320	T	T	T
0.6674435903661509	0.4487391941660414	0.1696350965572143	T	T	T
0.9386834361052585	0.4496269689429395	0.1488730327485417	T	T	T
0.5701950958026065	0.6255470378265184	0.4143491580971387	T	T	T
0.5877535771450156	0.4951938244457312	0.4369194384031970	T	T	T
0.5793848526175515	0.3614660220811599	0.4387944766833690	T	T	T
0.8002515141737426	0.6286970874321954	0.3624029773476430	T	T	T
0.7891312380842253	0.5114597828649210	0.4495080021521206	T	T	T
0.8197185193599803	0.3830730636730194	0.4372933080610604	T	T	T
0.0089075155903227	0.5586534313207214	0.2278604674912877	T	T	T
0.0226414228028200	0.3573732635894633	0.2178609748819318	T	T	T
0.8550424060852944	0.4321640285259730	0.7881924120257419	T	T	T
0.7927065375531149	0.4328643709846806	0.6114377846525795	T	T	T
0.6938065497531499	0.4200765988879426	0.4765462535143383	T	T	T
0.5944738541339990	0.4269473195685636	0.6072153644681652	T	T	T
0.6029786404931449	0.4403897667716423	0.8030982283444164	T	T	T
0.7290610578753423	0.4748879266062396	0.7700045063275860	T	T	T
0.8591047393026875	0.6828592369411921	0.7453582339087743	T	T	T
0.8171758567344489	0.6390091396024439	0.5566032875820629	T	T	T
0.6940419571403659	0.6465156932718313	0.4819766160244236	T	T	T
0.5884343799255928	0.6668300397212282	0.5994993436987133	T	T	T
0.5970159459798300	0.6596521674870418	0.7954522234964740	T	T	T
0.7209052663797637	0.6434236546102496	0.7310899011388282	T	T	T
0.8295900271516938	0.5469372654045835	0.6918594225016295	T	T	T
0.5813753081621047	0.5471661285833811	0.6868748026420431	T	T	T
0.9296359886179045	0.3781014450201843	0.9314436995640248	T	T	T
0.9120433290669138	0.5105062652915838	0.9298218888260823	T	T	T

Structure files (CONTCAR) involved in this work:

0.8938874709332191	0.6415329368039668	0.9275650960753892	T	T	T
0.6984022653909228	0.3741702987684936	0.8942033695481392	T	T	T
0.6732085521304346	0.5029664303870911	0.9420445348162755	T	T	T
0.6913658840585263	0.6370488239292456	0.9285366446266117	T	T	T
0.4864553937835798	0.4534185674654666	0.7167452623400909	T	T	T
0.4817977807507349	0.6325977894975930	0.7074417775267471	T	T	T
0.6442611251539331	0.9387195123371426	0.2825875185511380	T	T	T
0.7018347572849147	0.9311330531724056	0.1062068581239830	T	T	T
0.8035175525195249	0.9380930361081551	0.9764162595238659	T	T	T
0.9017480780766175	0.9269201774205382	0.1107765984498494	T	T	T
0.8999922908750925	0.9451384955918148	0.3085005639343970	T	T	T
0.7734197131689254	0.9636126086565883	0.2638462162941509	T	T	T
0.6435290786524054	0.1700008996879324	0.2526701691507499	T	T	T
0.6976906025171357	0.1574278289678457	0.0767582191064842	T	T	T
0.8115180995230056	0.1470916443869995	0.9781395455608501	T	T	T
0.9159854533463611	0.1664015333699769	0.0968981007967413	T	T	T
0.9002986364777447	0.1546749576898334	0.2938494379235921	T	T	T
0.7741402885793198	0.1444838956429085	0.2385617538725545	T	T	T
0.6846032792097653	0.0504669534828592	0.1932107519810606	T	T	T
0.9212553587748145	0.0469574465164019	0.1819136271550339	T	T	T
0.5726789633895381	0.8735614753327013	0.4171727082159903	T	T	T
0.5862344679819851	0.0050723085407866	0.4348778238993734	T	T	T
0.5993935133615264	0.1374050242014012	0.4336206824886817	T	T	T
0.8112117638760284	0.8702382980139685	0.3971553423005777	T	T	T
0.8191821606119184	1.0005969495490423	0.4420482855826638	T	T	T
0.8071054777327478	0.1351072612332543	0.4314163892035416	T	T	T
0.0133493353050550	0.9517815980550031	0.2162301655909693	T	T	T
0.0188214393495286	0.1343171425960267	0.2117224289515788	T	T	T
0.8613114293594581	0.0557920095561602	0.7817566352922046	T	T	T
0.8056859113348707	0.0731126087346947	0.6048429499245342	T	T	T
0.7031686707125067	0.0583214296022926	0.4778400499083562	T	T	T
0.6013632651769409	0.0734086209574041	0.6048592971884712	T	T	T
0.6069761391073860	0.0493257750454117	0.8019583251739322	T	T	T
0.7326296909564778	0.0301807673763977	0.7566178830613502	T	T	T
0.8587282976749022	0.8369175260096828	0.7669696584182295	T	T	T
0.8067674585981369	0.8312847599965694	0.5881521696349146	T	T	T
0.6951178791782625	0.8487454765648630	0.4841146120145280	T	T	T
0.5904015631261023	0.8273085987380706	0.6021590141591774	T	T	T
0.6036016885496884	0.8500826538993478	0.7965900364589510	T	T	T
0.7298299907227079	0.8635544963244496	0.7431057337171328	T	T	T
0.8218356894550247	0.9492932185910057	0.6763143970357340	T	T	T
0.5813829163259202	0.9511970587328088	0.6703479727510900	T	T	T
0.9335652852996160	0.1289727068460036	0.9071757273718085	T	T	T
0.9175237371583522	1.0001091627794871	0.9443972806499253	T	T	T
0.9144120624710470	0.8671724544098880	0.9400694661548789	T	T	T
0.6971645125595239	0.1284351483066956	0.8826956939067452	T	T	T
0.6898942465780048	0.0010694835113434	0.9400107751523904	T	T	T
0.6956711253257477	0.8662698245183950	0.9362321938664729	T	T	T
0.4918475294126106	0.0462857917462904	0.7142367672721002	T	T	T
0.4854141088534299	0.8630056373881375	0.7116745856527921	T	T	T
0.3554949256303466	0.4356074298000921	0.7167256671726135	T	T	T
0.2983830194638388	0.4298012074325238	0.8948301489523522	T	T	T
0.1981720748403590	0.4559142271886230	0.0238991458591395	T	T	T

Structure files (CONTCAR) involved in this work:

0.0944547525488562	0.4378207167762684	0.9018992426038080	T	T	T
0.1018771016363980	0.4356900950677501	0.7037115686845997	T	T	T
0.2272950222766412	0.4683921249379032	0.7398682434895991	T	T	T
0.3571254663636632	0.6689547800722659	0.7406313768002616	T	T	T
0.3033754343063784	0.6589355516474622	0.9168651008031515	T	T	T
0.1880008249757534	0.6449193279420484	0.0109680073689449	T	T	T
0.0810912276669710	0.6653822198617749	0.8977123236190114	T	T	T
0.1029587692228055	0.6627306749517841	0.7030997805565447	T	T	T
0.2279629790135857	0.6384880744921456	0.7561989616511258	T	T	T
0.3210597878943737	0.5489759242464278	0.8085573242932778	T	T	T
0.0793364124297971	0.5493339664762528	0.8008605332674832	T	T	T
0.4310753452924600	0.3745207190068520	0.5802750157102111	T	T	T
0.4159870044264249	0.5056199644143596	0.5694035644825263	T	T	T
0.3934720669307296	0.6367629265419575	0.5567370353231605	T	T	T
0.1980345117104966	0.3689653163079765	0.6142495987743626	T	T	T
0.1743008771910622	0.4964575264335706	0.5631075352498428	T	T	T
0.1925819050536300	0.6305118126302305	0.5639489518281525	T	T	T
0.9853334849901925	0.4527354310523807	0.7905666306058368	T	T	T
0.9814004201986825	0.6374738882721187	0.7745846804504627	T	T	T
0.1416979798096241	0.5633925179358157	0.2223031976768298	T	T	T
0.1976883674488283	0.5626390378990082	0.3966383957865764	T	T	T
0.2943647011983511	0.5476568791619812	0.5326862658849973	T	T	T
0.3888220511226141	0.5644867216902382	0.3947322513997436	T	T	T
0.3947392161743457	0.5569137074220146	0.1976623807672426	T	T	T
0.2691100070214415	0.5290283223423995	0.2371560865094959	T	T	T
0.1475106325101027	0.3223072993459876	0.2395430860800890	T	T	T
0.1929361907395243	0.3408382338465092	0.4211186002514817	T	T	T
0.3101540132192049	0.3516440031556176	0.5106523340630160	T	T	T
0.4139911702266894	0.3282546243909163	0.3924667981798846	T	T	T
0.3932785576519200	0.3401170964617087	0.1946022620670793	T	T	T
0.2728774284978500	0.3564822319250577	0.2637364237767367	T	T	T
0.1757317180495849	0.4457496557507184	0.3015102914237953	T	T	T
0.4113113688911533	0.4474712668277624	0.3098661426772433	T	T	T
0.0675401947300109	0.6267671727936706	0.0866529003357326	T	T	T
0.0768239579040474	0.4929754160421602	0.0819723060202685	T	T	T
0.1054106858710090	0.3633567535846112	0.0609165018767049	T	T	T
0.3009563078028599	0.6269406710813810	0.1097099728394578	T	T	T
0.3200656621186853	0.4981329682261349	0.0598414062146637	T	T	T
0.2930078920867222	0.3658338204005153	0.0665751162166144	T	T	T
0.5043279286959037	0.5419818164575545	0.2987361691264729	T	T	T
0.5119742347222133	0.3624032135204788	0.2686163922247612	T	T	T
0.4378281481493607	0.7486490389813748	0.6359297561919597	T	T	T
0.1990332557388321	0.7486067043646807	0.6508809294059869	T	T	T
0.2685109846343374	0.7480710595686261	0.0550318064875759	T	T	T
0.1068328217637011	0.7486840635751844	0.0474731060293066	T	T	T
0.0670806439085981	0.2467212122457400	0.1298898375610283	T	T	T
0.3016463458293789	0.2475595538117813	0.1524413576136811	T	T	T
0.2300052189602748	0.2485986007480972	0.5539499080509195	T	T	T
0.3941704745751681	0.2497114467342655	0.5472763175935431	T	T	T
0.5574718433257031	0.2481650164318939	0.3475821971509397	T	T	T
0.8161668380187456	0.2525966360047144	0.3406211455257615	T	T	T
0.7285804969020869	0.2496426886166659	0.9394842751604470	T	T	T
0.8931787841738490	0.2514662863364485	0.9497822636224839	T	T	T

Structure files (CONTCAR) involved in this work:

0.9440867591690006	0.7527349591180001	0.8563602817698889	T	T	T
0.6900795129004692	0.7523406847095975	0.8376630188794175	T	T	T
0.7791479516954514	0.7464929882599538	0.4441538964521551	T	T	T
0.6108790529283236	0.7485131566627926	0.4471485304853346	T	T	T
0.9438190280228111	0.4983613611871236	0.5035356534705895	T	T	T
0.0473353544841074	0.7433704562972533	0.5070324450473721	T	T	T
0.9146778613123800	0.4368031181150039	0.4116559543529544	T	T	T
0.8793380418619609	0.5526780336413372	0.5563629486503971	T	T	T
0.0438468560097188	0.7830954456842546	0.4649306226819653	T	T	T
0.0603054863308485	0.6268749919348605	0.3226596503312382	T	T	T
0.9954044890429671	0.5772491754316389	0.3807740234113967	T	T	T
0.9741615860919964	0.6467163211798921	0.2986327047256899	T	T	T
0.0476619972775794	0.7610926644402144	0.5749669633642169	T	T	T
1.0098829417048054	0.6062901897468197	0.3144174565660113	T	T	T

Figure 2(a) Ga-IS

1.0000000000000000

20.0219993591000005 0.0000000000000000 0.0000000000000000

0.0000000000000000 19.8990001678000006 0.0000000000000000

0.0000000000000000 0.0000000000000000 13.3830003737999998

93 3 193 1 6 1

Selective dynamics

Direct

0.4218535263509722	0.0571493549471711	0.6480621783635740	T	T	T
0.3009930426280221	0.0268336055798244	0.7891971078729654	T	T	T
0.2798649472190959	0.0604824123584748	0.0125564137349485	T	T	T
0.1201048157933897	0.0632633678614951	0.0123205109774034	T	T	T
0.0670518968425782	0.0288941088995145	0.7991042412032598	T	T	T
0.1763645011047572	0.0555514966770261	0.6510519083569406	T	T	T
0.4195589490851646	0.8271326124360456	0.6702106915850621	T	T	T
0.3016023397863279	0.8684681358613844	0.8090926444563067	T	T	T
0.2669431061873340	0.8282841518982380	0.0293307096496349	T	T	T
0.1119266120518958	0.8263275624160045	0.0172200103485949	T	T	T
0.0610534720982372	0.8695591887099141	0.8025857089458839	T	T	T
0.1789223529702397	0.8276798350378840	0.6734978466452191	T	T	T
0.0754079496497653	0.9427241949319765	0.1505997367288927	T	T	T
0.1963914901844603	0.9725793956273634	0.2930341568863213	T	T	T
0.2168596826333200	0.9365571408917646	0.5142176716373825	T	T	T
0.3765128883101525	0.9335843362088596	0.5155510930850085	T	T	T
0.4301757192074476	0.9693460245824355	0.3044471819970909	T	T	T
0.3207861463900983	0.9446463111498176	0.1551082387187463	T	T	T
0.0785334970793699	0.1720958592461983	0.1645883319852359	T	T	T
0.1960568831684171	0.1299566636577438	0.3071270312448675	T	T	T
0.2308130746194621	0.1728084135794319	0.5244259559398117	T	T	T
0.3854345248170361	0.1737922075139053	0.5122428494954008	T	T	T
0.4365362214915223	0.1275601070438057	0.3021402537153293	T	T	T
0.3189667509454210	0.1674181080182322	0.1714794487002962	T	T	T
0.5811590826197133	0.5574184695661799	0.3465028215214829	T	T	T
0.6931793846631962	0.5320427711363038	0.1881870098915641	T	T	T
0.7118478528233325	0.5634667841776846	0.9719004741332142	T	T	T
0.8701339470374734	0.5573251654552607	0.9715460225618031	T	T	T
0.9340185282962565	0.5275128212548452	0.1833464934697631	T	T	T
0.5782911940056650	0.3284888895184537	0.3304354543153849	T	T	T
0.7052919909607667	0.3743604675390628	0.2146860064936504	T	T	T

Structure files (CONTCAR) involved in this work:

0.7360127535444647	0.3302862570604432	0.9923168031781628	T	T	T
0.8874545671466336	0.3265761304946295	0.9792103150562070	T	T	T
0.9356447777219401	0.3708639796295401	0.1977644165972947	T	T	T
0.9250504651473150	0.4347310331566021	0.8345657613350213	T	T	T
0.7820876639230221	0.4439706912942754	0.4768719134496564	T	T	T
0.6224761427484822	0.4337948684708834	0.4886710615626981	T	T	T
0.5665570552234058	0.4664374945944871	0.7044028264174074	T	T	T
0.6738480612297906	0.4341705758572445	0.8481776011906561	T	T	T
0.9172751247299757	0.6714533362065040	0.8264135791513283	T	T	T
0.7984193821376735	0.6320632732992451	0.6981753271952869	T	T	T
0.7668043893503551	0.6671394656539746	0.4796389499492193	T	T	T
0.6109508350266779	0.6706772983513787	0.4855046967936474	T	T	T
0.5642786380637972	0.6249713465343945	0.7039233818483126	T	T	T
0.6801951425686781	0.6811331161026075	0.8265998855200110	T	T	T
0.5748780881143531	0.9434756818473815	0.3643064548914197	T	T	T
0.6951325876119441	0.9722819927886803	0.2215045889130423	T	T	T
0.7175141625215318	0.9435283890428678	0.9978512436451652	T	T	T
0.8777354603013592	0.9332985218401930	0.9956595641064112	T	T	T
0.9310398264462592	0.9689858336586354	0.2075636425277878	T	T	T
0.8200858759658303	0.9366810059411250	0.3535482480636105	T	T	T
0.5807412388660538	0.1744124689772164	0.3348917079761407	T	T	T
0.6990250957369568	0.1312343701655294	0.2011844505196478	T	T	T
0.7315731536325814	0.1722389616118107	0.9799415933870534	T	T	T
0.8863526443282055	0.1722708283931382	0.9942067249412929	T	T	T
0.9342556932239177	0.1277641853866669	0.2066987034272358	T	T	T
0.8201794077050835	0.1690746668929108	0.3416028199090491	T	T	T
0.9232942262813424	0.0566787508410158	0.8614692516858540	T	T	T
0.8044603197913602	0.0293540498555842	0.7214708800912248	T	T	T
0.7809398847150177	0.0548570670093227	0.4956671368990015	T	T	T
0.6209579898154161	0.0675266306974152	0.4942579889720307	T	T	T
0.5668356752561152	0.0333886604481961	0.7028361410808515	T	T	T
0.6778058697044074	0.0598795413054773	0.8516386238490270	T	T	T
0.9164957571789429	0.8242096017144789	0.8402311507378997	T	T	T
0.8012820358160013	0.8730365150141779	0.7056117669323996	T	T	T
0.7674515862246949	0.8285408792548807	0.4886440798111451	T	T	T
0.6121408575389822	0.8260161908619779	0.4973880392236651	T	T	T
0.5619097998999223	0.8765063154130033	0.7040044975384205	T	T	T
0.6764540012696543	0.8374598538724669	0.8381478881728910	T	T	T
0.4223644036708691	0.4455423444954008	0.6392048892670559	T	T	T
0.3036534872373551	0.4729704659516329	0.7877586689983502	T	T	T
0.2844910394023756	0.4325116030489440	0.0054973311933821	T	T	T
0.1259106471004543	0.4308565165405014	0.0011743921364840	T	T	T
0.0730388314173283	0.4721238590000567	0.7941497233655710	T	T	T
0.1819424209975224	0.4491583748841208	0.6455352751342716	T	T	T
0.4236658256163679	0.6721081253611274	0.6631833010381030	T	T	T
0.3017041820501163	0.6296957342448550	0.7992945043989437	T	T	T
0.2691788363209255	0.6720936112571110	0.0176426301405286	T	T	T
0.1148790946254223	0.6732698229951879	0.0075962402952499	T	T	T
0.0649397147131126	0.6293542823308655	0.7981511059488113	T	T	T
0.1796206881739906	0.6691492307427751	0.6631546162092619	T	T	T
0.0792149573076060	0.5528929652614991	0.1341309179350318	T	T	T
0.1997555524754233	0.5275732533011990	0.2808563767225181	T	T	T
0.2220506971718521	0.5676282361779528	0.5016906663873968	T	T	T

Structure files (CONTCAR) involved in this work:

0.3830536915806562	0.5703623780089444	0.5030540673314405	T	T	T
0.4337904941402755	0.5277180418403731	0.2940525055401935	T	T	T
0.3262726315477877	0.5523760161606432	0.1422862767936124	T	T	T
0.0808524813732490	0.3272187457662028	0.1570503868105178	T	T	T
0.1969461145916540	0.3693337819120046	0.3026815497905488	T	T	T
0.2314765275006536	0.3294348534525895	0.5219370843590667	T	T	T
0.3858314789881234	0.3271050341484099	0.5083394570263451	T	T	T
0.4342149050373649	0.3705802684359298	0.2952977652622693	T	T	T
0.3181026867879524	0.3261111762098494	0.1665471566343300	T	T	T
0.8125888670663812	0.5669163126619736	0.3201055425209560	T	T	T
0.8279878554738787	0.3271757994786100	0.3530937783400248	T	T	T
0.7962364758331901	0.4738000954041794	0.7200756322136357	T	T	T
0.3562082135461324	0.0624799125891613	0.7185536008092370	T	T	T
0.2998148920214803	0.0657519195140353	0.8955883482547691	T	T	T
0.1997267501978470	0.0510359536340985	0.0269302224361851	T	T	T
0.1007593326204272	0.0657370582876666	0.8950326853278057	T	T	T
0.1014758765230468	0.0566511046870559	0.6973436552762777	T	T	T
0.2276666011557325	0.0324166996236528	0.7385364150182383	T	T	T
0.3571891635947040	0.8263041500571191	0.7476369396020388	T	T	T
0.3039305175211950	0.8434386539700043	0.9240228507071961	T	T	T
0.1891810010002075	0.8519144432577548	0.0206840101045600	T	T	T
0.0838933480232313	0.8317021837245946	0.9042483942135817	T	T	T
0.1013787914711699	0.8368383182438421	0.7083618746731233	T	T	T
0.2275597405816470	0.8547024887754162	0.7625743203884099	T	T	T
0.3194965781963575	0.9479408865160934	0.8036139806215772	T	T	T
0.0793333116079964	0.9485932329240825	0.8103828970197711	T	T	T
0.4298771098596816	0.1265430950707582	0.5850412989962379	T	T	T
0.4163286256096157	0.9945077472940582	0.5701988945165724	T	T	T
0.3971179581163824	0.8622518999078608	0.5657391949891846	T	T	T
0.1937263510953571	0.1304931420641324	0.6115170585290031	T	T	T
0.1790841099945695	0.0023242748679664	0.5589502510634574	T	T	T
0.1923734150947638	0.8684961253756285	0.5704220047814275	T	T	T
0.9880375600711204	0.0456804488728508	0.7904672822421190	T	T	T
0.9810926869066421	0.8595501015350280	0.7871144305559454	T	T	T
0.1416142073504147	0.9386777918187263	0.2198889688884762	T	T	T
0.1977120469206710	0.9302515967028171	0.3968353994880900	T	T	T
0.2968311070086571	0.9463219554889122	0.5293573597874968	T	T	T
0.3962603247799663	0.9300558352150929	0.3983312829311885	T	T	T
0.3957512378024930	0.9446560261754797	0.2008585483627101	T	T	T
0.2697541515553112	0.9696706845933534	0.2419420130273409	T	T	T
0.1418837268672775	0.1697853463828949	0.2398989948158317	T	T	T
0.1934193982709829	0.1620340323578517	0.4182074382463412	T	T	T
0.3080799389716304	0.1480444602819091	0.5149721325236456	T	T	T
0.4132287821997593	0.1708110299480836	0.3988471776906977	T	T	T
0.3963878591452215	0.1551466058586328	0.2042965930842229	T	T	T
0.2705373229582335	0.1389492692356029	0.2600123614713752	T	T	T
0.1769539026280285	0.0507025784322508	0.3132057346675339	T	T	T
0.4180541430653761	0.0492772131689350	0.3211489690586689	T	T	T
0.0668889673521775	0.8713690323028729	0.0924082723464750	T	T	T
0.0806207186322538	0.0022835445425002	0.0675258510284635	T	T	T
0.0979381492839693	0.1345564035252735	0.0607270462509248	T	T	T
0.3028727301195815	0.8688929750126491	0.1192702139085853	T	T	T
0.3172818998705651	0.9953018775158782	0.0598918153170800	T	T	T

Structure files (CONTCAR) involved in this work:

0.3038681145296493	0.1291542746216550	0.0668899900231210	T	T	T
0.5091146291417630	0.9527068920778134	0.2948389487382883	T	T	T
0.5164493507457806	0.1361652644953395	0.2855117561683613	T	T	T
0.6421349686433899	0.5660262290749571	0.2689493796078040	T	T	T
0.6734083439066083	0.5614811404488478	0.0782737251479872	T	T	T
0.7911462689938489	0.5471060499688036	0.9876608473522168	T	T	T
0.9096775261822643	0.5573524527178151	0.0778204575891337	T	T	T
0.9000232410875810	0.5699078304410037	0.2785113712850489	T	T	T
0.7689550499541014	0.5527053467116616	0.2123199403281930	T	T	T
0.6401933490922502	0.3326311847578154	0.2538939328136181	T	T	T
0.7288176143242140	0.3371416423000042	0.1119776707256506	T	T	T
0.8116845880685588	0.3540677832141270	0.9607896777590881	T	T	T
0.9104357134488765	0.3368893727727595	0.0935606082032336	T	T	T
0.9047552691925489	0.3358310737367063	0.2943378979893652	T	T	T
0.7642733681417795	0.3725757986973974	0.2961221175302882	T	T	T
0.6816540170463412	0.4508381597567421	0.1898555145318213	T	T	T
0.9133209175046133	0.4501392411446048	0.1942416862317486	T	T	T
0.5674274512917776	0.6279394676918884	0.4048241112697823	T	T	T
0.5984131401502850	0.5006728794720843	0.4302720693722719	T	T	T
0.5942018898366328	0.3670572312018479	0.4348306721390571	T	T	T
0.8040099595187797	0.6425035793965108	0.3806458067788583	T	T	T
0.8048427131034757	0.4995340398156358	0.4005377592997945	T	T	T
0.8296660954255657	0.3736050235619146	0.4732241922538947	T	T	T
0.0131854970426204	0.5407253651866029	0.2028399377255923	T	T	T
0.0173519267862332	0.3689903132630832	0.1995647557563487	T	T	T
0.8715693245807259	0.4227008192869661	0.7408430049297010	T	T	T
0.8144930573158575	0.4654043689278851	0.5890627062359570	T	T	T
0.7038163957795618	0.4307254950758050	0.4919103004663157	T	T	T
0.5948726411452867	0.4339939452037882	0.6017212803884746	T	T	T
0.5992277260719163	0.4280445966788662	0.7995425730322410	T	T	T
0.7299062820158042	0.4281644284843225	0.7618211127746832	T	T	T
0.8633919323821999	0.6747024940553317	0.7363483164146558	T	T	T
0.8015871135719337	0.6312533292816553	0.5768623668433577	T	T	T
0.6880481563666976	0.6457685674018450	0.4801958682201075	T	T	T
0.5822958193899055	0.6585660950048933	0.5971468210404538	T	T	T
0.6039615709268631	0.6632404353413719	0.7932656086999543	T	T	T
0.7295160485866035	0.6701064623758270	0.7309627093694999	T	T	T
0.8013223018464828	0.5577124823178394	0.7461885869033509	T	T	T
0.5849922183754472	0.5461324043356441	0.7050922844247793	T	T	T
0.9355663030529371	0.3677917838923150	0.9014305828685210	T	T	T
0.8975114351641480	0.4952749512179366	0.9032456603280110	T	T	T
0.8883542750255486	0.6284392147067592	0.9198407449691501	T	T	T
0.6821212353886992	0.3758501769608671	0.9327504221006748	T	T	T
0.6784281537541972	0.5079979968762061	0.8995780318801465	T	T	T
0.7038359736463136	0.6371968940905575	0.9220345550719102	T	T	T
0.4861357486349860	0.4568192375333311	0.7112804752061379	T	T	T
0.4840032892102855	0.6336310857670711	0.7216317595505899	T	T	T
0.6401605075486643	0.9371421610787465	0.2933549177713672	T	T	T
0.6908585790337654	0.9383544025003800	0.1116926968058749	T	T	T
0.7983965910314126	0.9492530673269215	0.9925721492216724	T	T	T
0.9031274431248235	0.9288003238084102	0.1103449601623367	T	T	T
0.8954028801647240	0.9408214496727965	0.3083914281870506	T	T	T
0.7696471524024560	0.9593616626653869	0.2647208995717207	T	T	T

Structure files (CONTCAR) involved in this work:

0.6415651556067559	0.1751714764072858	0.2555388664701752	T	T	T
0.6965842689624324	0.1504047119530156	0.0838690887804603	T	T	T
0.8092929196178815	0.1475223825683543	0.9830284423907258	T	T	T
0.9090625601264719	0.1706939961711811	0.1102731068855434	T	T	T
0.8975845747210940	0.1561317807367004	0.3059001172215332	T	T	T
0.7722217432771217	0.1471494312775903	0.2473486723372389	T	T	T
0.6805272109660336	0.0522957187284092	0.2161943243542837	T	T	T
0.9165284219762739	0.0486196373174081	0.1909755639902215	T	T	T
0.5661059452914259	0.8747658188914329	0.4287015641133252	T	T	T
0.5799814385022799	0.0068555232791994	0.4406667857523132	T	T	T
0.6044695500445627	0.1376572029201952	0.4375240665748592	T	T	T
0.8043122424093312	0.8603064309098443	0.3907472426746779	T	T	T
0.8127323754677604	0.9867091626428461	0.4486885270708214	T	T	T
0.8058692144524429	0.1203778188963298	0.4365645188127587	T	T	T
0.0107087301222251	0.9553978171444371	0.2208253711168808	T	T	T
0.0148859919556728	0.1365312810102495	0.2184138664047239	T	T	T
0.8578504694492750	0.0684046032834331	0.7918900104506790	T	T	T
0.8071150680742107	0.0607208073675380	0.6101306849826287	T	T	T
0.6999388943974623	0.0497307409097161	0.4905840163798487	T	T	T
0.5967253151135736	0.0761706299559393	0.6094207035389232	T	T	T
0.6026357088803422	0.0555058170813325	0.8066269688546797	T	T	T
0.7290183985076695	0.0378443220125888	0.7634219052482720	T	T	T
0.8539996614507785	0.8249483350887914	0.7632530484731817	T	T	T
0.8042598690963061	0.8574572793077095	0.5875649072469855	T	T	T
0.6892858165882672	0.8513765657554799	0.4897257949932623	T	T	T
0.5870754721828249	0.8288806754962152	0.6128295967375266	T	T	T
0.5998252038527170	0.8543658351975552	0.8061643138798686	T	T	T
0.7259500585033578	0.8607081214067591	0.7474909409170039	T	T	T
0.8244485218952988	0.9502581530711751	0.7239362134490861	T	T	T
0.5795001445953147	0.9542516002258523	0.6784528684340216	T	T	T
0.9346702347014499	0.1236176961492532	0.9288973063398771	T	T	T
0.9165424106749214	0.9925399637122467	0.9358001306363235	T	T	T
0.8957592927244562	0.8618026844131990	0.9434373088068497	T	T	T
0.6930987868413467	0.1362550670106231	0.8873993777025504	T	T	T
0.6848586760796280	0.0099249749518933	0.9470351922030034	T	T	T
0.6942168122407040	0.8760013910825961	0.9408834235067829	T	T	T
0.4874956155939500	0.0477358841277749	0.7174708235518921	T	T	T
0.4818097071179537	0.8675525804142126	0.7203822419455790	T	T	T
0.3559611545079449	0.4423535817041184	0.7081571766606771	T	T	T
0.3055324272095490	0.4275059101173895	0.8885386408443949	T	T	T
0.2046792353643312	0.4470227819378465	0.0155577898416936	T	T	T
0.1059830768876893	0.4278256880832956	0.8834849053741323	T	T	T
0.1054586201225547	0.4539463757327766	0.6862074155831266	T	T	T
0.2295031180760319	0.4702235011862115	0.7385455905004150	T	T	T
0.3562119392320255	0.6662274039528597	0.7293838445013989	T	T	T
0.3013179906710164	0.6674214068100781	0.9065032836144056	T	T	T
0.1917300821783954	0.6466245378774644	0.0131438730052267	T	T	T
0.0901620554344902	0.6742807980057890	0.8920110557839251	T	T	T
0.1023813130913283	0.6549016416606079	0.6967364378087595	T	T	T
0.2283255418515111	0.6356784674719407	0.7470427315015584	T	T	T
0.3206320059101628	0.5508609085194962	0.8146818416508381	T	T	T
0.0829350815521579	0.5510927971763024	0.8207248320192733	T	T	T
0.4309731740236344	0.3751637427939940	0.5791623497625977	T	T	T

Structure files (CONTCAR) involved in this work:

0.4169689097170277	0.5060521991679110	0.5579374383900557	T	T	T
0.4106263648979649	0.6390483064574326	0.5536113026354457	T	T	T
0.1954250720332027	0.3728109682141465	0.6092952975531958	T	T	T
0.1908747597399270	0.4999452646937499	0.5514705152265407	T	T	T
0.1913575584064517	0.6344858011928878	0.5544092236455640	T	T	T
0.9943919438183855	0.4545688324025647	0.7805196073292464	T	T	T
0.9850725590504510	0.6368619434054494	0.7818414999967658	T	T	T
0.1429256557558602	0.5593807433142786	0.2081879196188510	T	T	T
0.1993362645027332	0.5698147557988946	0.3850539331129283	T	T	T
0.3023300900720969	0.5660146511777953	0.5152114118741054	T	T	T
0.4029118507374250	0.5712259853314592	0.3860639124165033	T	T	T
0.4005008722166536	0.5545974569243981	0.1905883072568457	T	T	T
0.2725373313750623	0.5337917334934730	0.2294899807481414	T	T	T
0.1405847428896507	0.3305423671667995	0.2386123134211005	T	T	T
0.1934659188323238	0.3411959667026636	0.4161316101182848	T	T	T
0.3087283259562881	0.3537071773931046	0.5110948084436941	T	T	T
0.4122688394672949	0.3286001945157082	0.3941076631149727	T	T	T
0.3950686427822490	0.3406491543749652	0.1983325836139826	T	T	T
0.2703188894372772	0.3561648313106716	0.2547166941131991	T	T	T
0.1815097216394506	0.4495889368761823	0.3028639530506680	T	T	T
0.4145710856063758	0.4491126964038941	0.3116978075126582	T	T	T
0.0688069722108651	0.6227149733432142	0.0734156224141103	T	T	T
0.0846633503956724	0.4912883711338125	0.0551946792335656	T	T	T
0.1062915939542250	0.3594158927619375	0.0514278382606150	T	T	T
0.3102293124838624	0.6256229068996859	0.0953384837465023	T	T	T
0.3242639148768234	0.4949385596463003	0.0560608552489725	T	T	T
0.3023310021689838	0.3619927187295673	0.0599317163385962	T	T	T
0.5138568601026208	0.5367943797052632	0.2860185576700829	T	T	T
0.5136406799160156	0.3625446474901253	0.2761979457319015	T	T	T
0.4417158570046311	0.7505399209227264	0.6462114876671947	T	T	T
0.1937085306285340	0.7487801434051065	0.6519263101475445	T	T	T
0.2724136372258386	0.7490380168168542	0.0564997817239927	T	T	T
0.1079081223885936	0.7483507285306530	0.0531845022706321	T	T	T
0.0610283155826323	0.2495397133650528	0.1371506058548633	T	T	T
0.3047321959496045	0.2465668279224857	0.1531904713602685	T	T	T
0.2268349257661697	0.2514617482420576	0.5552504913015426	T	T	T
0.3902008298571360	0.2509439535293509	0.5510893557784939	T	T	T
0.5608788615937854	0.2513990212696058	0.3602923885740026	T	T	T
0.8081469495464404	0.2447801949611730	0.3760568567873506	T	T	T
0.7262231786464994	0.2522394790310472	0.9607927994111307	T	T	T
0.8937808449726958	0.2478998533645722	0.9503761451091819	T	T	T
0.9342536612341164	0.7464814288574289	0.8666481137698696	T	T	T
0.6843968798556688	0.7585385795957578	0.8616791119891474	T	T	T
0.7737908818884449	0.7480829852789839	0.4890084927028440	T	T	T
0.6045882330184114	0.7496666027474177	0.4571288114146057	T	T	T
0.9837285077247913	0.6250816838415005	0.3910899287631295	T	T	T
0.8862211180627710	0.4010188420212870	0.5918965563732712	T	T	T
0.9602652028134457	0.3824312813493620	0.5771460078440782	T	T	T
0.9352068717857023	0.5942135908967288	0.3258792694053412	T	T	T
0.9549311162553664	0.5871866053785624	0.5323982276837214	T	T	T
0.9175076888051024	0.6640995219968389	0.4920836512769995	T	T	T
0.0026490219851922	0.6639645780338483	0.5343817585421746	T	T	T
0.0275146792484264	0.6038047169862750	0.3873279965322283	T	T	T

Structure files (CONTCAR) involved in this work:

0.9640830995422078 0.6354159612777792 0.4944329026783194 T T T

Figure 2(a) Ga-TS

1.0000000000000000

20.0219993591000005 0.0000000000000000 0.0000000000000000

0.0000000000000000 19.8990001678000006 0.0000000000000000

0.0000000000000000 0.0000000000000000 13.3830003737999998

93 3 193 1 6 1

Selective dynamics**Direct**

0.4209944805352205 0.0572795870221403 0.6471784574613639 T T T

0.2998597059628265 0.0262198543695733 0.7876014595103276 T T T

0.2793702488350928 0.0590103178824760 0.0115093248993311 T T T

0.1196766003907929 0.0609752658566499 0.0112644650680715 T T T

0.0661739067382213 0.0289734023974808 0.7976963963818776 T T T

0.1753126477293510 0.0562676005194355 0.6500594310027182 T T T

0.4183295604157205 0.8270506614331163 0.6684463865126937 T T T

0.3007454105143270 0.8675875249703823 0.8077848677792790 T T T

0.2666403834685550 0.8274215221969681 0.0282157832817465 T T T

0.1116409763652948 0.8250704183602631 0.0164603594519907 T T T

0.0602010540060094 0.8695174741227600 0.8017969920807936 T T T

0.1777139129537829 0.8275033897845724 0.6721249051361522 T T T

0.0750805643152301 0.9407347943870229 0.1496578395734272 T T T

0.1959639324088999 0.9717560816104419 0.2916952131319122 T T T

0.2158358021441311 0.9375196397427347 0.5135594318073063 T T T

0.3752977600107413 0.9343127829097665 0.5145220343658794 T T T

0.4294367666604121 0.9692328433683666 0.3036650625041290 T T T

0.3205267401785308 0.9434712335518483 0.1539711715429681 T T T

0.0783075667649060 0.1708904493423961 0.1635303453099392 T T T

0.1955904981022138 0.1291520435674885 0.3059906852182668 T T T

0.2301959592438100 0.1727141820037626 0.5231538064816734 T T T

0.3848350843589026 0.1740069938240914 0.5116114681475721 T T T

0.4359957757034283 0.1275377491327198 0.3013573422488707 T T T

0.3183750313133051 0.1665858191858031 0.1702737801668341 T T T

0.5781451895290231 0.5571290205536487 0.3487615938526300 T T T

0.6899041933765981 0.5367282210442799 0.1920401869198267 T T T

0.7122322896414124 0.5624320029583683 0.9736428484574674 T T T

0.8707929797389342 0.5570922240599425 0.9733901218268826 T T T

0.9336226703121489 0.5285666556289688 0.1856452039925630 T T T

0.5775834941234933 0.3294902940067291 0.3297809667794683 T T T

0.7051993296883023 0.3774242069398104 0.2173843312640892 T T T

0.7354903282704792 0.3314347853270627 0.9936622359867053 T T T

0.8873420382516582 0.3255093377476023 0.9787793159237780 T T T

0.9366875674698981 0.3706501627392517 0.1950582304825185 T T T

0.9242999386693057 0.4345875218621592 0.8350154666188448 T T T

0.7810224716490269 0.4451397604871696 0.4776423730380502 T T T

0.6227931311281781 0.4330505297632440 0.4890313026823931 T T T

0.5657594096142650 0.4668632358253114 0.7040128128392809 T T T

0.6736771896037785 0.4339727139099451 0.8468006189341680 T T T

0.9166685519390925 0.6708130852460229 0.8253212801003141 T T T

0.7958823955682873 0.6318282042981518 0.7029543357082090 T T T

0.7679585106231265 0.6677541038415105 0.4821402601382653 T T T

0.6127041123330627 0.6705907390442801 0.4838469753146534 T T T

0.5663924464815350 0.6254691918797075 0.7031126471298175 T T T

Structure files (CONTCAR) involved in this work:

0.6785114234563203	0.6812954543571064	0.8317979102095420	T	T	T
0.5743596303150417	0.9435424051118237	0.3641635193439195	T	T	T
0.6949401930722053	0.9720417360589145	0.2222914528615878	T	T	T
0.7165421495382202	0.9447656872534658	0.9974244585996924	T	T	T
0.8769163542230075	0.9327906728329513	0.9949923630703298	T	T	T
0.9308721554221536	0.9687746242614322	0.2066764626532555	T	T	T
0.8201319738902845	0.9357569203805569	0.3526774275317839	T	T	T
0.5800380577899761	0.1749099168217589	0.3343053805989967	T	T	T
0.6994220833351215	0.1314363012700270	0.2033466241461579	T	T	T
0.7306799422771868	0.1721652582446469	0.9818708181912331	T	T	T
0.8855918514560212	0.1719280387197561	0.9940176570707880	T	T	T
0.9337698142261489	0.1276989963251491	0.2065771101357761	T	T	T
0.8207604530824991	0.1703749662219382	0.3430909045192861	T	T	T
0.9225715890819757	0.0564485393447014	0.8611701847916818	T	T	T
0.8034862151352429	0.0300007859295277	0.7217628450053722	T	T	T
0.7804628629262829	0.0550545158521316	0.4950103566081570	T	T	T
0.6203105614397375	0.0680366807900300	0.4939553398064417	T	T	T
0.5658704839657067	0.0335171920425337	0.7026390121575347	T	T	T
0.6768903099863870	0.0617295248307241	0.8508020956658716	T	T	T
0.9156966461167965	0.8237392020388302	0.8399793881875123	T	T	T
0.7995780373227755	0.8732715218914208	0.7080233020361678	T	T	T
0.7675145109615018	0.8291343149278114	0.4904147321318473	T	T	T
0.6116526779057689	0.8258138651994578	0.4970641449818241	T	T	T
0.5610460667285920	0.8763705846868198	0.7036402661086567	T	T	T
0.6743759453254673	0.8371709991386017	0.8403549704446162	T	T	T
0.4218113088125878	0.4459898167951495	0.6372724646293716	T	T	T
0.3019599544180702	0.4723999556830229	0.7843998611054142	T	T	T
0.2847027367429336	0.4309577580844695	0.0024433943453441	T	T	T
0.1259223714568876	0.4297234828790033	0.9993030846402545	T	T	T
0.0726606921957795	0.4718104421621486	0.7925293403512235	T	T	T
0.1798818179748365	0.4487762110073754	0.6417456373782185	T	T	T
0.4234756937261752	0.6719425773736428	0.6576549301876172	T	T	T
0.3005101734668834	0.6292405550678791	0.7940970820212898	T	T	T
0.2691436277626648	0.6714620891850284	0.0123047865827095	T	T	T
0.1150039384623816	0.6718019678780137	0.0031480875029201	T	T	T
0.0645137572897336	0.6291498464386903	0.7945716884609231	T	T	T
0.1780906023285606	0.6690796786355556	0.6575303244513534	T	T	T
0.0784950950417276	0.5521062366963467	0.1316549188563480	T	T	T
0.1998474249185637	0.5275222565824786	0.2757781722263798	T	T	T
0.2202899282068217	0.5671914654867319	0.4984107358289875	T	T	T
0.3803724004866140	0.5700018595387136	0.5012455774605541	T	T	T
0.4296585073681836	0.5262182926541190	0.2930805891218118	T	T	T
0.3265929235195811	0.5517656926903776	0.1372946458308360	T	T	T
0.0813636159101918	0.3257116510290256	0.1534670799499094	T	T	T
0.1978560784178681	0.3691627817962711	0.2975361730264434	T	T	T
0.2309189793211374	0.3295733651197432	0.5180801641517833	T	T	T
0.3853381304544612	0.3272888511373478	0.5071304356134574	T	T	T
0.4329674722829187	0.3696298583975042	0.2933693575987667	T	T	T
0.3189061387497077	0.3248556505581259	0.1629550419858067	T	T	T
0.8161840914927849	0.5676810865342363	0.3193213250790936	T	T	T
0.8294264083926666	0.3285642093638864	0.3533886731550755	T	T	T
0.7957165834421811	0.4737436438550700	0.7203178568558621	T	T	T
0.3550653811313075	0.0620508032511009	0.7171620182912686	T	T	T

Structure files (CONTCAR) involved in this work:

0.2991601075131767	0.0645255397766861	0.8944830748642846	T	T	T
0.1993214577570424	0.0490024330948052	0.0257891979078909	T	T	T
0.1003697375758059	0.0647735411645109	0.8940254520985509	T	T	T
0.1003814882743212	0.0574471202475809	0.6962049504350271	T	T	T
0.2264333852272817	0.0322108732231629	0.7373013462153526	T	T	T
0.3564752986293317	0.8252299506795736	0.7467938925869354	T	T	T
0.3034183947233096	0.8436338633802589	0.9230961156258198	T	T	T
0.1888005830377473	0.8509977666990847	0.0204000105693115	T	T	T
0.0832990190816228	0.8325130790148102	0.9038872911898590	T	T	T
0.1002297970951233	0.8360152076777625	0.7077190819258411	T	T	T
0.2266856875320864	0.8526294577211390	0.7619048299389237	T	T	T
0.3180599850358355	0.9471065334713181	0.8006536258896266	T	T	T
0.0784088118987020	0.9485588244129252	0.8072699337540248	T	T	T
0.4291511078166859	0.1269297488531851	0.5849272215693982	T	T	T
0.4158378266038349	0.9949505050566214	0.5686184115898659	T	T	T
0.3951273935303306	0.8629097386393846	0.5650600525785378	T	T	T
0.1932947280648143	0.1312771007405655	0.6114735117911771	T	T	T
0.1778359242289217	0.0034332980390684	0.5573216919321160	T	T	T
0.1912792589749981	0.8697395983834694	0.5705016259847719	T	T	T
0.9871814568908835	0.0458468168202815	0.7897878379496827	T	T	T
0.9801956658629081	0.8592829149959831	0.7868563684133490	T	T	T
0.1412149773628877	0.9372937380913956	0.2191148898637794	T	T	T
0.1971199329960402	0.9301640338991999	0.3961926862590832	T	T	T
0.2957488740716629	0.9476786734997060	0.5287896678860258	T	T	T
0.3949436065394157	0.9301730380118340	0.3973305361842749	T	T	T
0.3954480890382777	0.9441732415171820	0.1999514338558369	T	T	T
0.2693161980914875	0.9684861966096401	0.2406185356546864	T	T	T
0.1415228162146893	0.1692260071254501	0.2391129654847442	T	T	T
0.1926475492565622	0.1602667913372665	0.4175636281930504	T	T	T
0.3075335357556677	0.1481147618867071	0.5142717709677621	T	T	T
0.4127283211159907	0.1705903506836832	0.3982817758613832	T	T	T
0.3958367654212897	0.1548895190201031	0.2033933536671755	T	T	T
0.2701821427033109	0.1385381887436864	0.2594366590727806	T	T	T
0.1763804749755169	0.0498837064177925	0.3107244454971552	T	T	T
0.4175542093192118	0.0491837486583518	0.3200405853653619	T	T	T
0.0665133451764615	0.8685242082971122	0.0937331350158123	T	T	T
0.0805318143129921	0.9989309586252954	0.0644802396966096	T	T	T
0.0972886394918377	0.1315492495729859	0.0610988320654786	T	T	T
0.3028148819068328	0.8675237029332862	0.1185411017548545	T	T	T
0.3170547295518615	0.9938502721821594	0.0584505043933246	T	T	T
0.3031660084880998	0.1275528344650758	0.0663074571080658	T	T	T
0.5084234534153690	0.9525031944839346	0.2950646175722280	T	T	T
0.5159154228985260	0.1362996553259102	0.2849741635068270	T	T	T
0.6334262080529025	0.5703477254881595	0.2642065856867800	T	T	T
0.6718647946565164	0.5591855902996539	0.0779653195031467	T	T	T
0.7915771090203599	0.5476824015101156	0.9914105065143701	T	T	T
0.9125675130407298	0.5582247265373894	0.0763236266161996	T	T	T
0.8980959450169047	0.5656097765305150	0.2771141063702190	T	T	T
0.7617972778374442	0.5656703236018495	0.2205306479353921	T	T	T
0.6396400041424978	0.3348303450171213	0.2536113445459565	T	T	T
0.7281092773355501	0.3431959857961810	0.1122362860689368	T	T	T
0.8114853658332428	0.3531549570751744	0.9609185543261551	T	T	T
0.9110702233353506	0.3334197042883828	0.0930160608614648	T	T	T

Structure files (CONTCAR) involved in this work:

0.9053156629678784	0.3375008890269032	0.2930901372110923	T	T	T
0.7641663977443445	0.3724439043592233	0.2983058539020222	T	T	T
0.6829702313044298	0.4550704083935624	0.2001239298317384	T	T	T
0.9161314405031662	0.4491533810467119	0.1843239536222435	T	T	T
0.5648869763971651	0.6264501471956653	0.4111009898517737	T	T	T
0.6021453402552834	0.5003727178151209	0.4285869385133906	T	T	T
0.5930597572261026	0.3669672467920632	0.4351366577258924	T	T	T
0.8165286869855010	0.6435206110942507	0.3916430102928000	T	T	T
0.7973952552540170	0.5029307921176325	0.4016953489236814	T	T	T
0.8312996527044250	0.3765936699534069	0.4722916563140556	T	T	T
0.0139885194954657	0.5409130791461457	0.2017568230701591	T	T	T
0.0183775434568817	0.3663303013770009	0.1986470391471078	T	T	T
0.8712852074389156	0.4229699199991169	0.7403946447483817	T	T	T
0.8146826671662160	0.4674106127016643	0.5891181035496368	T	T	T
0.7038199919511823	0.4270885863318423	0.4962924232016007	T	T	T
0.5930653484419859	0.4345174745157096	0.6008594098523835	T	T	T
0.5985161761116277	0.4287322143795618	0.7993258522085828	T	T	T
0.7289797100163733	0.4275484091799508	0.7593688614834330	T	T	T
0.8627901948432848	0.6739434863745912	0.7348433761807321	T	T	T
0.7956354430075192	0.6296006307307268	0.5815585498633062	T	T	T
0.6901286195036055	0.6476564011974910	0.4646351198006183	T	T	T
0.5925091779961883	0.6588261886370846	0.5996665880756028	T	T	T
0.6027355289431594	0.6625439611121746	0.7967489743417226	T	T	T
0.7287610915039074	0.6720294664404977	0.7367266894010891	T	T	T
0.7989993403262035	0.5574612912283524	0.7500786239921897	T	T	T
0.5851656093144613	0.5462854062356098	0.7049456125482587	T	T	T
0.9350135437487340	0.3672569913181046	0.9008776022403410	T	T	T
0.8957654000026052	0.4947800109121284	0.9029805898785979	T	T	T
0.8879965132069312	0.6276136964528025	0.9178970338992113	T	T	T
0.6818263758560721	0.3750707048745965	0.9304661447303020	T	T	T
0.6802093081138256	0.5074899939728706	0.8987817258590213	T	T	T
0.7031256371041731	0.6368001997066361	0.9256440094150326	T	T	T
0.4851246102080740	0.4579840858412659	0.7101537158475475	T	T	T
0.4857416583128022	0.6350572423288067	0.7132826886292514	T	T	T
0.6394990835392967	0.9366357172566147	0.2930532381492916	T	T	T
0.6889954138548456	0.9412634428532163	0.1108196436172679	T	T	T
0.7975491534398441	0.9487326492754029	0.9928745139267471	T	T	T
0.9028426465235898	0.9286835259494201	0.1094572051519650	T	T	T
0.8954457254031293	0.9402681770772108	0.3076788088246794	T	T	T
0.7693718486134777	0.9550491087004540	0.2627141722239926	T	T	T
0.6410262584953802	0.1754130171791661	0.2552607834667429	T	T	T
0.6965844491473030	0.1473204975078605	0.0850395035436589	T	T	T
0.8084224750006904	0.1473978698127269	0.9824885749185754	T	T	T
0.9079642922001357	0.1704489643470952	0.1103427397891087	T	T	T
0.8976273865878615	0.1556282127056660	0.3064365729833997	T	T	T
0.7721522355734276	0.1501912054728583	0.2486101910600376	T	T	T
0.6827433294949578	0.0524826942207324	0.2229187439154718	T	T	T
0.9162138365605392	0.0483822318843141	0.1907720892579931	T	T	T
0.5657429584883760	0.8749400722090764	0.4290164895625385	T	T	T
0.5798813657884789	0.0070934502685537	0.4400103449948111	T	T	T
0.6035924726494436	0.1381614001797668	0.4372221081426064	T	T	T
0.8058650581976077	0.8595432340772323	0.3928981355767108	T	T	T
0.8113508611046258	0.9871881463608669	0.4456756102128335	T	T	T

Structure files (CONTCAR) involved in this work:

0.8053413730138388	0.1211126716709215	0.4372274612739087	T	T	T
0.0104953158745395	0.9547469726845180	0.2196165399107001	T	T	T
0.0143764046077602	0.1363886642440627	0.2180962375772051	T	T	T
0.8572415135680688	0.0689537231214639	0.7916064957577253	T	T	T
0.8077954357600862	0.0588564612148592	0.6090958051136003	T	T	T
0.6994003810186493	0.0505151729400971	0.4914103310770924	T	T	T
0.5955227120980893	0.0761451695172354	0.6089296421633255	T	T	T
0.6016498995042268	0.0562701407524300	0.8062002336637496	T	T	T
0.7279040914564291	0.0412013258755462	0.7614930994688283	T	T	T
0.8532634489607864	0.8247333041128193	0.7627932803743671	T	T	T
0.8026415551224988	0.8598541694202876	0.5892491904589485	T	T	T
0.6891139271826526	0.8503255633422432	0.4882888501977672	T	T	T
0.5872399835651695	0.8289593683936790	0.6127313121060132	T	T	T
0.5981027661623929	0.8538437617278931	0.8062903884488645	T	T	T
0.7246049711006222	0.8587281225859593	0.7495118741750639	T	T	T
0.8215520045417908	0.9504678965934956	0.7288289076064055	T	T	T
0.5787203461724966	0.9542315214324526	0.6790335417234459	T	T	T
0.9340891093546174	0.1225451946521042	0.9300926791515958	T	T	T
0.9156337621565533	0.9915014979798892	0.9339614056668557	T	T	T
0.8946744521524336	0.8609596150640252	0.9433330866426174	T	T	T
0.6914793318400363	0.1378998900329792	0.8882913363743983	T	T	T
0.6852748348939115	0.0111104065463589	0.9450192661939182	T	T	T
0.6919704939122679	0.8772651168164700	0.9416931926836083	T	T	T
0.4864210167536916	0.0474724274997603	0.7169969911646957	T	T	T
0.4808564151404412	0.8670831965927821	0.7184443106653018	T	T	T
0.3550814686101296	0.4426252410405785	0.7054112529818415	T	T	T
0.3039073900211889	0.4265693131784587	0.8846820903055460	T	T	T
0.2049434340309896	0.4444117323955010	0.0151976175674844	T	T	T
0.1071720560658884	0.4282177972820670	0.8809406836022908	T	T	T
0.1036971765385316	0.4532409453238951	0.6837465808287190	T	T	T
0.2282390584051654	0.4694381186900964	0.7339555506425586	T	T	T
0.3565645524099674	0.6637259887456048	0.7246076042119927	T	T	T
0.2997816826851797	0.6687216535911087	0.8999201412023580	T	T	T
0.1919386964691668	0.6453874987694541	0.0083832723288513	T	T	T
0.0911004667339209	0.6746652976814929	0.8866902374764980	T	T	T
0.1000552422993092	0.6543942646044042	0.6903444802683788	T	T	T
0.2273395890870992	0.6354907444631566	0.7403086566098680	T	T	T
0.3178309084434435	0.5504073641526032	0.8124006739863211	T	T	T
0.0831363989072561	0.5512317817744786	0.8167597650187486	T	T	T
0.4307842402997122	0.3756022835983750	0.5773002891851668	T	T	T
0.4160174754905631	0.5064289848853769	0.5556801609795082	T	T	T
0.4098314611946327	0.6392350760867266	0.5479752125688444	T	T	T
0.1932560269409288	0.3728049074088103	0.6040541185643834	T	T	T
0.1875413246409402	0.5003581386200330	0.5482769751764436	T	T	T
0.1879936023575807	0.6347322838372311	0.5481156294117092	T	T	T
0.9938110852040370	0.4549561112671852	0.7816035581389943	T	T	T
0.9845871582047729	0.6372238980871840	0.7782190307159375	T	T	T
0.1436798583770351	0.5601596442075742	0.2032844328981859	T	T	T
0.2003397418771753	0.5689208316081017	0.3809794189038390	T	T	T
0.2999836866030274	0.5661347796721501	0.5189155330646081	T	T	T
0.3955954353521969	0.5694113530041728	0.3828527098957078	T	T	T
0.4004727139388520	0.5541314200175748	0.1873498327581227	T	T	T
0.2726392454347391	0.5344098769010333	0.2245225653187945	T	T	T

Structure files (CONTCAR) involved in this work:

0.1425505255906352	0.3294528207423751	0.2327987834069157	T	T	T
0.1944704120224444	0.3410024974567537	0.4110824516615461	T	T	T
0.3082843513994613	0.3541361642868672	0.5102941696157384	T	T	T
0.4114785379694357	0.3279410660524667	0.3927368258627453	T	T	T
0.3960250406656275	0.3374006330370123	0.1960402975075440	T	T	T
0.2715849937782887	0.3565806106832874	0.2503169850715316	T	T	T
0.1820277102689619	0.4493343744372698	0.2973040009893077	T	T	T
0.4098140611829202	0.4474751812902307	0.3073873022089180	T	T	T
0.0687154556245840	0.6208230510529479	0.0669972290485700	T	T	T
0.0849947571160198	0.4898246474649383	0.0536657149865728	T	T	T
0.1052482441611140	0.3577564849587078	0.0468698570947600	T	T	T
0.3115178837640748	0.6244170139428038	0.0875341555500639	T	T	T
0.3247686813280302	0.4935085628502987	0.0522723799099142	T	T	T
0.3045414507499332	0.3605181141894405	0.0556976709454271	T	T	T
0.5096434390477028	0.5344918716320884	0.2940355822468537	T	T	T
0.5128177334001982	0.3640519142396916	0.2763670829183270	T	T	T
0.4402070081203232	0.7507443549223137	0.6420513870279565	T	T	T
0.1916538452052754	0.7487749477286522	0.6471578782381100	T	T	T
0.2722933081099839	0.7479157398863344	0.0534898185182554	T	T	T
0.1079948546971773	0.7466348174359809	0.0496969077554671	T	T	T
0.0618198493925363	0.2479168787109174	0.1334373330681885	T	T	T
0.3038971126624068	0.2454849346740317	0.1504269158871915	T	T	T
0.2261284481261977	0.2516862196616582	0.5517470202788448	T	T	T
0.3895926153822368	0.2511930745369955	0.5503012897011519	T	T	T
0.5601444314825605	0.2520624264200795	0.3582501537962183	T	T	T
0.8107779358407979	0.2460251276530065	0.3789268086180214	T	T	T
0.7247815204761605	0.2525006910222765	0.9680013141310811	T	T	T
0.8932967728546414	0.2469379508012727	0.9482217322008540	T	T	T
0.9337948088481245	0.7459230424502749	0.8651898064752228	T	T	T
0.6814768915228976	0.7586731882583647	0.8674375368830547	T	T	T
0.7760251810587024	0.7484779738021589	0.4936866049267759	T	T	T
0.6036955323266022	0.7495032527799521	0.4566548753274534	T	T	T
0.0101276833864261	0.6680972907525528	0.4834473903368097	T	T	T
0.8870338540316218	0.4033127440213512	0.5911399507710925	T	T	T
0.9613781086240216	0.3855358372573023	0.5773082360335642	T	T	T
0.0370186642417321	0.6350315327160064	0.4472352201447989	T	T	T
0.9053525629754594	0.6223513509505937	0.5024815132821820	T	T	T
0.9305837351500081	0.6407118820995704	0.3699562934807592	T	T	T
0.9064851219872450	0.7112475534069342	0.4569283624215987	T	T	T
0.0203821295128600	0.6619540161750141	0.5548053532550131	T	T	T
0.9173329907492027	0.6583976323196878	0.4442941865929744	T	T	T

Figure 2(a) Ga-FS

1.0000000000000000

20.0219993591000005 0.0000000000000000 0.0000000000000000

0.0000000000000000 19.8990001678000006 0.0000000000000000

0.0000000000000000 0.0000000000000000 13.3830003737999998

93 3 193 1 6 1

Direct

0.4222432230342856 0.0572897720387266 0.6483779820160794

0.3016510458160340 0.0264746843556360 0.7891521447634756

0.2799699590334399 0.0591628329698498 0.0125250208757969

0.1204172468645082 0.0622373101567470 0.0120719561767850

0.0674798676783037 0.0283822806115568 0.7989780527182875

Structure files (CONTCAR) involved in this work:

0.1769713394382333	0.0552997944209552	0.6514576653385266
0.4192319812620253	0.8277090724334780	0.6695792943116643
0.3024737834197347	0.8684298758173949	0.8097627242212478
0.2675983786726069	0.8279357328071915	0.0299763576279308
0.1125882016213245	0.8257462232200098	0.0183655308623642
0.0619734626382478	0.8690739038090326	0.8034433141991627
0.1798348859862667	0.8278386655949300	0.6740967867182758
0.0756400301200773	0.9424214890176436	0.1506624083647374
0.1966152315462822	0.9723568144161787	0.2935027718935788
0.2168797248622295	0.9369555109791549	0.5141303717290266
0.3762872759293933	0.9344265715952575	0.5153026959944912
0.4305680949365641	0.9697935121296494	0.3045056852747920
0.3210734097030570	0.9440183009201789	0.1557994186835115
0.0792739353540396	0.1715534182592130	0.1644558284205581
0.1960988333648809	0.1296407970103923	0.3086674496590727
0.2319804322929790	0.1727194865884634	0.5256671625139578
0.3866633326010399	0.1741434526311341	0.5131626587963526
0.4364264906476689	0.1281590742013699	0.3019471110245938
0.3181534713780697	0.1668029846279430	0.1714932750018065
0.5770207162478688	0.5550844432744688	0.3520744636790434
0.6882719781760239	0.5374900223241568	0.1923154396708701
0.7130323277359286	0.5628888974072008	0.9749496324878723
0.8709127895097577	0.5571910376161118	0.9739644241258926
0.9333313051849870	0.5265740986673079	0.1845982991745324
0.5768100046161383	0.3303419236844325	0.3296655651069934
0.7062107746749243	0.3774499218744807	0.2183734303261655
0.7367973630223552	0.3313155463255871	0.9957444178943998
0.8885446097412176	0.3246316027418092	0.9785938580330374
0.9369695437642367	0.3695724159037970	0.1941418108344868
0.9244627901214493	0.4348992676053536	0.8354790606024524
0.7797681140195543	0.4439459570788116	0.4793982587198359
0.6225347878303829	0.4317806869649121	0.4918484048920828
0.5664921219217541	0.4657274223186808	0.7065747420724915
0.6748242807071592	0.4340588261334624	0.8491417999854127
0.9181595576759007	0.6699445208901782	0.8257983559482829
0.7971845002764312	0.6320032074767876	0.7047569825246142
0.7672378689026021	0.6681599206532413	0.4844302903181169
0.6153064936186587	0.6693945700062778	0.4815864069204673
0.5709226065254991	0.6243374240244269	0.7014836266378935
0.6803915593895311	0.6820536632499948	0.8338908253099830
0.5753549844358377	0.9433496139354322	0.3640769566556621
0.6956482195653868	0.9728659987816096	0.2221112819048646
0.7179227020197361	0.9455970718702571	0.9973276309914836
0.8782094440353004	0.9323159138357946	0.9956391032465161
0.9313704230499659	0.9690843061063741	0.2073609720518085
0.8205595249724381	0.9363922942208862	0.3530698902982187
0.5803660554539311	0.1753157062200346	0.3333445355170342
0.6997930881083813	0.1320583455631701	0.2025852608287177
0.7315503728308489	0.1724267138505547	0.9809946705530392
0.8863851526189077	0.1714640042292879	0.9921838034904832
0.9342739142764465	0.1278490444402479	0.2052363449086268
0.8214593880955305	0.1704225990184727	0.3424216181552643
0.9237433808659304	0.0553315897164091	0.8607304550750906

Structure files (CONTCAR) involved in this work:

0.8041357386203578	0.0294684841190803	0.7209438164192880
0.7810920198861198	0.0551668118616242	0.4949948253323795
0.6208107645881599	0.0682187133634009	0.4936910275455637
0.5671430747959766	0.0337705771639673	0.7024607139713067
0.6780549316692954	0.0621265923022905	0.8507155781817984
0.9173085984965391	0.8232991911539685	0.8408210360939322
0.8007897218729696	0.8720243918033193	0.7075386409301774
0.7678855496299618	0.8295843691717063	0.4894037773298874
0.6123704426445222	0.8255891083300236	0.4968543105802322
0.5618618735970938	0.8770723170805611	0.7029104135303488
0.6751245037511507	0.8375032125000934	0.8402978627238930
0.4227047886619089	0.4460152389614984	0.6400760837083391
0.3039146441082805	0.4719883740506877	0.7874808317312167
0.2853298679010997	0.4323245517017587	0.0051174412949646
0.1269538981890491	0.4311919897785161	0.0027732360206893
0.0731209133330826	0.4714295270060783	0.7963564119875040
0.1811700147809200	0.4482958038638860	0.6473609243449174
0.4259974059288172	0.6727631114669210	0.6595103271351379
0.3048393243943707	0.6287943952363289	0.7989072486444900
0.2697694514043677	0.6714251741061378	0.0174458192170930
0.1151215541252977	0.6724393384741836	0.0106642295830577
0.0661090520373835	0.6285635598139792	0.8005115578556201
0.1808809105040557	0.6695779842300846	0.6637338541007980
0.0786397348316591	0.5519523283428077	0.1376630246002892
0.2002044332964383	0.5264826549960366	0.2821583964733066
0.2202277587002011	0.5667373155196210	0.5048159840237825
0.3795390379844754	0.5703383061725263	0.5066041887394583
0.4273187687159126	0.5246615450325997	0.2990660513802856
0.3264105307703380	0.5516944517844879	0.1419449151977892
0.0823811132573753	0.3264045472750553	0.1578086981525441
0.1976178392123519	0.3681954853114419	0.3041939903868150
0.2326934242438035	0.3291214547276547	0.5236065839143602
0.3870309059175606	0.3269600289230105	0.5094863273622227
0.4319467737033196	0.3688004510194915	0.2953766002306144
0.3174059427655815	0.3247007986320808	0.1660702334285245
0.8149188392852630	0.5635793572642470	0.3180469416194767
0.8299672536033512	0.3282672480633497	0.3543685846023606
0.7959292390048048	0.4733798994895232	0.7212941837765564
0.3565051747458632	0.0628773011850763	0.7186134977631874
0.3003520254042055	0.0650677785870884	0.8957576177866480
0.1998978278548970	0.0487414033668993	0.0255912405479354
0.1003624691666846	0.0656281889722018	0.8951198831689087
0.1021191925323667	0.0566345096373333	0.6977597184781669
0.2282153042050442	0.0311652344991889	0.7385399455378349
0.3579198850417469	0.8255537921603524	0.7487581862486148
0.3046688650007685	0.8442183305156361	0.9250230781085206
0.1898066903412404	0.8515588863636716	0.0217697566825763
0.0847981322583474	0.8313632696137956	0.9052004010362784
0.1022777744474875	0.8364347306467967	0.7091350231303239
0.2283691922831511	0.8547666186973319	0.7634547850347745
0.3211117826586072	0.9477051209245986	0.8028107551591718
0.0803102843840924	0.9481603988890849	0.8104520212628374
0.4311387160725006	0.1265989145946606	0.5855489315157780

Structure files (CONTCAR) involved in this work:

0.4166622867716515	0.9947809380727659	0.5702948649812697
0.3953590962238869	0.8628884473936386	0.5660539630660179
0.1952354317312209	0.1301833497965690	0.6128607897210131
0.1787991161065313	0.0025738373061844	0.5586651672132216
0.1933749639594337	0.8690247268649065	0.5714286667053452
0.9883206178446193	0.0443787504306306	0.7894555878883757
0.9819053423298719	0.8590495277677668	0.7884599904599947
0.1419405793667042	0.9390012676822699	0.2196955605996103
0.1974828065220350	0.9296005148301716	0.3969689357394319
0.2967790662613677	0.9481400790459998	0.5279650774330535
0.3970155915733794	0.9303830890799316	0.3985317219186283
0.3961791507177602	0.9446244945178129	0.2012093964026502
0.2700762024347769	0.9694005387936402	0.2425336158501543
0.1414584449658842	0.1690073798473930	0.2419142620734394
0.1942570586895101	0.1618705930321134	0.4196997739409440
0.3093489458077323	0.1483254150382582	0.5156811028701771
0.4141388048814401	0.1710684423893482	0.3995368053455424
0.3956882401002085	0.1556929638983518	0.2046838147697476
0.2703691105858622	0.1384201981620919	0.2607685567565761
0.1772779958421756	0.0503109789492139	0.3149519492775807
0.4183511426438085	0.0497118980288746	0.3209177646442722
0.0672652475462809	0.8707765927425746	0.0933561965337285
0.0803402235086836	0.0014756131602490	0.0667947325112414
0.0997034133851379	0.1335170678107599	0.0615073343013994
0.3033593038687066	0.8680357579048221	0.1207197995937009
0.3176059503897541	0.9941646874256095	0.0599825826600050
0.3033017250821153	0.1277161015571312	0.0675707974243682
0.5096097332133731	0.9532842411363940	0.2949968357073200
0.5162060513353210	0.1370234142379123	0.2837061832419502
0.6285937698080195	0.5667393558424327	0.2622394850176840
0.6712329609192438	0.5597180953802379	0.0781031061627191
0.7919560534813995	0.5477868743341630	0.9958403951773562
0.9142275352422575	0.5583654154780426	0.0756761514320683
0.8953786922109733	0.5613792099423026	0.2756955200629868
0.7573282892501639	0.5716041520142908	0.2253561064997989
0.6389873766532226	0.3375596809668201	0.2540412145848789
0.7293047227001821	0.3411890449129633	0.1148659511664276
0.8127207138978014	0.3531328111274752	0.9634076826172466
0.9133131238867348	0.3303666869956676	0.0927006769468761
0.9051515356619004	0.3375139348720962	0.2926203595332161
0.7640876868348734	0.3722114821570700	0.3009717246316219
0.6875216626589471	0.4556983571615172	0.1983551412692806
0.9149335575921108	0.4473920355344114	0.1789505799588247
0.5652605710708961	0.6259473469590107	0.4117582862569958
0.6047126444177128	0.5008281739919062	0.4331851722512589
0.5912533899661537	0.3674898377429897	0.4355519999843307
0.8214888503058329	0.6424639465383718	0.3953218695421349
0.7920228328057971	0.5034978430772702	0.4038997000891953
0.8322427835063494	0.3774741370187373	0.4722740054710748
0.0131366300085059	0.5384103121920064	0.2048826004824471
0.0185558937185272	0.3671088225740066	0.2001151814520335
0.8720634466177573	0.4233065668185162	0.7398912365828958
0.8138837330400643	0.4676390558331352	0.5895953852781760

Structure files (CONTCAR) involved in this work:

0.7033960346517388	0.4234080631413107	0.4996755059674827
0.5925759445860818	0.4322188425459698	0.6034676494399428
0.5995565307663762	0.4281828416306427	0.8021825860060261
0.7299054349962065	0.4265740013888940	0.7615862102654553
0.8653736813095013	0.6723247842402482	0.7334852412400390
0.7935139769098624	0.6301771075443814	0.5828257510988907
0.6924049167930696	0.6459315501089831	0.4541300259826087
0.6012823383557442	0.6560169250650808	0.5989403069559970
0.6057075106814478	0.6613092774193562	0.7964035346740057
0.7319713012223965	0.6746043225330752	0.7402022263193362
0.7978877998099694	0.5573159576870689	0.7503137846970943
0.5875442506511587	0.5447699962027559	0.7052435526384587
0.9354266859564645	0.3674691917303818	0.9010915496432739
0.8940478047105020	0.4944364468171269	0.9030757842780002
0.8865162441147425	0.6277028435393375	0.9177131503955926
0.6831986465152948	0.3763354239805192	0.9345413730565412
0.6816595295890567	0.5083241168737384	0.8988872074375308
0.7049753097961081	0.6375651119713548	0.9277153221082739
0.4858108261897104	0.4576814669548686	0.7138149047387523
0.4906867188581296	0.6356563352738707	0.7076013392094574
0.6405776149105847	0.9369264864752801	0.2929612752852871
0.6904383138819137	0.9415981593464231	0.1108167921185923
0.7989033157685596	0.9486612520102492	0.9926758266386992
0.9034311233715916	0.9284203326067557	0.1105316395973728
0.8959209915678926	0.9409908814154240	0.3086725377545792
0.7701460445649397	0.9569745363707343	0.2633681291521608
0.6414834307197925	0.1762414333601613	0.2544257778699075
0.6973468307771422	0.1477614073075267	0.0842241207926749
0.8091046186960752	0.1471300323882574	0.9811359755842788
0.9086222948517003	0.1701566497540351	0.1085227248547891
0.8981840755724704	0.1565937657497937	0.3046436411390113
0.7724297665899891	0.1507177270547426	0.2482583575691404
0.6826686441842146	0.0531767880410836	0.2222547975647610
0.9162657296005843	0.0485349741731439	0.1906060253950972
0.5666823363897384	0.8738200317781853	0.4271089706165239
0.5810397777129374	0.0061164473520709	0.4413984385167249
0.6034971533316991	0.1378273049575600	0.4359301838647498
0.8056992899425557	0.8597787553751463	0.3916489398597963
0.8113299783288407	0.9862066952142097	0.4478819996743477
0.8069216696458615	0.1201091989657924	0.4355922680974140
0.0109592449738460	0.9554973979350578	0.2208832342779036
0.0148660566043719	0.1362567398224543	0.2166144090127725
0.8583254603207314	0.0672468942136767	0.7912275172353189
0.8081581735950172	0.0597966626830560	0.6090927811856529
0.7000468641055319	0.0514958289851054	0.4907684250106653
0.5963254759992923	0.0768644944499798	0.6087871314823033
0.6028436306802917	0.0561062102626499	0.8062653516015964
0.7287922199510727	0.0407418334547451	0.7615524493020733
0.8548934843334883	0.8248765502918953	0.7635349331935075
0.8042531697545930	0.8566878637431089	0.5891169422278776
0.6896599598853862	0.8510506783437891	0.4894961356465035
0.5870507989890313	0.8289658882172098	0.6119352078293046
0.5991478075820778	0.8544927467912373	0.8052670952169770

Structure files (CONTCAR) involved in this work:

0.7258608131864959 0.8569593566069300 0.7490078925600376
0.8215615225557299 0.9497722114161744 0.7254294382597484
0.5804570860564218 0.9546357290814321 0.6776395720953360
0.9348823832294447 0.1219569511554749 0.9286267418574012
0.9171284977861962 0.9909104643726753 0.9346648243785092
0.8959603782666855 0.8603657915623787 0.9443479241544511
0.6922792811570033 0.1386013332783771 0.8871140667864369
0.6870222078876533 0.0125076164785247 0.9460239844804806
0.6927897944480473 0.8788218593457207 0.9403823790955751
0.4877669167675194 0.0472746610422087 0.7179111101515782
0.4817061469827285 0.8686128000656135 0.7183451130724732
0.3556266322708484 0.4407670173216026 0.7072326058897178
0.3065893867838682 0.4265204020794770 0.8882336383070082
0.2058487941430758 0.4480007372169866 0.0143102713127348
0.1056071161230042 0.4269656981801659 0.8857016163684127
0.1049878988953322 0.4511461990983983 0.6889777671119728
0.2294409367153003 0.4702577741190110 0.7393078586519177
0.3629415408565886 0.6641793740496167 0.7340694934242626
0.3017500421963420 0.6662475187639026 0.9061898134541319
0.1922990495334569 0.6463214810796007 0.0140905196370787
0.0895213999136023 0.6731884879241135 0.8955946951260039
0.1047353449524206 0.6559182326964029 0.7014602701900056
0.2330583731390536 0.6360022019575481 0.7423310045276381
0.3220694386134381 0.5496313479783420 0.8143009476094072
0.0851548290411537 0.5503836746491577 0.8212085733829434
0.4325227430496697 0.3766642812663538 0.5775616262314294
0.4174127428847073 0.5080931552278350 0.5611182410494909
0.4081778880857419 0.6407172605303696 0.5507331442572804
0.1966267584538837 0.3724294133548876 0.6108225168025309
0.1876505239322315 0.4995783214497927 0.5534318797263477
0.1879431612708722 0.6346572340474123 0.5536220698010004
0.9940456792104179 0.4560568020424393 0.7836201655523294
0.9862547221321595 0.6352468173022017 0.7835362107748359
0.1425778655848166 0.5586561690774886 0.2119033171824736
0.2026347690379753 0.5685743336060604 0.3865350442996910
0.2997550657759562 0.5654138697243762 0.5276091258157675
0.3927405992494455 0.5684820373152335 0.3876202847458238
0.4001472698750597 0.5535151921739419 0.1928070431525463
0.2720233196566351 0.5325854853075106 0.2276534167207318
0.1413109886540985 0.3289132290265145 0.2408278198792968
0.1947704043691605 0.3402459582120620 0.4177619464271751
0.3099569390849157 0.3534687419758106 0.5128567078714811
0.4125065736988826 0.3261802828810128 0.3947016582110967
0.3947913903488014 0.3368693937883987 0.1981588978719622
0.2707589025535435 0.3547704050481413 0.2553962339867445
0.1826660817436732 0.4484338412010355 0.3046401981790727
0.4070452538500323 0.4459415840002545 0.3117905374509458
0.0696898654768828 0.6226180879414400 0.0779718533935647
0.0862127295751377 0.4916783699618577 0.0565366847481903
0.1091187188089023 0.3594938265595320 0.0536572358622130
0.3111910599621858 0.6251841507213010 0.0951661301703130
0.3257763501943963 0.4945661140559034 0.0552077399722191
0.3022709250057174 0.3618336643922991 0.0603079174697887

Structure files (CONTCAR) involved in this work:

0.5073409378560908 0.5308092376740287 0.3036988126405124
0.5117613531118897 0.3644780460731611 0.2763893595970033
0.4420561614516330 0.7516512071617637 0.6434433806389472
0.1951298244015542 0.7491454140130194 0.6515537095345021
0.2735164953953411 0.7485515912045491 0.0555712290124195
0.1086524945358918 0.7480219454047218 0.0548790074379217
0.0628076052785236 0.2488356270579201 0.1356412961593884
0.3028141923193589 0.2454726212339597 0.1511739159504574
0.2281972199733517 0.2511746262142742 0.5571990372048912
0.3919590670190806 0.2510296847170113 0.5533538170223851
0.5607111313157895 0.2525334963778684 0.3574915270412512
0.8112989005925521 0.2457447086301124 0.3799799251010479
0.7258845890411736 0.2528318973637312 0.9675107280488086
0.8938868759266618 0.2463935234270068 0.9457686983442889
0.9345163253658237 0.7453070664682144 0.8654990528832390
0.6807712892576958 0.7593052304997396 0.8703043520089467
0.7745692981430279 0.7483579328793325 0.4886170014003681
0.6064113771089659 0.7486655748215439 0.4573543595920361
0.0426485678527696 0.6354569295271572 0.4432879147817032
0.8883003208185871 0.4058438615664012 0.5906119299589830
0.9627828395841230 0.3895692324657219 0.5752315925401926
0.0579355421979285 0.6174232051079493 0.3796561177442683
0.9210308912020851 0.6191500469053052 0.4376306058735263
0.8905528028167923 0.6983880933908088 0.4822661634927874
0.9116219173358689 0.6882236680276630 0.3523018198743155
0.0836542688568910 0.6455764148536406 0.4796550869968373
0.8916449618203182 0.6636070359410704 0.4188276884818068

Figure 2(a) Cu-IS

Si Al O Cu H C

1.0000000000000000

20.0219999999999985 0.0000000000000000 0.0000000000000000

0.0000000000000000 19.8990000000000009 0.0000000000000000

0.0000000000000000 0.0000000000000000 13.3829999999999991

93 3 196 3 5 1

Selective dynamics

Direct

0.4229288788235088 0.0532097363686105 0.6426107455590608 T T T
0.3025519287439287 0.0259977817517393 0.7875306744588323 T T T
0.2792510208010242 0.0633432206717487 0.0070097737500476 T T T
0.1192492563408575 0.0630570884848108 0.0066400684986088 T T T
0.0661795528116327 0.0242155802665977 0.7947249139341354 T T T
0.1778277771927287 0.0512023620469895 0.6480799610878889 T T T
0.4207602008703819 0.8267668160340149 0.6646427409325265 T T T
0.3041482650693167 0.8687593567657640 0.8080231052278927 T T T
0.2678807051331229 0.8278824568926758 0.0271592171036942 T T T
0.1133518789281478 0.8252706203439161 0.0160731202460305 T T T
0.0644115840323157 0.8637013660472224 0.7989773938428720 T T T
0.1843471941128514 0.8266579779269591 0.6705276664011830 T T T
0.0767896159729010 0.9427609014716657 0.1472930245483163 T T T
0.1976881851314342 0.9719209000373025 0.2903770626604921 T T T
0.2192507251123096 0.9335772119604542 0.5091485545781367 T T T
0.3783101961575815 0.9301991688915393 0.5091881398562550 T T T
0.4302555501335380 0.9698218697577121 0.2993732564935802 T T T

Structure files (CONTCAR) involved in this work:

0.3210588274483632	0.9471711160948644	0.1494777736426863	T	T	T
0.0797788322287983	0.1699635409817684	0.1621630269882750	T	T	T
0.1967467901026380	0.1286631159056456	0.3071016211790490	T	T	T
0.2304261269100304	0.1713443784997153	0.5242706080182651	T	T	T
0.3853249918146989	0.1717691033471901	0.5098051638433833	T	T	T
0.4344006578075581	0.1273280330629822	0.2993122079249507	T	T	T
0.3174434777422194	0.1681318702731249	0.1698145804176309	T	T	T
0.5757141957772602	0.5577285224839833	0.3497412892626215	T	T	T
0.6920748605608191	0.5299050732595239	0.2090524064767142	T	T	T
0.7147788889260256	0.5488770668587919	0.9803265253774098	T	T	T
0.8726758824590357	0.5628756672387450	0.9862627091809172	T	T	T
0.9317009972160133	0.5266057123481804	0.1942729594667980	T	T	T
0.8173012552784702	0.5607548894862281	0.3329009455489799	T	T	T
0.5808389527695736	0.3263276274651933	0.3295122326654479	T	T	T
0.7004586553851999	0.3722410216247736	0.2039971172407001	T	T	T
0.7341020008253002	0.3301443065109350	0.9862823176780569	T	T	T
0.8888508672605522	0.3282810653247148	0.9943728616737941	T	T	T
0.9375887098445639	0.3693829742746865	0.2038159548895390	T	T	T
0.8227094185400120	0.3310452464048816	0.3405714934711723	T	T	T
0.9258091415676601	0.4421171673842340	0.8548010170688485	T	T	T
0.8084603686072859	0.4675911270651792	0.7140606517492158	T	T	T
0.7808762399846417	0.4440712197684233	0.4907628443192334	T	T	T
0.6218305588512808	0.4333193342291840	0.4881802678696581	T	T	T
0.5645348739040326	0.4637929566698891	0.6998471077079451	T	T	T
0.6804033155764420	0.4298419668406476	0.8314678258710145	T	T	T
0.7984095191547771	0.6215386112569049	0.6983028814327994	T	T	T
0.6090035467110591	0.6706633340267952	0.4823037964302516	T	T	T
0.5661330263681300	0.6221659489298594	0.7008832828134883	T	T	T
0.6773821221345124	0.6689297558002605	0.8344264464596172	T	T	T
0.5761786956662319	0.9419142686654245	0.3510104868123315	T	T	T
0.6944858420234012	0.9739349482827119	0.2082410624218307	T	T	T
0.7169828852849591	0.9513731751109830	0.9843486348835989	T	T	T
0.8778573334729232	0.9470128751727932	0.9842678632759316	T	T	T
0.9337402031645926	0.9691457172756196	0.1989087496466602	T	T	T
0.8165522366789545	0.9309049973377586	0.3276300694323285	T	T	T
0.5801677115499101	0.1726716524759062	0.3251846072024722	T	T	T
0.7008942583869564	0.1305219947985061	0.1978913132782884	T	T	T
0.7358027573120325	0.1683746702683478	0.9797418339922737	T	T	T
0.8917150655588885	0.1750569381594997	0.9797548101822738	T	T	T
0.9366771537534226	0.1273714223055716	0.1983493524629710	T	T	T
0.8217532249337222	0.1760673466834594	0.3305009851753791	T	T	T
0.9218473937616343	0.0665198790622000	0.8408614629018640	T	T	T
0.8070207211326202	0.0342693173883120	0.6984410618134479	T	T	T
0.7828181666856813	0.0555850503057241	0.4728019334938010	T	T	T
0.6229867655255641	0.0664094363955011	0.4832795004545317	T	T	T
0.5677508893807204	0.0337565665081900	0.6948377352246140	T	T	T
0.6837466233932711	0.0681719244812164	0.8255539431435071	T	T	T
0.9150132118953422	0.8301219576139260	0.8297480706436212	T	T	T
0.7992825020328128	0.8774794960081169	0.6975332597692053	T	T	T
0.7686519510877122	0.8297369807519187	0.4837979847416971	T	T	T
0.6102217555844774	0.8251406799117200	0.4901904715181191	T	T	T
0.5631184618655488	0.8757242701450727	0.7033410006497330	T	T	T
0.4218972511293729	0.4426576873371257	0.6483363248132386	T	T	T

Structure files (CONTCAR) involved in this work:

0.3025565181635569	0.4723549098618716	0.7923149069988358	T	T	T
0.2816887735829389	0.4342099461018883	0.0119295244213013	T	T	T
0.1224307698459311	0.4323560912298418	0.0116993049217536	T	T	T
0.0711235063433240	0.4702793753372067	0.7998607130738598	T	T	T
0.1803080128797907	0.4467928074840937	0.6518499110875963	T	T	T
0.4227355000043251	0.6715504604444696	0.6657612114813710	T	T	T
0.3061375047726861	0.6286998176655072	0.8090244629193213	T	T	T
0.2689119596689449	0.6713745430331154	0.0271200462511628	T	T	T
0.1150983924474462	0.6721812099079539	0.0120846402975351	T	T	T
0.0673417565365330	0.6294889103695563	0.7977856558248891	T	T	T
0.1864088657772180	0.6687411462188825	0.6685924996194700	T	T	T
0.0763352658461605	0.5552959850610278	0.1440356843074639	T	T	T
0.1964781866226783	0.5256920718033958	0.2875811140653740	T	T	T
0.2209890947274335	0.5624149417255639	0.5086545506517983	T	T	T
0.3803208093862339	0.5650708237809380	0.5114239141408247	T	T	T
0.4307603784747741	0.5257365854572532	0.3001609109888221	T	T	T
0.3222465796711314	0.5523443688408614	0.1496170156835591	T	T	T
0.0810395557237817	0.3245038384629443	0.1657314861690243	T	T	T
0.1970048058888335	0.3681631988697656	0.3078378929707450	T	T	T
0.2330060293247956	0.3277872287760836	0.5262686467821053	T	T	T
0.3880030354163993	0.3243755023508129	0.5137745662573762	T	T	T
0.4363332040679542	0.3689364154286955	0.3014322971077719	T	T	T
0.3188538391239701	0.3269812097678475	0.1727352738743813	T	T	T
0.7651907848738120	0.6682929636577412	0.4837397999386530	T	T	T
0.9163958001755074	0.6743320454991428	0.8209333561906085	T	T	T
0.6762539633603395	0.8293960070012811	0.8384915568004049	T	T	T
0.3571216876337017	0.0586732271784659	0.7127801181941311	T	T	T
0.3007428478368070	0.0694356021844333	0.8904331381334954	T	T	T
0.1991169192540614	0.0520857899939937	0.0177754717387265	T	T	T
0.0974799509821555	0.0637527901369438	0.8901992193103229	T	T	T
0.1027214572598038	0.0498133203731384	0.6935824182604092	T	T	T
0.2292306682894610	0.0283933830351848	0.7357827603825913	T	T	T
0.3589568285996631	0.8281755184680430	0.7433323585164607	T	T	T
0.3045744756182961	0.8386067328925801	0.9203979568799208	T	T	T
0.1902170554638304	0.8519220728889113	0.0189591297416205	T	T	T
0.0869372353855667	0.8276609840416838	0.9020014325313416	T	T	T
0.1067195447581395	0.8348036412391835	0.7046501551644366	T	T	T
0.2304156720226843	0.8588714369813256	0.7585543281820049	T	T	T
0.3219521870264402	0.9483630294764227	0.8113391535152211	T	T	T
0.0760330002518316	0.9439270816866758	0.8104257995375198	T	T	T
0.4301965920230756	0.1217860064958366	0.5774563109252832	T	T	T
0.4189365289563433	0.9897536303544440	0.5660238426348398	T	T	T
0.3966056888031400	0.8577933970400186	0.5577726082396255	T	T	T
0.1937620426532773	0.1268215474121326	0.6095272919752519	T	T	T
0.1811344090045207	0.9986901425564180	0.5552289614021002	T	T	T
0.1962090272010574	0.8648541234489975	0.5647914525889158	T	T	T
0.9873138422537624	0.0403978135887895	0.7818423721534349	T	T	T
0.9868490747672094	0.8448045031996250	0.7779336546856407	T	T	T
0.1432577519788445	0.9390199273197712	0.2156953562599042	T	T	T
0.1993842658749763	0.9272986896127164	0.3919270766365581	T	T	T
0.2989955851863102	0.9450095005596535	0.5228322885535426	T	T	T
0.3981154565751944	0.9276881205128187	0.3918160387194384	T	T	T
0.3961100284940686	0.9479963500411897	0.1943444903212790	T	T	T

Structure files (CONTCAR) involved in this work:

0.2705212218891133	0.9711192097270449	0.2376283519802576	T	T	T
0.1433331718979977	0.1666465537269134	0.2364038154830316	T	T	T
0.1932162921796764	0.1623674440299080	0.4171594948917273	T	T	T
0.3077399266757538	0.1469934355363688	0.5134529892169915	T	T	T
0.4112671070491316	0.1718481837034702	0.3949726096972034	T	T	T
0.3950104223672158	0.1538229300534204	0.2001278206824815	T	T	T
0.2709959812168604	0.1379580163354297	0.2594744709858688	T	T	T
0.1780832579842284	0.0493853456925935	0.3154212443286315	T	T	T
0.4170263798212867	0.0491507407989455	0.3214011955540690	T	T	T
0.0676747108163608	0.8715494665792212	0.0889249338213376	T	T	T
0.0811795693950479	0.0022462043110045	0.0641534649068527	T	T	T
0.0971400435541779	0.1342760916262268	0.0559807305915722	T	T	T
0.3044535577358027	0.8712862544151894	0.1134214856283043	T	T	T
0.3166552979483145	0.9984796842610096	0.0551834583392182	T	T	T
0.3004312419400588	0.1322123097689067	0.0638319986744714	T	T	T
0.5089862000167170	0.9541460661766266	0.2861031747271499	T	T	T
0.5141659275760804	0.1355137454385256	0.2808539466601636	T	T	T
0.6356781956928839	0.5710542255388084	0.2694897496989955	T	T	T
0.6824107308650473	0.5440101720832702	0.0905143074621325	T	T	T
0.7949493270790313	0.5397401852391785	0.9830633729763686	T	T	T
0.9011486318411837	0.5666227191698060	0.0994206824949601	T	T	T
0.8941184091344963	0.5507481084583919	0.2962098086919513	T	T	T
0.7664634482444144	0.5563124452002053	0.2393370948762252	T	T	T
0.6416686017639476	0.3259500490620312	0.2493865635329195	T	T	T
0.6994630584876569	0.3634057103946029	0.0840091588061559	T	T	T
0.8118928365872806	0.3539140712767285	0.9858584859828469	T	T	T
0.9120598323658071	0.3241941829393011	0.1104878854445459	T	T	T
0.8992332871958990	0.3464237790710122	0.3050729075610668	T	T	T
0.7730493709226464	0.3506251808828314	0.2480998776655448	T	T	T
0.6856091490355571	0.4502317791062398	0.2333765596902083	T	T	T
0.9198978652036323	0.4471927960733562	0.1773563488182532	T	T	T
0.5584737789754717	0.6244909843438883	0.4143147916643466	T	T	T
0.5960217027244823	0.4968547644835403	0.4240431846273780	T	T	T
0.6056767874345006	0.3634546117195796	0.4306913674983034	T	T	T
0.8176007294845824	0.6380574100387821	0.3796454161208032	T	T	T
0.7976047884615343	0.5069142769836452	0.4171274226309786	T	T	T
0.8063607465360163	0.3749191376040555	0.4392867728937545	T	T	T
0.0095048624776844	0.5459505453062855	0.2124769181877924	T	T	T
0.0176052954746496	0.3615059408835933	0.2191827736196912	T	T	T
0.8633666171785067	0.4268224589722350	0.7806105854533287	T	T	T
0.8202742766644785	0.4534066751457791	0.5957472215704301	T	T	T
0.7012242036567935	0.4404927148653379	0.5088877423845475	T	T	T
0.5822155264169360	0.4300972103335085	0.5930355995049468	T	T	T
0.6054915747272528	0.4248922512630423	0.7871861069152926	T	T	T
0.7337905221347256	0.4410122769469417	0.7418308501081247	T	T	T
0.8539501698843431	0.6739793861065104	0.7347057030942655	T	T	T
0.7924262069518064	0.6176404121097155	0.5797833919285309	T	T	T
0.6838940828556299	0.6492535640989044	0.4550061138181667	T	T	T
0.5926002637365998	0.6589983559650212	0.6009464105313854	T	T	T
0.6008083020747624	0.6550213998413116	0.8005416684737721	T	T	T
0.7258008183118543	0.6414407348542788	0.7481834376138941	T	T	T
0.8167274330679217	0.5463496363685727	0.7425669117514114	T	T	T
0.5850142037589511	0.5427089091711794	0.6985214648371758	T	T	T

Structure files (CONTCAR) involved in this work:

0.9359332135749827	0.3794294998373240	0.9315515181938651	T	T	T
0.9156537696629968	0.5097999277426798	0.9215183610992917	T	T	T
0.8868724698164936	0.6367770233881883	0.9354340257199771	T	T	T
0.6964473030876320	0.3600623335530691	0.8889653701936714	T	T	T
0.6821664934508453	0.4942631377647848	0.9071516846123151	T	T	T
0.6936906908009888	0.6259678803202722	0.9421377256485634	T	T	T
0.4853950373763765	0.4536018195945111	0.7221369250446088	T	T	T
0.4858347076595949	0.6308050462812949	0.7123997440237299	T	T	T
0.6381041645586506	0.9354382138698800	0.2729713569346899	T	T	T
0.6794370779752197	0.9668399528613151	0.0892833626363808	T	T	T
0.7975401025884790	0.9497981461877891	0.0036237970547270	T	T	T
0.9150459445318035	0.9384022291774449	0.0902291557800032	T	T	T
0.8929698264041441	0.9309963929962437	0.2865600938325319	T	T	T
0.7669372868986740	0.9401411952927498	0.2310329656444068	T	T	T
0.6368495552100326	0.1722871211746009	0.2380591447273499	T	T	T
0.7022767819173333	0.1325797716348601	0.0768192785045733	T	T	T
0.8146188193125892	0.1487591170052681	0.9740648310582908	T	T	T
0.9192342601103072	0.1621412301257055	0.0918022856117262	T	T	T
0.8973612268143996	0.1656879063731430	0.2882015602838201	T	T	T
0.7699966660243953	0.1638226478491523	0.2381443610580820	T	T	T
0.6950186161073741	0.0534444657112707	0.2378930871534799	T	T	T
0.9149375723434459	0.0487921110300147	0.1990737934700803	T	T	T
0.5674090625224698	0.8741272044049340	0.4164454744166205	T	T	T
0.5864753484415810	0.0051246322765272	0.4257140793252724	T	T	T
0.6079974462413278	0.1364514128411065	0.4252912575869111	T	T	T
0.8025570954231288	0.8600892313048897	0.3820738431654925	T	T	T
0.8061777362497048	0.9941306688034759	0.4022884569147355	T	T	T
0.8057743804693320	0.1264926856888118	0.4231534506839092	T	T	T
0.0128443410188378	0.9565416137543116	0.2190330982533899	T	T	T
0.0167262916000245	0.1336397016781240	0.2170114397860398	T	T	T
0.8617657019443493	0.0772146492525574	0.7615553084399215	T	T	T
0.8189186683691535	0.0486980359203871	0.5807391618321462	T	T	T
0.7026547596008509	0.0533220906923167	0.4877993805837377	T	T	T
0.5922799349314254	0.0727895474847141	0.5945831900010696	T	T	T
0.6065176899293647	0.0665556151702989	0.7901863557972333	T	T	T
0.7323274992677101	0.0599000072845905	0.7289657175174292	T	T	T
0.8602243549475959	0.8312593805774871	0.7417521915864527	T	T	T
0.7999637332082356	0.8727476359806332	0.5765210079399288	T	T	T
0.6885166339578248	0.8445225112101091	0.4781232924428772	T	T	T
0.5872011141058230	0.8334237498195554	0.6054162197715012	T	T	T
0.5951346070510772	0.8466013058624379	0.8041453495079114	T	T	T
0.7298979007912136	0.8544923017862202	0.7449581797325430	T	T	T
0.8169846252706285	0.9556615913205524	0.7272665400469229	T	T	T
0.5839937715545224	0.9543614106858814	0.6849975582584361	T	T	T
0.9375901100405847	0.1372115736271706	0.8969155011048799	T	T	T
0.9010922506116417	0.0153002180700947	0.9300398399372587	T	T	T
0.8986081389392501	0.8840435312670857	0.9156626136610468	T	T	T
0.6980589728315320	0.1392884014306755	0.8815876239453135	T	T	T
0.6967547235618158	0.0053284142310115	0.9011156966888469	T	T	T
0.6984973331236682	0.8738111258030902	0.9520891695841065	T	T	T
0.4883604746007588	0.0460350667172519	0.7130371155923920	T	T	T
0.4815561958029454	0.8707152939351223	0.7101603977683071	T	T	T
0.3548469322434811	0.4380644262278783	0.7156105172520952	T	T	T

Structure files (CONTCAR) involved in this work:

0.3002715893068268	0.4279818541277883	0.8942628733522765	T	T	T
0.2017553835896383	0.4452165049391642	0.0276049527528935	T	T	T
0.1037063614561825	0.4302014128502103	0.8942093421995491	T	T	T
0.1050400877843673	0.4450136537096112	0.6963433630871801	T	T	T
0.2292049973509889	0.4728818771848385	0.7407906645678863	T	T	T
0.3621876783660699	0.6684016938717838	0.7457846377433152	T	T	T
0.3045707899798231	0.6614945333058392	0.9195394331610676	T	T	T
0.1917467258518981	0.6454353765906848	0.0210416340560836	T	T	T
0.0921967607454188	0.6708163970838275	0.8964166600746433	T	T	T
0.1092334507200862	0.6562417407465463	0.7008085957476223	T	T	T
0.2336973046505726	0.6370064963660755	0.7555320158227966	T	T	T
0.3246279013838964	0.5492341159654162	0.8168573939823339	T	T	T
0.0829688175134924	0.5500944679596773	0.8170047219858864	T	T	T
0.4307670463546351	0.3724462458838275	0.5877282990331740	T	T	T
0.4194553245327126	0.5046479870434351	0.5687787600263170	T	T	T
0.3992506146461730	0.6370665128037507	0.5610114927904570	T	T	T
0.2002268441865755	0.3718213233010081	0.6154184646659445	T	T	T
0.1824207336621215	0.4986371665322479	0.5579899173679236	T	T	T
0.1996945721029753	0.6326027316454624	0.5614575219880029	T	T	T
0.9925054356330697	0.4521782682717477	0.7886301421383584	T	T	T
0.9899176722807186	0.6430975458155206	0.7775638600127602	T	T	T
0.1400625625792029	0.5608647384777016	0.2178817022671738	T	T	T
0.1992241882438407	0.5668794318866971	0.3920710372687352	T	T	T
0.3007329251235859	0.5505759670051574	0.5212934977571884	T	T	T
0.4017604168436993	0.5675667381841383	0.3949108451353054	T	T	T
0.3962991112403398	0.5520884760389950	0.1978654573200982	T	T	T
0.2689267784143939	0.5292821730036086	0.2344414960130736	T	T	T
0.1433576343874303	0.3258941377751398	0.2427274607860557	T	T	T
0.1938822501730290	0.3410904609057172	0.4217689006909497	T	T	T
0.3106697746958609	0.3498924541463811	0.5117743771056255	T	T	T
0.4182921201514891	0.3269389118880730	0.4016323025760987	T	T	T
0.3964020731409559	0.3376386096751919	0.2061171689142635	T	T	T
0.2713701639606526	0.3570773575794720	0.2613895497874563	T	T	T
0.1769393251590475	0.4473867040588445	0.3057505161449955	T	T	T
0.4143326355394455	0.4466107142360735	0.3179926138509099	T	T	T
0.0676173824078896	0.6243341260723065	0.0805955007101666	T	T	T
0.0816501124306348	0.4925402959424034	0.0671037016255058	T	T	T
0.1006828554669724	0.3612999965541220	0.0613935562825497	T	T	T
0.3072702596793745	0.6280740663676446	0.1117419106092600	T	T	T
0.3200644832353182	0.4995886619916616	0.0568679529961666	T	T	T
0.3047486914077819	0.3656285882714924	0.0678315244819716	T	T	T
0.5101981014410207	0.5366664997061961	0.2859872727525757	T	T	T
0.5162707639530399	0.3638554137442466	0.2805258965898718	T	T	T
0.4426517227763688	0.7491944189972423	0.6452816604901819	T	T	T
0.2022251948732020	0.7480201078869034	0.6544467379824304	T	T	T
0.2720275243881546	0.7495879820260568	0.0597732878643012	T	T	T
0.1084782247851110	0.7481575007376297	0.0552250555530877	T	T	T
0.0616258259921971	0.2477424520389382	0.1389282641585405	T	T	T
0.3037526137884976	0.2478723381003260	0.1559613553625142	T	T	T
0.2265801286453494	0.2494917416179005	0.5581839275984274	T	T	T
0.3920331991939218	0.2475502569830563	0.5540772833938143	T	T	T
0.5617461442384913	0.2493221672970150	0.3555647728811549	T	T	T
0.8140911980965361	0.2527123938269120	0.3704555450756619	T	T	T

Structure files (CONTCAR) involved in this work:

0.7269455818285445	0.2492388593971800	0.9867088965223447	T	T	T
0.8955275339634835	0.2535650354178224	0.9490257374134567	T	T	T
0.9163576076530303	0.7549651633847655	0.8836506304896792	T	T	T
0.6896108723344511	0.7445523076400916	0.8726191350333098	T	T	T
0.7856108036953893	0.7516309913191448	0.4940933501217150	T	T	T
0.5941972367981231	0.7488204986999365	0.4555758062032462	T	T	T
0.8001526652781282	0.6740767294655496	0.0736299257676592	T	T	T
0.7009789424826204	0.7699520527171165	0.1169002261857240	T	T	T
0.8401560684924226	0.7967485369770548	0.0583177021487806	T	T	T
0.9331517406862120	0.6808259527494359	0.3884032396572673	T	T	T
0.7143404680924204	0.6981956122788431	0.0434728432483530	T	T	T
0.7564245053670108	0.8235945240785468	0.0469486580624665	T	T	T
0.8593469319011853	0.7196501792175611	0.9966193296048936	T	T	T
0.8678529001071394	0.6605231203419318	0.3804684008204241	T	T	T
0.9454751704187898	0.7406864220156391	0.5131593916651536	T	T	T
0.0051215785430551	0.6734407243077014	0.5027238194219582	T	T	T
0.9205563917113790	0.6560898422370492	0.5406673315958166	T	T	T
0.9584904486868728	0.6441132734280492	0.3581610757318841	T	T	T
0.9525893158107325	0.6877632479014761	0.4933963374208288	T	T	T

Figure 2(a) Cu-TS

Si Al O Cu H C

1.0000000000000000

20.0219999999999985 0.0000000000000000 0.0000000000000000

0.0000000000000000 19.8990000000000009 0.0000000000000000

0.0000000000000000 0.0000000000000000 13.3829999999999991

93 3 196 3 5 1

Selective dynamics

Direct

0.4226141214419629	0.0533042214391157	0.6422758727454486	T	T	T
0.3020639201253080	0.0260638639511597	0.7868771107130187	T	T	T
0.2792313971459404	0.0631424860667862	0.0068076682040806	T	T	T
0.1192943423698227	0.0627816490713295	0.0067266540720432	T	T	T
0.0660516265418535	0.0239425848973468	0.7942622379333900	T	T	T
0.1773319721359744	0.0514692866779397	0.6473147171439416	T	T	T
0.4209246713028167	0.8265805791110721	0.6635703149995100	T	T	T
0.3042029560456854	0.8686395108798067	0.8073044329877912	T	T	T
0.2680822612978968	0.8277026692659222	0.0263455977588350	T	T	T
0.1135924808152468	0.8250449018938718	0.0149257269162604	T	T	T
0.0641978849927578	0.8631802410361736	0.7977224036618936	T	T	T
0.1844201989447083	0.8263790083219312	0.6696723561378545	T	T	T
0.0767585882694404	0.9422632403943342	0.1469838609255751	T	T	T
0.1977264929442358	0.9717875787496318	0.2896997433405410	T	T	T
0.2190706486454305	0.9338007663139040	0.5088364076763647	T	T	T
0.3779510279195068	0.9302167751137519	0.5091585450692884	T	T	T
0.4298808652529821	0.9696748481843790	0.2993390492159429	T	T	T
0.3211820807917404	0.9469617517471076	0.1487728482954169	T	T	T
0.0797207273539071	0.1698323868517458	0.1612399025551745	T	T	T
0.1968971470152874	0.1285591536748301	0.3059916439119165	T	T	T
0.2301180660749741	0.1714623664189724	0.5232083267252813	T	T	T
0.3849720528579450	0.1717736191293059	0.5091663954553914	T	T	T
0.4345281935203168	0.1270990234204794	0.2991143198313967	T	T	T
0.3178958420541992	0.1679862037089031	0.1692610072569628	T	T	T
0.5767149225282148	0.5569947451303813	0.3506545844211831	T	T	T

Structure files (CONTCAR) involved in this work:

0.6937248133945819	0.5283257870532080	0.2111088987325685	T	T	T
0.7139310260453845	0.5485832628383515	0.9830742814890294	T	T	T
0.8720016746258570	0.5629307993091284	0.9869573886257907	T	T	T
0.9313505326776829	0.5282773174335841	0.1957972727464355	T	T	T
0.8176446188676180	0.5630634619372937	0.3337599931991627	T	T	T
0.5809968706334551	0.3260754402967473	0.3295791515837790	T	T	T
0.7006071188806502	0.3714168800825431	0.2056096210787709	T	T	T
0.7341661997027674	0.3305567872962556	0.9870175840378469	T	T	T
0.8891081563797717	0.3286524406712000	0.9949311466716092	T	T	T
0.9374130337569478	0.3709071179671672	0.2042066167743145	T	T	T
0.8234019816765752	0.3309368259498087	0.3422285054243629	T	T	T
0.9254841858888979	0.4424247468972524	0.8550133305319010	T	T	T
0.8082957381037253	0.4681071490265843	0.7139110056585063	T	T	T
0.7816628416050995	0.4441226163930760	0.4899006850056040	T	T	T
0.6224610532211761	0.4325310484370749	0.4886006946531585	T	T	T
0.5646855577178627	0.4632052270262313	0.6997833732028069	T	T	T
0.6802418036968801	0.4305146814428949	0.8324838655444363	T	T	T
0.7971736261515153	0.6219149808479778	0.6974172008674259	T	T	T
0.6043777945364430	0.6736584812377786	0.4839564933159602	T	T	T
0.5654026217479169	0.6216108164209339	0.7022857533926514	T	T	T
0.6764799696782895	0.6687672075157899	0.8385408265763004	T	T	T
0.5762198895532030	0.9434551636874405	0.3517245698751383	T	T	T
0.6948172529175498	0.9749139336773049	0.2091637513814230	T	T	T
0.7166991501474048	0.9518654520536713	0.9850918938900196	T	T	T
0.8776036729020879	0.9462625145821632	0.9838026923074029	T	T	T
0.9334727381880448	0.9678256525431647	0.1982973317482463	T	T	T
0.8164216066405919	0.9306700610150224	0.3284702896261908	T	T	T
0.5801761313933501	0.1728524189924390	0.3256598002700980	T	T	T
0.7015022181263483	0.1312188034981922	0.1988655792725548	T	T	T
0.7356489603901025	0.1688926264184965	0.9803997580362132	T	T	T
0.8916157818220349	0.1752398152099014	0.9802592257328183	T	T	T
0.9368731316592632	0.1262190364170618	0.1981644816975259	T	T	T
0.8226180896240323	0.1758283025510744	0.3312281439449604	T	T	T
0.9217956865233445	0.0662544593191988	0.8419380215856682	T	T	T
0.8063490333216781	0.0343832820033944	0.6992908344548771	T	T	T
0.7826745756010832	0.0553744306399777	0.4734970632422449	T	T	T
0.6230064269330894	0.0675266575407791	0.4839042811101628	T	T	T
0.5675492083331040	0.0347648885139255	0.6953466965869578	T	T	T
0.6832961719419023	0.0686475502046187	0.8263943200277142	T	T	T
0.9143297935613031	0.8298461885280666	0.8274181754330211	T	T	T
0.7974353886354055	0.8773438863593961	0.6987628327655804	T	T	T
0.7686397231145111	0.8272508965526941	0.4839332273917971	T	T	T
0.6078957045244466	0.8230689430870498	0.4907808206419338	T	T	T
0.5636737303747713	0.8767644581454539	0.7040090910651792	T	T	T
0.4218501791408186	0.4425345588388390	0.6478605022946359	T	T	T
0.3022639461107428	0.4723269078559114	0.7916844032739099	T	T	T
0.2818114990781664	0.4338099962397681	0.0114869604600726	T	T	T
0.1224901361038975	0.4319847978756967	0.0107572480284359	T	T	T
0.0710969415159008	0.4705037740002925	0.7991066986035760	T	T	T
0.1800783541334192	0.4467637795852213	0.6509042837209723	T	T	T
0.4226839038793252	0.6712489687381522	0.6656594839107677	T	T	T
0.3054693437688301	0.6287275496037563	0.8079465958674149	T	T	T
0.2692615922382651	0.6712665923427849	0.0262728004205152	T	T	T

Structure files (CONTCAR) involved in this work:

0.1155855497202977	0.6719200843007523	0.0105395760401594	T	T	T
0.0674497835912133	0.6299274137951582	0.7965225039382979	T	T	T
0.1862258710100709	0.6685309146287876	0.6672069153046915	T	T	T
0.0762832671251292	0.5552341697865795	0.1424887404054969	T	T	T
0.1966049020879884	0.5260553170964419	0.2858963470526291	T	T	T
0.2212524985463435	0.5623016391961461	0.5071347167945148	T	T	T
0.3809229592562412	0.5650614768642053	0.5102453865059876	T	T	T
0.4320102732216401	0.5260105902089343	0.2990916538883379	T	T	T
0.3229082153142895	0.5523119072208644	0.1489324561408286	T	T	T
0.0805062186841478	0.3246607049010714	0.1649836619004433	T	T	T
0.1970435845163688	0.3683824125098432	0.3062558078281859	T	T	T
0.2327037318935627	0.3279980233066109	0.5250270820284986	T	T	T
0.3877411253091937	0.3244585996920709	0.5132313904825314	T	T	T
0.4367008394576813	0.3692143882172567	0.3011213049503866	T	T	T
0.3193577262801823	0.3269058042131176	0.1720235913281115	T	T	T
0.7648956392152894	0.6672504414284807	0.4783921923442205	T	T	T
0.9151497426859656	0.6735173311854242	0.8191180029955859	T	T	T
0.6745773771569818	0.8292917172913601	0.8421953508026720	T	T	T
0.3567856173276471	0.0587301294235124	0.7124126415768499	T	T	T
0.3000273152544047	0.0692765965565239	0.8899477910280503	T	T	T
0.1991324850196837	0.0517040566122439	0.0186944165578357	T	T	T
0.0979395918355586	0.0624644829799033	0.8901143915116346	T	T	T
0.1023167840593896	0.0501731873888799	0.6932491134442696	T	T	T
0.2288659209389238	0.0286139501723827	0.7347751240718390	T	T	T
0.3594066590155729	0.8285254711562945	0.7427828357778147	T	T	T
0.3048362172689026	0.8384955713960199	0.9196530359994849	T	T	T
0.1904066538966521	0.8517817538922516	0.0176265318876494	T	T	T
0.0867863440615053	0.8276856079675484	0.9010253049039799	T	T	T
0.1065531993686407	0.8338016174583764	0.7035512398455481	T	T	T
0.2304227472943511	0.8581459051570836	0.7579830374366089	T	T	T
0.3212706161853572	0.9483663154438969	0.8105210365651689	T	T	T
0.0756563055729585	0.9434241129453325	0.8080508266868591	T	T	T
0.4298164039779032	0.1216977465203911	0.5767679992484313	T	T	T
0.4188455727887432	0.9895248222097938	0.5661593674940896	T	T	T
0.3961124727380924	0.8575067286169855	0.5569424030757376	T	T	T
0.1932200825629674	0.1269699642259396	0.6083686345524133	T	T	T
0.1804120541760769	0.9986570640295060	0.5547012399777739	T	T	T
0.1959874699829038	0.8649116734013295	0.5641885462260030	T	T	T
0.9871703755770043	0.0402767797328305	0.7824413132603057	T	T	T
0.9867134991014018	0.8437222096789431	0.7764248214016052	T	T	T
0.1430580980590183	0.9384953829763656	0.2157130681148588	T	T	T
0.1996705979310275	0.9273355606921422	0.3914679127704200	T	T	T
0.2987040160437944	0.9453726697115270	0.5234361615735142	T	T	T
0.3972866283910700	0.9277690190096644	0.3916292405690491	T	T	T
0.3961262840403668	0.9477147178548049	0.1940829837491785	T	T	T
0.2703986758145752	0.9708651986967777	0.2366041872753877	T	T	T
0.1435377911727570	0.1663556538218021	0.2350217754038271	T	T	T
0.1931141629543170	0.1622967965226782	0.4159858142997134	T	T	T
0.3074054573626785	0.1469175428004796	0.5129589946088882	T	T	T
0.4109282911039014	0.1717557111852474	0.3943553240775113	T	T	T
0.3954850567359148	0.1535560996421993	0.1995559847080129	T	T	T
0.2712626424158087	0.1377629365411508	0.2587385381888663	T	T	T
0.1781510212432265	0.0492556784008603	0.3144833116122843	T	T	T

Structure files (CONTCAR) involved in this work:

0.4166620945995343	0.0489878865327846	0.3210409920920551	T	T	T
0.0679669105402893	0.8712734942866075	0.0879396863453361	T	T	T
0.0808969862945710	0.0023456654247643	0.0648338237861310	T	T	T
0.0970821998998955	0.1343656427525404	0.0547338676955856	T	T	T
0.3045136214608797	0.8711145453175548	0.1126905680119964	T	T	T
0.3170020832999407	0.9982909324616341	0.0544686713789182	T	T	T
0.3007620528002300	0.1320071668316933	0.0633046373069741	T	T	T
0.5086476603030236	0.9536594321250775	0.2870570753557666	T	T	T
0.5144958380752990	0.1346143891841306	0.2819988478443375	T	T	T
0.6384880811354052	0.5704322429368254	0.2737126817371732	T	T	T
0.6812116980951430	0.5423274723352186	0.0926920939357544	T	T	T
0.7942144321857774	0.5398854749259123	0.9845696388112953	T	T	T
0.9017930658730878	0.5678217515657378	0.0989834232110912	T	T	T
0.8949917158651409	0.5522212382764911	0.2973552444078316	T	T	T
0.7693319810240207	0.5514621241214989	0.2361660458040930	T	T	T
0.6416413934985072	0.3243759943199767	0.2492736004972351	T	T	T
0.7002267194658173	0.3634570274740981	0.0853688479130661	T	T	T
0.8120685726166124	0.3537070704911015	0.9854786924764007	T	T	T
0.9119180313337987	0.3251727074118291	0.1111458237295858	T	T	T
0.8994502609118993	0.3475107720038251	0.3056351025672910	T	T	T
0.7729022527615790	0.3492106002945368	0.2500806378608971	T	T	T
0.6842341231211297	0.4487772637688107	0.2358121546186003	T	T	T
0.9200994670651932	0.4485045864313789	0.1772763984778485	T	T	T
0.5584813534464643	0.6229990814508316	0.4161711155827443	T	T	T
0.5949355332768324	0.4957049587537299	0.4252606341458748	T	T	T
0.6062279613686780	0.3626381877611429	0.4309321674142799	T	T	T
0.8111471020426727	0.6371533632850441	0.3775846828326383	T	T	T
0.7995304988892957	0.5047435831913479	0.4146595456232844	T	T	T
0.8063147419914127	0.3732034663985331	0.4419464334893502	T	T	T
0.0100650440447857	0.5459314852716665	0.2110414501622853	T	T	T
0.0175343118579343	0.3618790028357967	0.2189385747764735	T	T	T
0.8631726981062224	0.4272781541838260	0.7806809033775979	T	T	T
0.8200899238618359	0.4533752836552001	0.5960585307751430	T	T	T
0.7016978297726544	0.4406737866579008	0.5082939433465175	T	T	T
0.5831326986152943	0.4287498929929288	0.5938712943133393	T	T	T
0.6052918735516962	0.4251289750081529	0.7882247951157338	T	T	T
0.7335959508891177	0.4420973361975508	0.7429805546769672	T	T	T
0.8555759118701655	0.6737389256399782	0.7278164617820188	T	T	T
0.7851726865950498	0.6179720075727330	0.5803842589417177	T	T	T
0.6808800462766921	0.6644833649720667	0.4559913237340101	T	T	T
0.5909099485308780	0.6593082449984367	0.6028025706210507	T	T	T
0.6006994403840780	0.6534304040010268	0.8021361969350191	T	T	T
0.7276760637506073	0.6430890406801463	0.7551369182396462	T	T	T
0.8170061172107727	0.5470433279846597	0.7416580221449272	T	T	T
0.5844375733963817	0.5423129642233928	0.6976925668433468	T	T	T
0.9360220638330072	0.3795923799563121	0.9313955332508610	T	T	T
0.9149743508060665	0.5100246227827929	0.9216799393762765	T	T	T
0.8848271140688858	0.6365574777087085	0.9332217833192111	T	T	T
0.6963734341778494	0.3607537293865848	0.8900458979106645	T	T	T
0.6814710971539779	0.4949464320122815	0.9080636764504486	T	T	T
0.6921904225858060	0.6260552057799421	0.9466142368963446	T	T	T
0.4853856909538189	0.4532578271650086	0.7214853509645754	T	T	T
0.4850243399522083	0.6305526747182241	0.7147178843329314	T	T	T

Structure files (CONTCAR) involved in this work:

0.6379980186467079	0.9368609223427108	0.2735561875301010	T	T	T
0.6799749245429996	0.9686248804756482	0.0902301198808526	T	T	T
0.7973783552312413	0.9498451351542075	0.0030372620665670	T	T	T
0.9145001797179497	0.9364481531439297	0.0899949355597145	T	T	T
0.8927520839820383	0.9299687092921415	0.2867982770349539	T	T	T
0.7665949672007215	0.9395601364575322	0.2323998411708648	T	T	T
0.6368352319463964	0.1721355459225274	0.2385372581499982	T	T	T
0.7027675297449566	0.1328339185283400	0.0778020941576664	T	T	T
0.8144412793448216	0.1493140436827912	0.9737171296817650	T	T	T
0.9186165106084541	0.1614432350069769	0.0923807169944965	T	T	T
0.8980098809312856	0.1636417828177130	0.2891249729623362	T	T	T
0.7703947872060685	0.1649053782041218	0.2390245470397641	T	T	T
0.6966717454922005	0.0541513327176610	0.2396443165264825	T	T	T
0.9151438445022450	0.0474870648396871	0.1980924647747120	T	T	T
0.5696836325916339	0.8766652678252626	0.4193284359395903	T	T	T
0.5854704473459952	0.0073456604937039	0.4252473484933388	T	T	T
0.6089076309732970	0.1377909762979672	0.4262622533575285	T	T	T
0.8028916518302025	0.8596882554696295	0.3838736117303252	T	T	T
0.8064000798700096	0.9933624417821053	0.4039110486886445	T	T	T
0.8057120175194338	0.1258900719433731	0.4232803458409378	T	T	T
0.0124897764991424	0.9548477676552605	0.2187093880605108	T	T	T
0.0170335844131262	0.1325350748143890	0.2157983190408318	T	T	T
0.8615235620240784	0.0763968311982295	0.7627568635513124	T	T	T
0.8186352062896369	0.0486091505875458	0.5816032272313915	T	T	T
0.7024694050607405	0.0526774631956164	0.4881230064507079	T	T	T
0.5924869254891378	0.0738231123179848	0.5953216238039432	T	T	T
0.6060410160150863	0.0673657090620993	0.7910406222653327	T	T	T
0.7318808515828682	0.0606169171760483	0.7296337788932694	T	T	T
0.8608446068220175	0.8317979330627312	0.7370938020895250	T	T	T
0.7940045590061706	0.8729905341897107	0.5774295623339725	T	T	T
0.6881234281886164	0.8299526011551579	0.4731458587361596	T	T	T
0.5914941980757544	0.8354000703607800	0.6075696940660813	T	T	T
0.5941707315174211	0.8482182381548286	0.8061900450574421	T	T	T
0.7301172545299979	0.8528450871235723	0.7501716884910713	T	T	T
0.8152666010901458	0.9554749769495586	0.7274879157532562	T	T	T
0.5840686137333659	0.9554693217584632	0.6857691441209646	T	T	T
0.9374021009099833	0.1370784586297657	0.8975036586809910	T	T	T
0.9017448951464665	0.0149076654716015	0.9313600897933737	T	T	T
0.8977706562431602	0.8840508844049670	0.9129499244535079	T	T	T
0.6975820048896992	0.1395561364880546	0.8826872593980831	T	T	T
0.6964074828855563	0.0053671357865321	0.9011766925193246	T	T	T
0.6970451338550409	0.8743294830337657	0.9549203367836138	T	T	T
0.4880457696498338	0.0465854532018695	0.7128285539224936	T	T	T
0.4821376710640337	0.8707195521657062	0.7073383974367344	T	T	T
0.3547498684729784	0.4382879687259179	0.7151255278926086	T	T	T
0.2999998257288579	0.4280275692483894	0.8936195817848486	T	T	T
0.2018845440386360	0.4440093787487386	0.0278014500469254	T	T	T
0.1045680123275435	0.4305508891872852	0.8928454240261455	T	T	T
0.1046924227527184	0.4454921340092485	0.6951094897067204	T	T	T
0.2289635337814562	0.4726996766673840	0.7399601591716009	T	T	T
0.3608707429043375	0.6685086734014702	0.7436478399492618	T	T	T
0.3043066226270350	0.6619960721935656	0.9181031069017157	T	T	T
0.1921596994271575	0.6452041005039120	0.0204973221023565	T	T	T

Structure files (CONTCAR) involved in this work:

0.0937707881122127	0.6712597404195273	0.8941792670640327	T	T	T
0.1082598899890873	0.6567730178832947	0.6977566906840206	T	T	T
0.2325970577723726	0.6367243833502771	0.7549953051297041	T	T	T
0.3239817984778602	0.5493566410856823	0.8161909374351453	T	T	T
0.0829019173567384	0.5505724167540671	0.8151808805611598	T	T	T
0.4304832331941950	0.3721932961968421	0.5875817101685391	T	T	T
0.4192413353930593	0.5043080969650764	0.5679503875834970	T	T	T
0.4001799130946469	0.6367807993891955	0.5604602677394601	T	T	T
0.1996271716122204	0.3717480188759173	0.6142913430623553	T	T	T
0.1828729759652775	0.4986127973809468	0.5569855052523677	T	T	T
0.1993775905706916	0.6324465085379157	0.5600651121800919	T	T	T
0.9924177974731266	0.4526834721657613	0.7891401956768378	T	T	T
0.9901010547133743	0.6445485371988589	0.7768524667693470	T	T	T
0.1405735277163589	0.5613396488626551	0.2156742672299544	T	T	T
0.1987962098415603	0.5669624490626670	0.3908694356247310	T	T	T
0.3010680795747709	0.5512756644800813	0.5193611875353511	T	T	T
0.4027597930629825	0.5677177195285037	0.3939419179419281	T	T	T
0.3970726495291643	0.5520493812370073	0.1968633899602308	T	T	T
0.2695190901704602	0.5300778385553543	0.2341700275910598	T	T	T
0.1434155353339079	0.3261332643473642	0.2410901057933704	T	T	T
0.1938739262486698	0.3415470496044722	0.4203737366245405	T	T	T
0.3104189896111053	0.3500615129358344	0.5113085798485467	T	T	T
0.4180463018279250	0.3272833632743410	0.4011747358292809	T	T	T
0.3967691429281861	0.3377506954756399	0.2058611416968315	T	T	T
0.2714634714229131	0.3570634063444527	0.2600976027411855	T	T	T
0.1772666548488663	0.4476763326829505	0.3038134099460987	T	T	T
0.4150385758951752	0.4470037146884172	0.3172424180231063	T	T	T
0.0677129799081957	0.6240570559438212	0.0780214323320147	T	T	T
0.0821901076610639	0.4926155642117823	0.0653709759948385	T	T	T
0.0998100934049031	0.3610318645803695	0.0600011241277938	T	T	T
0.3081647489119698	0.6279768012141679	0.1102446698274590	T	T	T
0.3200204482642557	0.4992822842467227	0.0565461548947007	T	T	T
0.3056097465889309	0.3652470755350369	0.0667490281981403	T	T	T
0.5114940046898082	0.5370484580715781	0.2848330608418027	T	T	T
0.5166330736555675	0.3640993587294829	0.2807634856094836	T	T	T
0.4427339712667068	0.7489344899575412	0.6452268247504079	T	T	T
0.2021694399342703	0.7477621147207200	0.6527547521179221	T	T	T
0.2721629028678876	0.7494793341579922	0.0591933308686154	T	T	T
0.1087248885779119	0.7479173602466126	0.0538802396918576	T	T	T
0.0612273820627323	0.2476145652791331	0.1389706290135065	T	T	T
0.3043244934781880	0.2477156074166186	0.1554985682763519	T	T	T
0.2262029916387857	0.2496365319100842	0.5567661370986676	T	T	T
0.3916168775751298	0.2475372997166960	0.5533099376498468	T	T	T
0.5606180954263722	0.2492506924102935	0.3552155300278492	T	T	T
0.8166245864459299	0.2522034667776258	0.3718091870350287	T	T	T
0.7265210540206869	0.2496045146434710	0.9871201640125304	T	T	T
0.8963984408300414	0.2537151554467217	0.9502460075679772	T	T	T
0.9144801404560858	0.7546617250923331	0.8808616236421118	T	T	T
0.6863883306780261	0.7446502939233084	0.8772516488451593	T	T	T
0.7957846095764071	0.7507221360347218	0.4962348959142965	T	T	T
0.5795149409518860	0.7498727731963829	0.4593552373856978	T	T	T
0.8001069425489746	0.6744202784268689	0.0739613669850444	T	T	T
0.7011191249679171	0.7696422480295088	0.1209687106102113	T	T	T

Structure files (CONTCAR) involved in this work:

0.8396559418527503	0.7971193671347996	0.0559081692048736	T	T	T
0.9948806072393273	0.7174079522734774	0.4681871766646084	T	T	T
0.7136802673376131	0.6977602637015978	0.0478541546122620	T	T	T
0.7552878276662026	0.8234273031531975	0.0488661943566856	T	T	T
0.8581162151433507	0.7196932099639295	0.9948619785937451	T	T	T
0.9973076358569395	0.6804686572919346	0.4198735797160351	T	T	T
0.9057723700916932	0.7832306540896233	0.4425509461889162	T	T	T
0.9032075455300815	0.7381479657913330	0.5660774759420663	T	T	T
0.8870791379871098	0.6913384681938262	0.4457708219877717	T	T	T
0.0145089967824859	0.7004920640691893	0.5304907969744376	T	T	T
0.902791843332150	0.7366576350282198	0.4847779886387900	T	T	T

Figure 2(a) Cu-FS

Si Al O Cu H C

1.0000000000000000

20.0219993591000005 0.0000000000000000 0.0000000000000000

0.0000000000000000 19.8990001678000006 0.0000000000000000

0.0000000000000000 0.0000000000000000 13.3830003737999998

93 3 196 3 5 1

Selective dynamics

Direct

0.4216897864324184	0.0534280772471200	0.6417257689534627	T	T	T
0.3015028314220362	0.0259161491555747	0.7865072333772530	T	T	T
0.2790791045464139	0.0627287321451911	0.0068746245484123	T	T	T
0.1191696371825006	0.0625080367757418	0.0066131882845609	T	T	T
0.0658500780112039	0.0240340127606700	0.7943136737138349	T	T	T
0.1769279234708413	0.0512482396439195	0.6470129283425817	T	T	T
0.4210208143470217	0.8263212401879311	0.6637735548578143	T	T	T
0.3040543426999966	0.8684262180897646	0.8068566087779281	T	T	T
0.2682425127333518	0.8274670224827051	0.0258106519971954	T	T	T
0.1139646087909564	0.8246799132894513	0.0146898997502246	T	T	T
0.0638045992241808	0.8633327345276429	0.7984452338000850	T	T	T
0.1836810474081627	0.8260178134621107	0.6698351117279741	T	T	T
0.0767356983436937	0.9417817897562277	0.1465327163599908	T	T	T
0.1976389059938206	0.9712628010931130	0.2897661775016771	T	T	T
0.2187097956981397	0.9333180835247310	0.5089067490125467	T	T	T
0.3776103962167411	0.9297233337571743	0.5094096675061676	T	T	T
0.4298514013821083	0.9686332205932124	0.2995393058552417	T	T	T
0.3211465383900386	0.9464048392091403	0.1487900353560746	T	T	T
0.0793088198129466	0.1694485038097555	0.1610136026634751	T	T	T
0.1966640151876068	0.1282504146704795	0.3058753555141741	T	T	T
0.2293912380295061	0.1714472659795791	0.5229829160902255	T	T	T
0.3842904902271583	0.1717818372279426	0.5081689266007493	T	T	T
0.4343476609161144	0.1261467642638494	0.2988909261527549	T	T	T
0.3179620481027527	0.1675535674873003	0.1690582285818769	T	T	T
0.5774776465990751	0.5567126961824700	0.3511518463489691	T	T	T
0.6928935062393762	0.5266999567312680	0.2099673794935267	T	T	T
0.7132184250882486	0.5486567169908466	0.9830506347823602	T	T	T
0.8711892109234571	0.5636186503848404	0.9870084088871387	T	T	T
0.9316764905766022	0.5280089924321490	0.1938302361807758	T	T	T
0.8170421854812898	0.5607964449833234	0.3304816865310147	T	T	T
0.5804887880567601	0.3254856319664776	0.3302233099116940	T	T	T
0.6991141629843290	0.3704950170305991	0.2049962804567969	T	T	T
0.7340240884093174	0.3308995302766561	0.9868530433050826	T	T	T

Structure files (CONTCAR) involved in this work:

0.8885639360260118	0.3289472613274580	0.9948355491924270	T	T	T
0.9384527599570858	0.3714041798923221	0.2019967896850047	T	T	T
0.8235022670019543	0.3324176550845176	0.3397065983041051	T	T	T
0.9248052612625461	0.4432016163891248	0.8548064901025909	T	T	T
0.8075650219911089	0.4690280507390232	0.7127056377453229	T	T	T
0.7811189495389447	0.4438265923618335	0.4894245796872085	T	T	T
0.6219853640188170	0.4318399566044282	0.4890431953081902	T	T	T
0.5642715835015809	0.4624241735754482	0.7002397238574861	T	T	T
0.6800112013431091	0.4309538563048437	0.8318630510093082	T	T	T
0.7964346604096385	0.6239800850705630	0.6966805942885389	T	T	T
0.6041450989432441	0.6747470699316755	0.4855636732387078	T	T	T
0.5660546521235289	0.6207462079919654	0.7029867900491232	T	T	T
0.6759429884004493	0.6693849820420656	0.8396318864603297	T	T	T
0.5765792894558928	0.9436881681683942	0.3513234624203951	T	T	T
0.6935999913633252	0.9774782315469985	0.2071780370460824	T	T	T
0.7162631923109561	0.9535715765781657	0.9842267134929005	T	T	T
0.8765266244385874	0.9467905308533245	0.9833912635715975	T	T	T
0.9332714373393201	0.9669651609599083	0.1962694416562611	T	T	T
0.8155181423852890	0.9350065951190280	0.3253336010810987	T	T	T
0.5795840285907649	0.1732494904177962	0.3254446397401651	T	T	T
0.6998514078160744	0.1333295574642833	0.1974986260057262	T	T	T
0.7353051687840548	0.1691981775150068	0.9793060750469090	T	T	T
0.8906857740281697	0.1755231721432735	0.9800094790350856	T	T	T
0.9362393740508672	0.1255130897668972	0.1967687711970845	T	T	T
0.8215080028658274	0.1765991669730496	0.3294167767554602	T	T	T
0.9219165884177721	0.0663451969982332	0.8422332821819218	T	T	T
0.8057546525367577	0.0351515156085232	0.6980826612264647	T	T	T
0.7817031880558316	0.0576539047537496	0.4733280675142290	T	T	T
0.6224901856829779	0.0678598338153082	0.4832621472219857	T	T	T
0.5665710917330834	0.0361323575292064	0.6947602998621687	T	T	T
0.6825354105614824	0.0694293641179936	0.8249026998501670	T	T	T
0.9130496678508919	0.8302614069908506	0.8265965679714846	T	T	T
0.7968419930758897	0.8770464639524971	0.6978093194674218	T	T	T
0.7665601993143212	0.8302007994848473	0.4791978887945940	T	T	T
0.6063795481260212	0.8219449415304666	0.4925340353926951	T	T	T
0.5636042870589055	0.8781448417644039	0.7050120250113873	T	T	T
0.4214399181840412	0.4424596044245193	0.6473313966843025	T	T	T
0.3021689382743007	0.4720260120220065	0.7915613087291714	T	T	T
0.2817478546343844	0.4337408698824794	0.0113665620938930	T	T	T
0.1224168270230526	0.4317359510186320	0.0103316860951465	T	T	T
0.0706973396662736	0.4705412252732475	0.7996606001599234	T	T	T
0.1797357149453641	0.4468945481947933	0.6511791901591065	T	T	T
0.4230056959416009	0.6710419337487126	0.6653110852201397	T	T	T
0.3057870970862875	0.6283992413018252	0.8075404757545980	T	T	T
0.2696875556869150	0.6709166314312281	0.0258880036410260	T	T	T
0.1162909111427808	0.6718272089095317	0.0105865403292034	T	T	T
0.0674962976991495	0.6294047497809385	0.7977633219736368	T	T	T
0.1857332986006970	0.6680060306782336	0.6672992488701296	T	T	T
0.0765583058297630	0.5550775673632622	0.1419391037932844	T	T	T
0.1968220533650053	0.5258658352685024	0.2857416756244030	T	T	T
0.2212461886405717	0.5623155247416423	0.5069079461020680	T	T	T
0.3809923063939046	0.5652112199777117	0.5097774900196085	T	T	T
0.4327875503088724	0.5266660981404401	0.2987098943341157	T	T	T

Structure files (CONTCAR) involved in this work:

0.3232310711095899	0.5522748308927007	0.1489534839164710	T	T	T
0.0810873136895907	0.3242687653924909	0.1649594748955622	T	T	T
0.1973471880969379	0.3680298324397879	0.3062522451807657	T	T	T
0.2320520255324802	0.3280194193171757	0.5254068732636145	T	T	T
0.3872354184464392	0.3246340575286547	0.5124018093215750	T	T	T
0.4368314357732899	0.3696497187795327	0.3004763590738406	T	T	T
0.3195496522204990	0.3268143570605399	0.1719135755838215	T	T	T
0.7647910929067844	0.6655531844175093	0.4720992547975030	T	T	T
0.9148889000564409	0.6739170631509298	0.8185187690868835	T	T	T
0.6743569518417826	0.8299704850318502	0.8428139800517805	T	T	T
0.3558607353684615	0.0590148818876073	0.7117295071093038	T	T	T
0.2998800115219895	0.0687242163165341	0.8899797255195608	T	T	T
0.1989987931942847	0.0513019334141823	0.0188163227142695	T	T	T
0.0979427422472653	0.0626717591725179	0.8899203203178571	T	T	T
0.1019306632923579	0.0496355950605762	0.6928264403278984	T	T	T
0.2281988003623589	0.0286455137553497	0.7349784188315694	T	T	T
0.3596615084072424	0.8282905159418235	0.7429823421872429	T	T	T
0.3052038527638583	0.8386833785532455	0.9194017858312824	T	T	T
0.1907016744294702	0.8517946739599190	0.0169157101033485	T	T	T
0.0868201911229797	0.8271484064365826	0.9009829996922339	T	T	T
0.1060741550009191	0.8346868188009978	0.7039840425095985	T	T	T
0.2303891891668084	0.8575894303529435	0.7577234974314724	T	T	T
0.3210745016106299	0.9482150921510089	0.8092946910234369	T	T	T
0.0749154655028039	0.9436335694587957	0.8094797012555078	T	T	T
0.4290472137026879	0.1215143809975435	0.5756389644059613	T	T	T
0.4184206512861846	0.9891717592903259	0.5663890316174025	T	T	T
0.3962051708569646	0.8570884669015552	0.5570892563377686	T	T	T
0.1926699271226059	0.1268028086257078	0.6081599791922750	T	T	T
0.1803879098205821	0.9984884745554384	0.5544313339927900	T	T	T
0.1956353274339181	0.8646205255561299	0.5644077689788454	T	T	T
0.9871628061503582	0.0412678632588644	0.7817382449902499	T	T	T
0.9859728320495007	0.8447627984372256	0.7784887649436055	T	T	T
0.1428197370001227	0.9383302936522526	0.2157427562587954	T	T	T
0.1994845925554610	0.9268226517825263	0.3914907990955268	T	T	T
0.2984294959497420	0.9448297453065789	0.5234380024932550	T	T	T
0.3972793421681302	0.9269788846921484	0.3919879536669229	T	T	T
0.3961157116141418	0.9470153274303383	0.1942236464874851	T	T	T
0.2703644785364538	0.9700774490524774	0.2367213026873111	T	T	T
0.1429718467501975	0.1655644055382678	0.2349886890390438	T	T	T
0.1924778570136284	0.1621569536676030	0.4157249861545999	T	T	T
0.3067441542991153	0.1470642686498448	0.5124933919287503	T	T	T
0.4101449863117694	0.1712351894635305	0.3932769225059019	T	T	T
0.3954618367781285	0.1519595924771887	0.1989131755533831	T	T	T
0.2710222002202742	0.1379030137761920	0.2586387878456393	T	T	T
0.1784826254920814	0.0488383972643555	0.3145500599978879	T	T	T
0.4171938304009229	0.0479669390297757	0.3214525577262854	T	T	T
0.0682091549164591	0.8710202218813246	0.0872078170918440	T	T	T
0.0807618592276245	0.0021024604515064	0.0646621178402193	T	T	T
0.0968137741611458	0.1340695797054169	0.0545443085859554	T	T	T
0.3047157054680891	0.8706195311296125	0.1124425507893963	T	T	T
0.3170347913005508	0.9980498685022002	0.0548467643114615	T	T	T
0.3004308795454366	0.1317755393824958	0.0631059997097548	T	T	T
0.5085947721874455	0.9518115354022647	0.2872491587958179	T	T	T

Structure files (CONTCAR) involved in this work:

0.5144341987335891	0.1337999125835715	0.2825886160588822	T	T	T
0.6402143397395649	0.5701343340839315	0.2757746266020090	T	T	T
0.6794203982539536	0.5421007920562428	0.0921338440875590	T	T	T
0.7934752144186644	0.5398332315895249	0.9856183497926329	T	T	T
0.9015948599454346	0.5691888292745084	0.0986838216034241	T	T	T
0.8942418482194990	0.5489420021527258	0.2958386663632797	T	T	T
0.7697001413992552	0.5465876778433584	0.2324942216655452	T	T	T
0.6416821695100907	0.3224885002024460	0.2508058463975664	T	T	T
0.6980225076705481	0.3621142346781507	0.0847932942783838	T	T	T
0.8116354704001828	0.3549304745908911	0.9885197563524263	T	T	T
0.9130862076309282	0.3243778394501989	0.1102479385662299	T	T	T
0.8991646767384563	0.3506242515573284	0.3035288197319756	T	T	T
0.7723739182612919	0.3505364782227166	0.2482746268293201	T	T	T
0.6806484934325154	0.4475498357652966	0.2343201292277556	T	T	T
0.9224469053871744	0.4485358378186000	0.1707819432839919	T	T	T
0.5605581868400342	0.6225864477990807	0.4176186234848515	T	T	T
0.5941634950031133	0.4949128226530629	0.4255349979291969	T	T	T
0.6058993393827641	0.3619352420298765	0.4315143344861880	T	T	T
0.8075719226432575	0.6356154685615578	0.3700534509462033	T	T	T
0.7979825301953196	0.5051786326824770	0.4149943025730301	T	T	T
0.8058382060502772	0.3733532498078678	0.4404495927123451	T	T	T
0.0099108883876136	0.5471010161958091	0.2100833921269808	T	T	T
0.0182124205633734	0.3615661627047608	0.2191486183042030	T	T	T
0.8622022881816109	0.4288717539604583	0.7806032750558805	T	T	T
0.8197080736777848	0.4531028336353908	0.5953042091992061	T	T	T
0.7012091846039612	0.4402033543441011	0.5085156863393177	T	T	T
0.5828070995484238	0.4280497811604101	0.5943370080124589	T	T	T
0.6048591969890462	0.4242968459675058	0.7886671747478066	T	T	T
0.7327708638477557	0.4432597847152777	0.7418357104457132	T	T	T
0.8548096628975115	0.6751223021415095	0.7280134975103734	T	T	T
0.7840211140794564	0.6228716029547650	0.5793163833435234	T	T	T
0.6809193601327393	0.6725703491137992	0.4550286014218931	T	T	T
0.5938193628188921	0.6579391162526255	0.6041615451973116	T	T	T
0.6003219568378404	0.6526648319334615	0.8035550881730104	T	T	T
0.7271219570711559	0.6445892312149519	0.7554732227219446	T	T	T
0.8157192703041170	0.5483539082722863	0.7378393193263389	T	T	T
0.5846955281254387	0.5414093851230541	0.6986411728708819	T	T	T
0.9348986153123725	0.3798117093959846	0.9303715805923110	T	T	T
0.9141181552529068	0.5106021768908288	0.9218818365692707	T	T	T
0.8829271229207525	0.6371847673950023	0.9324631581648813	T	T	T
0.6973774312919309	0.3615138961999486	0.8893217471833371	T	T	T
0.6808322763260370	0.4955151384550913	0.9072083920370340	T	T	T
0.6920860705900468	0.6264429698551166	0.9473595306596740	T	T	T
0.4849218175008336	0.4528586658775329	0.7213604946534377	T	T	T
0.4857164382318973	0.6301437870847622	0.7129997238724215	T	T	T
0.6386712197376159	0.9377771272080450	0.2733578070735795	T	T	T
0.6782902190754829	0.9703924073603010	0.0885722177454339	T	T	T
0.7966419458661614	0.9546174061500140	0.0022983311792031	T	T	T
0.9133876204885266	0.9342390189991926	0.0891682145346167	T	T	T
0.8920280112429138	0.9308721261054748	0.2862522686510461	T	T	T
0.7668793658712481	0.9447900280760231	0.2285652316385701	T	T	T
0.6355336282190787	0.1746807811370141	0.2372854413631769	T	T	T
0.7010051270281494	0.1342172848373544	0.0764760278785968	T	T	T

Structure files (CONTCAR) involved in this work:

0.8138221403132498	0.1484219429717501	0.9742344377688984	T	T	T
0.9180308687391945	0.1624166066164141	0.0921803974930079	T	T	T
0.8965286970581938	0.1607824585606787	0.2888711783089391	T	T	T
0.7692073922263694	0.1663268113644003	0.2371632256734226	T	T	T
0.6936955507410766	0.0564306987358581	0.2387791800325074	T	T	T
0.9150903593217251	0.0466799617898569	0.1934285069836888	T	T	T
0.5723304506518787	0.8769558499061958	0.4196172737191348	T	T	T
0.5845408343158464	0.0080165891785925	0.4242673392254480	T	T	T
0.6102584026836219	0.1381126194971080	0.4248235960378212	T	T	T
0.7963010422140361	0.8646576507351335	0.3794818108319568	T	T	T
0.8071973407164063	0.9968115652807572	0.4025043970501981	T	T	T
0.8018656935952017	0.1288998197806847	0.4230973577254538	T	T	T
0.0120531581316779	0.9541947864101853	0.2175236143360175	T	T	T
0.0162568176062938	0.1324004785174620	0.2151731852662956	T	T	T
0.8608407191432779	0.0753253871534671	0.7639248459862841	T	T	T
0.818488898964908	0.0512326398031520	0.5808716445766310	T	T	T
0.7017116421910504	0.0513560909111595	0.4889033832580632	T	T	T
0.5911318517485850	0.0746749268196693	0.5940307899980755	T	T	T
0.6053112190010278	0.0694843022837916	0.7894885220244450	T	T	T
0.7312486317443492	0.0611528871114802	0.7283209120593473	T	T	T
0.8608724858896908	0.8322024332338275	0.7341450476238133	T	T	T
0.7924038172733557	0.8705407277463343	0.5759637412762857	T	T	T
0.6873619169948703	0.8215855788090821	0.4740576372204732	T	T	T
0.5930987694118601	0.8371479341413519	0.6090738197822634	T	T	T
0.5941230276334701	0.8501333867375387	0.8074386479982393	T	T	T
0.7299266849901459	0.8524239822421098	0.7499724514561177	T	T	T
0.8138533036941632	0.9556353998115062	0.7225800966631282	T	T	T
0.5834796125552033	0.9568500430705639	0.6861521024692762	T	T	T
0.9365845040106734	0.1376313157340195	0.8971279444637126	T	T	T
0.9040025022745979	0.0147258237694004	0.9322720958722411	T	T	T
0.8932650515446660	0.8844981542957641	0.9106091577432669	T	T	T
0.6975681121832034	0.1399789180386224	0.8813733159186568	T	T	T
0.6944961024175410	0.0055361207436801	0.8988542584859416	T	T	T
0.6976199221700896	0.8754643688887097	0.9549553422838901	T	T	T
0.4871162072424111	0.0473814173893383	0.7125513368696431	T	T	T
0.4822962715392918	0.8708077288349664	0.7069376841517702	T	T	T
0.3542986967239686	0.4379301403610222	0.7143692295119184	T	T	T
0.3004902687331411	0.4278597559031585	0.8936947056926173	T	T	T
0.2018003715947091	0.4443606341053276	0.0267552782957346	T	T	T
0.1038589396024363	0.4294267179919877	0.8927046604593427	T	T	T
0.1043038281166152	0.4462605554845633	0.6952435157405460	T	T	T
0.2286751309903994	0.4722686179356029	0.7406134999780914	T	T	T
0.3617665819305089	0.6680857528877165	0.7440161557522054	T	T	T
0.3047421632068778	0.6615247054205677	0.9178253784329542	T	T	T
0.1927068568696662	0.6445415384566160	0.0208031291097295	T	T	T
0.0944377763777328	0.6715105919181210	0.8945282403498190	T	T	T
0.1086958613340955	0.6549502577192778	0.6994380653020220	T	T	T
0.2333079595152817	0.6366806324695103	0.7543469591509619	T	T	T
0.3242627987006939	0.5489757614429543	0.8157634501889254	T	T	T
0.0829177638587330	0.5501342824498630	0.8184262699565121	T	T	T
0.4302318664711759	0.3723126299027957	0.5865550617781381	T	T	T
0.4192286398729931	0.5045269210375176	0.5679221189326726	T	T	T
0.4002276735959199	0.6370036902073630	0.5599952935919102	T	T	T

Structure files (CONTCAR) involved in this work:

0.1988540440473107	0.3716040032605304	0.6147397230304362	T	T	T
0.1835568894711391	0.4983196649760537	0.5569993727880628	T	T	T
0.1999770037352835	0.6323276947771886	0.5601692897372281	T	T	T
0.9918641056438638	0.4530885286062331	0.7893357212320604	T	T	T
0.9898484370749241	0.6433372139829997	0.7807094635440488	T	T	T
0.1408464116411220	0.5607860295122069	0.2150528173548327	T	T	T
0.1987114325351539	0.5666673981262009	0.3906438778378181	T	T	T
0.3012757204243930	0.5512534438370742	0.5179382194671621	T	T	T
0.4037138411999976	0.5681742644363118	0.3937920043229927	T	T	T
0.3975685646031839	0.5522581427531230	0.1965513675859036	T	T	T
0.2699063975422175	0.5303372955218471	0.2343763499009293	T	T	T
0.1440936300952155	0.3254302743254943	0.2408329174276320	T	T	T
0.1935356070284228	0.3415536950934772	0.4204858982049386	T	T	T
0.3098616094259912	0.3499854114370887	0.5115995843780761	T	T	T
0.4172680267375766	0.3277220810781685	0.4001398868121714	T	T	T
0.3970448203477431	0.3386927689817129	0.2047658651315344	T	T	T
0.2719428001909656	0.3563474325517175	0.2607921904796281	T	T	T
0.1777811610811639	0.4473200763624911	0.3029116694599435	T	T	T
0.4162138622368993	0.4476428931500757	0.3169814729482144	T	T	T
0.0681421867888413	0.6241384376538689	0.0780360835388348	T	T	T
0.0819059514820611	0.4922394441961759	0.0651098621365617	T	T	T
0.1003693390626727	0.3607490956390809	0.0601587516390884	T	T	T
0.3088704651595341	0.6279020393471799	0.1099030180531684	T	T	T
0.3202025665226930	0.4988874204948936	0.0570264825820579	T	T	T
0.3048678383529381	0.3649833643661416	0.0668297846346942	T	T	T
0.5123099560232942	0.5385024815059439	0.2842592884269103	T	T	T
0.5168341300405314	0.3640856022151457	0.2805325725318734	T	T	T
0.4433458659358630	0.7488057796299827	0.6456464216546969	T	T	T
0.2011203001710667	0.7474363050404045	0.6532749077216836	T	T	T
0.2723885609779178	0.7492315341081162	0.0583821387621798	T	T	T
0.1098320492066583	0.7477345340739613	0.0542981062561812	T	T	T
0.0613136018857550	0.2473535583578705	0.1388961568086068	T	T	T
0.3054011338193556	0.2474415029101246	0.1555186723626364	T	T	T
0.2255364810974352	0.2495630870115177	0.5567888496621781	T	T	T
0.3914298814201168	0.2475734208590289	0.5519305294852039	T	T	T
0.5587661609561864	0.2490645646521997	0.3563565128318924	T	T	T
0.8180688656787692	0.2534708720702123	0.3679807229146217	T	T	T
0.7272677079648547	0.2499697733720032	0.9849184757601457	T	T	T
0.8940540485083682	0.2540260675714024	0.9493644217833096	T	T	T
0.9127030958422518	0.7551961507373683	0.8802713107314527	T	T	T
0.6848820177307803	0.7453868313168327	0.8781813160447453	T	T	T
0.8015416707387411	0.7525274138313381	0.4814044487594658	T	T	T
0.5743576066118898	0.7497886056242726	0.4641451384344855	T	T	T
0.8000144071694409	0.6743517547232430	0.0743993289870046	T	T	T
0.6989775480265690	0.7673923434751245	0.1266893684427346	T	T	T
0.8355770393169611	0.7981961468592592	0.0511919191112813	T	T	T
0.9896278661247532	0.7131932590098224	0.3134602747481846	T	T	T
0.7125777220836251	0.6960460398379024	0.0524168351606238	T	T	T
0.7500766788907756	0.8214652735783563	0.0511679824807227	T	T	T
0.8556963642503836	0.7202461728568735	0.9929615216503329	T	T	T
0.9800459456300078	0.6813749322050857	0.2601103287917161	T	T	T
0.8933940177440992	0.7966323206976157	0.4389118593208371	T	T	T
0.8936371311999285	0.7518116351905221	0.5573701272707463	T	T	T

Structure files (CONTCAR) involved in this work:

0.8919264864543606 0.7074187686778420 0.4384659946633462 T T T
1.0343190207063788 0.7009296643359793 0.3355573147337210 T T T
0.8762379844379369 0.7521610936863413 0.4798001727262903 T T T

Figure S8(a)

Si Al O Zn H C

1.0000000000000000

20.021999999999985 0.0000000000000000 0.0000000000000000

0.0000000000000000 19.899000000000009 0.0000000000000000

0.0000000000000000 0.0000000000000000 13.382999999999991

93 3 194 2 5 1

Selective dynamics

Direct

0.4244399999999970 0.0580300000000022 0.6471700000000027 T T T
0.3067399999999978 0.0269899999999978 0.7922399999999996 T T T
0.2835400000000021 0.0581699999999969 0.0141199999999984 T T T
0.1246300000000033 0.0614899999999992 0.0117300000000000 T T T
0.0697400000000030 0.0301199999999966 0.8002600000000015 T T T
0.1818099999999987 0.0568700000000035 0.6600899999999967 T T T
0.4197800000000029 0.8261800000000008 0.6668599999999998 T T T
0.3061999999999969 0.8684000000000012 0.8090100000000007 T T T
0.2665799999999976 0.8288200000000003 0.0261799999999965 T T T
0.1123600000000025 0.8263499999999979 0.0084999999999980 T T T
0.0671000000000035 0.8727700000000027 0.7946400000000011 T T T
0.1857100000000003 0.8278400000000019 0.6698900000000023 T T T
0.0779500000000013 0.9400199999999970 0.1472199999999972 T T T
0.1955400000000012 0.9701499999999967 0.2912299999999988 T T T
0.2199799999999996 0.9393900000000031 0.5134899999999973 T T T
0.3790400000000034 0.9355300000000000 0.5123800000000003 T T T
0.4342299999999994 0.9674199999999971 0.3006400000000014 T T T
0.3213599999999985 0.9408900000000031 0.1602600000000010 T T T
0.0836299999999994 0.1709600000000009 0.1653999999999982 T T T
0.1957599999999999 0.1279299999999992 0.3084300000000013 T T T
0.2347800000000007 0.1688199999999966 0.5245699999999971 T T T
0.3894799999999989 0.1730400000000003 0.5084700000000026 T T T
0.4369099999999975 0.1257799999999989 0.2955299999999994 T T T
0.3165800000000019 0.1691799999999972 0.1719500000000025 T T T
0.5764100000000028 0.5544599999999988 0.3528799999999990 T T T
0.6904800000000009 0.5249000000000024 0.1974999999999980 T T T
0.7137600000000006 0.5688400000000016 0.9834800000000001 T T T
0.8728899999999982 0.5729400000000027 0.9814999999999969 T T T
0.8091000000000008 0.5494399999999970 0.3400600000000011 T T T
0.5735099999999989 0.3270100000000014 0.3284900000000022 T T T
0.6941500000000005 0.3709399999999974 0.1890799999999970 T T T
0.7305500000000009 0.3263800000000003 0.9785200000000032 T T T
0.8853300000000033 0.3260300000000029 0.9966000000000008 T T T
0.9438499999999976 0.3755999999999986 0.1916599999999988 T T T
0.9195100000000025 0.4440400000000011 0.8591399999999965 T T T
0.8006799999999998 0.4710499999999982 0.7175799999999981 T T T
0.7710399999999993 0.4353399999999965 0.4934700000000021 T T T
0.6126300000000029 0.4277200000000008 0.4891199999999998 T T T
0.5659700000000001 0.4680899999999966 0.7030099999999990 T T T
0.6757199999999983 0.4476099999999974 0.8540599999999969 T T T
0.9194400000000016 0.6778899999999979 0.8228200000000001 T T T

Structure files (CONTCAR) involved in this work:

0.7705399999999969	0.6667899999999989	0.4622400000000013	T	T	T
0.6151600000000030	0.6718499999999992	0.4850899999999996	T	T	T
0.5616500000000002	0.6265300000000025	0.6965300000000028	T	T	T
0.6756400000000014	0.6732799999999983	0.8212100000000007	T	T	T
0.5796300000000016	0.9438800000000001	0.3546800000000019	T	T	T
0.6999599999999973	0.9724099999999964	0.2101100000000002	T	T	T
0.7224399999999989	0.9351800000000026	0.9884800000000027	T	T	T
0.8831800000000030	0.9328000000000003	0.9923700000000011	T	T	T
0.9338800000000020	0.9678699999999978	0.2029300000000021	T	T	T
0.8234100000000026	0.9449299999999994	0.3515599999999992	T	T	T
0.5795400000000015	0.1717299999999966	0.3255800000000022	T	T	T
0.6998400000000018	0.1310599999999980	0.1890000000000001	T	T	T
0.7334200000000024	0.1709400000000016	0.9687600000000032	T	T	T
0.8881000000000014	0.1733800000000016	0.9837800000000030	T	T	T
0.9380799999999994	0.1254899999999992	0.1954899999999995	T	T	T
0.8225100000000012	0.1719799999999978	0.3254599999999996	T	T	T
0.9244699999999995	0.0552800000000033	0.8551900000000003	T	T	T
0.8053200000000018	0.0271100000000004	0.7049400000000006	T	T	T
0.7824600000000004	0.0659800000000033	0.4882100000000023	T	T	T
0.6218700000000013	0.0685599999999980	0.4879600000000011	T	T	T
0.5691500000000005	0.0311200000000014	0.6970900000000029	T	T	T
0.6818400000000011	0.0527099999999976	0.8440599999999989	T	T	T
0.9256699999999967	0.8300899999999984	0.8320599999999985	T	T	T
0.8042200000000008	0.8703999999999965	0.6932299999999998	T	T	T
0.7719400000000007	0.8251100000000022	0.4772800000000004	T	T	T
0.6165900000000022	0.8254700000000028	0.4874500000000026	T	T	T
0.5647499999999965	0.8740900000000025	0.6947800000000015	T	T	T
0.6802100000000024	0.8327799999999996	0.8274499999999989	T	T	T
0.4216100000000012	0.4427499999999966	0.6449500000000015	T	T	T
0.3025999999999982	0.4699499999999972	0.7899900000000031	T	T	T
0.2785999999999973	0.4380400000000009	0.0115699999999990	T	T	T
0.1202800000000011	0.4360599999999977	0.0125499999999974	T	T	T
0.0641999999999996	0.4690500000000029	0.7982000000000014	T	T	T
0.1773999999999987	0.4399999999999977	0.6574400000000011	T	T	T
0.4178100000000029	0.6725500000000011	0.6605599999999967	T	T	T
0.3030299999999997	0.6286599999999964	0.8044700000000020	T	T	T
0.2664199999999965	0.6702000000000012	0.0211200000000034	T	T	T
0.1122399999999999	0.6727300000000014	0.0048499999999976	T	T	T
0.0615299999999976	0.6277499999999989	0.7923299999999998	T	T	T
0.1818000000000026	0.6699199999999976	0.6693899999999999	T	T	T
0.0794199999999989	0.5591000000000008	0.1460300000000032	T	T	T
0.1962199999999967	0.5263500000000008	0.2907999999999973	T	T	T
0.2165699999999973	0.5581999999999994	0.5144000000000020	T	T	T
0.3761200000000002	0.5648800000000023	0.5098899999999986	T	T	T
0.4298799999999972	0.5290000000000035	0.2977699999999999	T	T	T
0.3203999999999994	0.5553700000000035	0.1531499999999966	T	T	T
0.0855299999999986	0.3232500000000016	0.1619699999999966	T	T	T
0.1967900000000000	0.3687100000000001	0.3064600000000013	T	T	T
0.2321600000000004	0.3282299999999978	0.5240200000000002	T	T	T
0.3867800000000017	0.3272300000000001	0.5057600000000022	T	T	T
0.4328599999999980	0.3709800000000030	0.2906100000000009	T	T	T
0.3145400000000009	0.3278400000000019	0.1688199999999966	T	T	T
0.9217700000000022	0.5302999999999969	0.1905399999999986	T	T	T

Structure files (CONTCAR) involved in this work:

0.8213099999999969	0.3352999999999966	0.3230799999999974	T	T	T
0.8009100000000018	0.6330000000000027	0.6886599999999987	T	T	T
0.3587599999999966	0.0640900000000002	0.7176499999999990	T	T	T
0.3125000000000000	0.0623099999999965	0.9011199999999988	T	T	T
0.2036900000000017	0.0438100000000006	0.0123999999999995	T	T	T
0.0968599999999995	0.0690600000000003	0.8988599999999991	T	T	T
0.1058000000000021	0.0609999999999999	0.7017600000000002	T	T	T
0.2307199999999980	0.0347000000000008	0.7514600000000016	T	T	T
0.3623199999999969	0.8242899999999977	0.7521300000000011	T	T	T
0.3076399999999992	0.8472500000000025	0.9256200000000021	T	T	T
0.1893299999999982	0.8526299999999978	0.0127600000000001	T	T	T
0.0856199999999987	0.8304600000000022	0.8947100000000034	T	T	T
0.1080699999999979	0.8416599999999974	0.7001899999999992	T	T	T
0.2325999999999979	0.8526799999999994	0.7625699999999966	T	T	T
0.3248699999999971	0.9474299999999971	0.7973900000000000	T	T	T
0.0879699999999985	0.9507699999999986	0.8111800000000002	T	T	T
0.4332800000000034	0.1273300000000006	0.5843199999999982	T	T	T
0.4183599999999998	0.9954499999999982	0.5696500000000029	T	T	T
0.3918099999999995	0.8642800000000008	0.5679999999999978	T	T	T
0.2032799999999995	0.1305800000000019	0.6202200000000033	T	T	T
0.1844299999999990	0.0018400000000014	0.5705099999999987	T	T	T
0.2042199999999994	0.8684500000000028	0.5684299999999993	T	T	T
0.9899599999999964	0.0406699999999987	0.7871400000000008	T	T	T
0.9873300000000000	0.8669500000000028	0.7734200000000016	T	T	T
0.1439700000000030	0.9321100000000015	0.2167900000000031	T	T	T
0.1904499999999985	0.9355300000000000	0.4007000000000005	T	T	T
0.2999000000000009	0.9530600000000007	0.5116799999999984	T	T	T
0.4072299999999984	0.9287899999999993	0.3996300000000019	T	T	T
0.3969900000000024	0.9367700000000028	0.2030200000000022	T	T	T
0.2716300000000018	0.9633499999999984	0.2505200000000016	T	T	T
0.1410100000000014	0.1733400000000032	0.2507900000000021	T	T	T
0.1933000000000007	0.1478800000000007	0.4254000000000033	T	T	T
0.3123799999999974	0.1468899999999991	0.5097700000000032	T	T	T
0.4186100000000010	0.1676399999999987	0.3959699999999984	T	T	T
0.3944899999999976	0.1570099999999996	0.2023000000000010	T	T	T
0.2701599999999971	0.1423300000000012	0.2639700000000005	T	T	T
0.1757800000000032	0.0493299999999977	0.2950099999999978	T	T	T
0.4176399999999987	0.0471999999999966	0.3110500000000016	T	T	T
0.0671999999999997	0.8713300000000004	0.0833999999999975	T	T	T
0.0846200000000010	0.0020900000000026	0.0690499999999972	T	T	T
0.1116900000000030	0.1324800000000010	0.0673499999999976	T	T	T
0.3000699999999981	0.8671000000000006	0.1202200000000033	T	T	T
0.3196200000000005	0.9957300000000018	0.0704300000000018	T	T	T
0.2990599999999972	0.1289599999999993	0.0696799999999982	T	T	T
0.5136299999999991	0.9545900000000032	0.2861400000000032	T	T	T
0.5165999999999968	0.1327799999999968	0.2734900000000025	T	T	T
0.6390099999999990	0.5572700000000026	0.2770000000000010	T	T	T
0.6955499999999972	0.5744200000000035	0.1017700000000019	T	T	T
0.7933299999999974	0.5581400000000016	0.9651599999999974	T	T	T
0.8910300000000007	0.5804199999999966	0.0982199999999978	T	T	T
0.8863500000000002	0.5335099999999997	0.3106799999999978	T	T	T
0.7636800000000008	0.5214399999999983	0.2506399999999971	T	T	T
0.6414699999999982	0.3359400000000008	0.2655299999999983	T	T	T

Structure files (CONTCAR) involved in this work:

0.6893000000000029	0.3313899999999990	0.0825699999999969	T	T	T
0.8076999999999970	0.3502200000000002	0.9959699999999998	T	T	T
0.9122899999999987	0.3223899999999986	0.1120999999999981	T	T	T
0.9059400000000011	0.3672499999999985	0.3015199999999965	T	T	T
0.7681499999999986	0.3678000000000026	0.2345899999999972	T	T	T
0.6700200000000009	0.4486500000000007	0.1684800000000024	T	T	T
0.9345900000000000	0.4500999999999991	0.1503399999999999	T	T	T
0.5707999999999984	0.6261200000000002	0.4098499999999987	T	T	T
0.5853499999999983	0.4958699999999965	0.4365900000000025	T	T	T
0.5793999999999997	0.3620200000000011	0.4383499999999998	T	T	T
0.7975500000000011	0.6290199999999970	0.3614800000000002	T	T	T
0.7915500000000009	0.5112799999999993	0.4483999999999995	T	T	T
0.8179700000000025	0.3818399999999968	0.4363799999999998	T	T	T
0.0103200000000001	0.5564200000000028	0.2220799999999983	T	T	T
0.0220399999999970	0.3595200000000034	0.2145500000000027	T	T	T
0.8546400000000034	0.4320900000000023	0.7868399999999980	T	T	T
0.7908600000000021	0.4330500000000015	0.6105500000000035	T	T	T
0.6931200000000004	0.4230200000000011	0.4728199999999987	T	T	T
0.5955200000000005	0.4276399999999967	0.6069200000000023	T	T	T
0.6023300000000020	0.4411500000000004	0.8035500000000013	T	T	T
0.7283800000000014	0.4746000000000024	0.7702000000000027	T	T	T
0.8602100000000021	0.6823300000000003	0.7433899999999980	T	T	T
0.8164799999999985	0.6385000000000005	0.5555200000000013	T	T	T
0.6929900000000018	0.6466899999999995	0.4837899999999991	T	T	T
0.5857499999999973	0.6662999999999997	0.5969699999999989	T	T	T
0.5968200000000010	0.6605100000000022	0.7934500000000000	T	T	T
0.7211599999999976	0.6444899999999976	0.7314500000000024	T	T	T
0.8281399999999977	0.5467799999999983	0.6916099999999972	T	T	T
0.5810800000000000	0.5474999999999994	0.6867099999999979	T	T	T
0.9292200000000008	0.3780599999999978	0.9298399999999987	T	T	T
0.9121999999999986	0.5102300000000000	0.9286699999999968	T	T	T
0.8955199999999977	0.6415399999999991	0.9256999999999991	T	T	T
0.6971699999999998	0.3740600000000001	0.8940300000000008	T	T	T
0.6735800000000012	0.5029800000000009	0.9427900000000022	T	T	T
0.6899599999999992	0.6369499999999988	0.9283799999999971	T	T	T
0.4866400000000013	0.4530000000000030	0.7157100000000014	T	T	T
0.4810599999999994	0.6327799999999968	0.7082100000000011	T	T	T
0.6443799999999982	0.9391000000000034	0.2827100000000016	T	T	T
0.7001199999999983	0.9322799999999987	0.1047399999999996	T	T	T
0.8031199999999998	0.9396399999999971	0.9772999999999996	T	T	T
0.9020599999999988	0.9261699999999990	0.1098199999999991	T	T	T
0.8988599999999991	0.9461200000000005	0.3072700000000026	T	T	T
0.7729399999999984	0.9647399999999990	0.2612600000000000	T	T	T
0.6428000000000011	0.1713799999999992	0.2504800000000031	T	T	T
0.6964200000000034	0.1571599999999975	0.0744800000000012	T	T	T
0.8111000000000033	0.1473000000000013	0.9782599999999988	T	T	T
0.9152100000000019	0.1672799999999981	0.0972799999999978	T	T	T
0.8991100000000003	0.1525699999999972	0.2935599999999994	T	T	T
0.7732299999999981	0.1449199999999990	0.2360600000000019	T	T	T
0.6828999999999965	0.0512000000000015	0.1929400000000001	T	T	T
0.9216699999999989	0.0466499999999996	0.1784699999999972	T	T	T
0.5721800000000030	0.8737300000000019	0.4160499999999985	T	T	T
0.5850900000000010	0.0052299999999974	0.4344499999999982	T	T	T

Structure files (CONTCAR) involved in this work:

0.599899999999981	0.1373400000000018	0.4315500000000014	T	T	T
0.8094800000000006	0.8695000000000022	0.3930099999999968	T	T	T
0.8169100000000000	0.9987500000000011	0.4419800000000009	T	T	T
0.8049200000000027	0.1331100000000021	0.4294099999999972	T	T	T
0.0129499999999965	0.9517200000000017	0.2170500000000004	T	T	T
0.0180799999999977	0.1347400000000007	0.2119700000000009	T	T	T
0.8594700000000017	0.0564099999999996	0.7833600000000018	T	T	T
0.8063399999999987	0.0724999999999980	0.6040399999999977	T	T	T
0.7018300000000011	0.0571699999999993	0.4809699999999992	T	T	T
0.5984199999999973	0.0747399999999985	0.6038100000000028	T	T	T
0.6061100000000010	0.0505399999999980	0.8009800000000027	T	T	T
0.7312799999999982	0.0302500000000023	0.7538899999999984	T	T	T
0.8590099999999978	0.8356599999999972	0.7646700000000024	T	T	T
0.8072099999999978	0.8328699999999998	0.5856700000000004	T	T	T
0.6944299999999970	0.8493899999999996	0.4842000000000013	T	T	T
0.5894100000000009	0.8281300000000016	0.6014600000000030	T	T	T
0.6037400000000019	0.8510500000000008	0.7955200000000033	T	T	T
0.7300600000000017	0.8625899999999973	0.7415499999999966	T	T	T
0.8221800000000030	0.9493300000000033	0.6778600000000026	T	T	T
0.5805099999999968	0.9522699999999986	0.6697500000000005	T	T	T
0.9331800000000001	0.1282799999999966	0.9083499999999987	T	T	T
0.9182399999999973	0.9985900000000001	0.9424700000000001	T	T	T
0.9119799999999998	0.8655400000000029	0.9394300000000015	T	T	T
0.6976099999999974	0.1287900000000022	0.8801800000000028	T	T	T
0.6893699999999967	0.0017199999999988	0.9381600000000034	T	T	T
0.6960699999999989	0.8671199999999999	0.9348900000000029	T	T	T
0.4904300000000035	0.0470699999999979	0.7153700000000001	T	T	T
0.4850500000000011	0.8640299999999996	0.7119500000000016	T	T	T
0.3556900000000027	0.4347100000000026	0.7148400000000024	T	T	T
0.3052199999999985	0.4320799999999991	0.8975500000000025	T	T	T
0.1989799999999988	0.4558400000000020	0.0159900000000022	T	T	T
0.0929300000000026	0.4342899999999972	0.8997299999999981	T	T	T
0.1018899999999974	0.4373199999999997	0.7015799999999999	T	T	T
0.2271500000000017	0.4629800000000017	0.7472899999999996	T	T	T
0.3570199999999986	0.6707299999999989	0.7404300000000035	T	T	T
0.3067300000000017	0.6550700000000020	0.9187599999999989	T	T	T
0.1890199999999993	0.6458299999999966	0.0078499999999977	T	T	T
0.0822399999999988	0.6677499999999981	0.8938500000000005	T	T	T
0.1040199999999984	0.6606999999999985	0.7010900000000007	T	T	T
0.2283299999999997	0.6417199999999994	0.7603099999999969	T	T	T
0.3211900000000014	0.5491299999999981	0.8009800000000027	T	T	T
0.0797499999999971	0.5489299999999986	0.8062299999999993	T	T	T
0.4312200000000033	0.3753200000000021	0.5777500000000018	T	T	T
0.4166299999999978	0.5067599999999999	0.5697199999999967	T	T	T
0.3935299999999984	0.6379700000000028	0.5567100000000025	T	T	T
0.1972700000000032	0.3654500000000027	0.6181199999999976	T	T	T
0.1831800000000001	0.4927199999999985	0.5655799999999971	T	T	T
0.1966200000000029	0.6286500000000004	0.5672100000000029	T	T	T
0.9850199999999987	0.4530200000000022	0.7882900000000035	T	T	T
0.9822899999999990	0.6367499999999993	0.7724100000000007	T	T	T
0.1415300000000030	0.5659500000000008	0.2213899999999995	T	T	T
0.1927200000000013	0.5622899999999973	0.3985699999999994	T	T	T
0.2971300000000028	0.5485899999999972	0.5191700000000026	T	T	T

Structure files (CONTCAR) involved in this work:

0.399099999999971	0.5672700000000006	0.3941900000000018	T	T	T
0.3956400000000002	0.558999999999975	0.1972000000000023	T	T	T
0.2699799999999968	0.533499999999965	0.2431300000000007	T	T	T
0.1459400000000031	0.322859999999986	0.2422600000000017	T	T	T
0.1916399999999996	0.3471199999999968	0.4225199999999987	T	T	T
0.3093399999999988	0.352499999999991	0.5111500000000007	T	T	T
0.4126199999999969	0.3297299999999979	0.3909599999999998	T	T	T
0.3927699999999987	0.3417000000000030	0.1940799999999996	T	T	T
0.2719999999999985	0.3562200000000004	0.2643699999999995	T	T	T
0.1753199999999993	0.447499999999980	0.2947399999999973	T	T	T
0.4139899999999983	0.449339999999994	0.3081000000000031	T	T	T
0.0682199999999966	0.6257299999999972	0.0804899999999975	T	T	T
0.0792599999999979	0.4922600000000017	0.0788599999999988	T	T	T
0.1079300000000032	0.3627400000000023	0.0611299999999986	T	T	T
0.2999300000000034	0.628999999999978	0.1124099999999970	T	T	T
0.3181799999999981	0.499699999999971	0.0645799999999994	T	T	T
0.2923800000000014	0.3669799999999981	0.0674500000000009	T	T	T
0.5094399999999979	0.5415700000000001	0.2881900000000002	T	T	T
0.5120300000000029	0.3620099999999979	0.2676999999999978	T	T	T
0.4381600000000034	0.7496099999999970	0.6360400000000013	T	T	T
0.1974200000000010	0.7485900000000001	0.6476600000000019	T	T	T
0.2700499999999977	0.7490400000000008	0.0487499999999983	T	T	T
0.1076400000000035	0.7488900000000029	0.0460899999999995	T	T	T
0.0664099999999976	0.2472199999999987	0.1309899999999971	T	T	T
0.3019499999999979	0.2482899999999972	0.1517499999999998	T	T	T
0.2286399999999986	0.2485100000000031	0.5449699999999993	T	T	T
0.3933800000000005	0.2505499999999969	0.5456000000000003	T	T	T
0.5575699999999983	0.2485100000000031	0.3478800000000035	T	T	T
0.8159500000000008	0.2509999999999977	0.3418399999999977	T	T	T
0.7282999999999973	0.2496200000000002	0.9380299999999977	T	T	T
0.8928999999999974	0.2513999999999967	0.9487900000000025	T	T	T
0.9456100000000021	0.7526900000000012	0.8530999999999977	T	T	T
0.6891400000000019	0.7527800000000013	0.8387699999999967	T	T	T
0.7778500000000008	0.7466500000000025	0.4447299999999998	T	T	T
0.6104899999999986	0.7489500000000007	0.4467199999999991	T	T	T
0.9374499999999983	0.4884100000000018	0.5144299999999973	T	T	T
0.0489600000000010	0.5568999999999988	0.5379999999999967	T	T	T
0.9140400000000000	0.4316699999999969	0.4131199999999993	T	T	T
0.8746200000000002	0.5508600000000001	0.5543300000000002	T	T	T
0.0170200000000023	0.5761200000000031	0.2885399999999976	T	T	T
0.0643000000000029	0.6552399999999992	0.4997899999999973	T	T	T
0.9836900000000028	0.6396599999999992	0.5506799999999998	T	T	T
0.0020099999999985	0.6139799999999980	0.4255799999999965	T	T	T
0.0114099999999979	0.5234900000000025	0.5328700000000026	T	T	T
0.0235699999999994	0.6183199999999971	0.5022000000000020	T	T	T

Figure S8(b)

Si Al O Cu H C

1.000000000000000

20.021999999999985 0.000000000000000 0.000000000000000

0.000000000000000 19.899000000000009 0.000000000000000

0.000000000000000 0.000000000000000 13.382999999999991

93 3 196 3 5 1

Selective dynamics

Structure files (CONTCAR) involved in this work:

Direct

0.4217215530797016	0.0536236050575312	0.6435060960843076	T	T	T
0.2996330025801127	0.0274388773685293	0.7851774373520157	T	T	T
0.2787377598441030	0.0638597902482447	0.0067666201400520	T	T	T
0.1186897990130227	0.0645892120562138	0.0078457143163047	T	T	T
0.0651183966139679	0.0222428456437409	0.7979969519745544	T	T	T
0.1727254065505493	0.0517006757293767	0.6472036017961494	T	T	T
0.4200207472176253	0.8279034878540891	0.6601020745330171	T	T	T
0.3046610053036472	0.8693831493504367	0.8060946325443292	T	T	T
0.2684505656031023	0.8282705688051178	0.0247675047380523	T	T	T
0.1137911339168943	0.8249067498470156	0.0118217368411348	T	T	T
0.0659382026220960	0.8624952060652554	0.7945741242972399	T	T	T
0.1860196837305992	0.8251384689269606	0.6671804873574867	T	T	T
0.0759757994754114	0.9421943371870203	0.1451225403246490	T	T	T
0.1960396567878981	0.9720463636279504	0.2885436110571283	T	T	T
0.2177040192836943	0.9346396296553146	0.5085539023649822	T	T	T
0.375942332294282	0.9320849559284623	0.5084205058382676	T	T	T
0.4284676958017926	0.9720656017271522	0.2985635067127053	T	T	T
0.3198217146947466	0.9470662283809566	0.1485410537630285	T	T	T
0.0785093524314556	0.1716615172116650	0.1604409900456274	T	T	T
0.1965024607102345	0.1290305445684813	0.3023409022604948	T	T	T
0.2275415341267476	0.1708681060378454	0.5219878566973306	T	T	T
0.3824464693245102	0.1714083721936985	0.5111983993898687	T	T	T
0.4333672042020164	0.1292807885444580	0.3010573342575648	T	T	T
0.3187207695561198	0.1686159516344706	0.1676672721238106	T	T	T
0.5772934189610857	0.5526512563770172	0.3437527513618719	T	T	T
0.6992742822208533	0.5320468823779436	0.2135142996849554	T	T	T
0.7180899971373604	0.5497831075196059	0.9835295546626855	T	T	T
0.8754603662800071	0.5663244438008728	0.9871378239362661	T	T	T
0.9324130948727982	0.5330737959178873	0.1976847572122872	T	T	T
0.8215730264659918	0.5683509412562346	0.3407244978552029	T	T	T
0.5805174413582218	0.3304110626853850	0.3276488037854419	T	T	T
0.7042481671372912	0.3747633028609996	0.2093150211261727	T	T	T
0.7344833980429333	0.3324744505791024	0.9898108007879585	T	T	T
0.8902838510713827	0.3303961850025581	0.9916033606885147	T	T	T
0.9365805450000740	0.3752554793021105	0.2032239819587622	T	T	T
0.8265214150215632	0.3314472435740988	0.3470902992197779	T	T	T
0.9268530453491320	0.4467303611463971	0.8546589458146694	T	T	T
0.8045622735026708	0.4722668491270824	0.7161089236107643	T	T	T
0.7842870677227076	0.4466053519443327	0.4907564448911853	T	T	T
0.6242529595775040	0.4351140099441064	0.4902352209675293	T	T	T
0.5646476854774313	0.4629040943941777	0.7024632693131008	T	T	T
0.6793444235727860	0.4308305630620060	0.8361788688240323	T	T	T
0.7927274727882513	0.6293451700169046	0.7001023396878894	T	T	T
0.5647342297254979	0.6219760144878684	0.7062671756871663	T	T	T
0.6732059584222599	0.6713654536002299	0.8443193982649910	T	T	T
0.5741183568728204	0.9504301913924872	0.3526377189099179	T	T	T
0.6975490631852940	0.9784529147993583	0.2161562282123431	T	T	T
0.7126449741353913	0.9529728393444304	0.9884833752347352	T	T	T
0.8753314021732657	0.9430082203152992	0.9854089896461119	T	T	T
0.9320624579415527	0.9681191346417916	0.2001186144430516	T	T	T
0.8173858834879031	0.9307970181779226	0.3357471570635986	T	T	T
0.5800254835877534	0.1758422689331377	0.3299411027125106	T	T	T

Structure files (CONTCAR) involved in this work:

0.7038108795876228	0.1339792660620696	0.2056767436543220	T	T	T
0.7343790500188829	0.1720509093835023	0.9861682887917790	T	T	T
0.8917659846198811	0.1770059909134253	0.9827794102689124	T	T	T
0.9363076763014987	0.1268386000825439	0.2002619645562238	T	T	T
0.8239852271429844	0.1776644419580704	0.3374150195483431	T	T	T
0.9184231027207488	0.0638345044568942	0.8487828781794392	T	T	T
0.8037102805595896	0.0359068556408550	0.7029879578113016	T	T	T
0.7808839953813830	0.0568097370613130	0.4768735452928571	T	T	T
0.6214418257699786	0.0722423291676075	0.4875831498248002	T	T	T
0.5670733456287387	0.0361640242638504	0.6993481629659761	T	T	T
0.6825542513752687	0.0723553173998280	0.8316180128496597	T	T	T
0.9172992955928334	0.8322332518276615	0.8254126571681893	T	T	T
0.7928644886221798	0.8769456180444350	0.7074833260017953	T	T	T
0.7645471510505590	0.8282909265305736	0.4865051106945228	T	T	T
0.6068229173095768	0.8290980952901083	0.4860568974278187	T	T	T
0.5638095047984959	0.8778968488371727	0.7010625036135734	T	T	T
0.4217306090827225	0.4413393147433924	0.6455357384916349	T	T	T
0.3031191222578720	0.4720411686948539	0.7898053796411231	T	T	T
0.2819232776249914	0.4345813727136626	0.0097581884495210	T	T	T
0.1225567140291988	0.4322160815531054	0.0068917376559653	T	T	T
0.0716913912669250	0.4720885559662785	0.7965672603321774	T	T	T
0.1810353129817283	0.4469373693639563	0.6493610698427018	T	T	T
0.4231746172954343	0.6725481642185387	0.6653510857532822	T	T	T
0.3058978130260950	0.6285624393644434	0.8061475027050966	T	T	T
0.2705447928491443	0.6713941248383490	0.0242829347997240	T	T	T
0.1166720105736723	0.6725526719957545	0.0077235953728000	T	T	T
0.0685829834280469	0.6302452701325367	0.7949569640511002	T	T	T
0.1871066084930863	0.6675739951414718	0.6663004528531127	T	T	T
0.0771425092717011	0.5554126297822497	0.1387798140591417	T	T	T
0.1965798259334314	0.5267000963759727	0.2839902516997545	T	T	T
0.2235494121497577	0.5624020421879673	0.5029675628836154	T	T	T
0.3841051882064865	0.5657030933166382	0.5079353106430941	T	T	T
0.4325474120826929	0.5238565860364026	0.2973241448187424	T	T	T
0.3228790562604351	0.5528102847642518	0.1486554381762800	T	T	T
0.0796695110247006	0.3266479622782630	0.1623945821982358	T	T	T
0.1960171650339625	0.3688103983346532	0.3053159122572489	T	T	T
0.2306279384079014	0.3275579592597849	0.5242864175290450	T	T	T
0.3855583672813991	0.3235057197948628	0.5119813024685561	T	T	T
0.4342219711326195	0.3690620658985495	0.3013822951017122	T	T	T
0.3181463669167586	0.3272691896511271	0.1704592283673552	T	T	T
0.7644026648948649	0.6703394732751936	0.4800003396390224	T	T	T
0.9170079174842374	0.6755886433480075	0.8164830522408201	T	T	T
0.6678094095903826	0.8306687764182876	0.8527998260204932	T	T	T
0.6091943251204843	0.6788001842645662	0.4865632542648991	T	T	T
0.3553614731263058	0.0602946684699816	0.7124090719299483	T	T	T
0.2977948405808939	0.0693554341087647	0.8893600500134744	T	T	T
0.1985901657282499	0.0555979219909126	0.0226863213676802	T	T	T
0.0990490101695358	0.0624113457480056	0.8907433121513062	T	T	T
0.0978822312881415	0.0508234815205163	0.6951205854267105	T	T	T
0.2263528282443552	0.0318222261313757	0.7336657737687859	T	T	T
0.3615191157169327	0.8297959269812518	0.7440789660889129	T	T	T
0.3061123711527742	0.8407245976705966	0.9192740514610575	T	T	T
0.1906921565140614	0.8517404548604476	0.0147821896743471	T	T	T

Structure files (CONTCAR) involved in this work:

0.0870331593076161	0.8256449771494093	0.8978432518602865	T	T	T
0.1084223687268663	0.8337953900453617	0.7004632581724257	T	T	T
0.2315888239648161	0.8562602152149188	0.7566429955110636	T	T	T
0.3192051937057700	0.9495803200611568	0.8066680441371896	T	T	T
0.0795248592431407	0.9423473438813308	0.8084961208381954	T	T	T
0.4289277813372598	0.1216911715150093	0.5768940060444996	T	T	T
0.4179542412066855	0.9894940260335477	0.5680247816812303	T	T	T
0.3911009966161226	0.8582232446268784	0.5552922025536895	T	T	T
0.1873503847908964	0.1264855384599907	0.6038706264765596	T	T	T
0.1760712369922979	0.9966057626329097	0.5575599664416978	T	T	T
0.1993143155891706	0.8638422694598547	0.5622427483898533	T	T	T
0.9847961082934693	0.0332218031550563	0.7968077143999399	T	T	T
0.9884299196792679	0.8452377015254132	0.7704441894796732	T	T	T
0.1418265887253884	0.9376909251328387	0.2147820333894536	T	T	T
0.1974107562288088	0.9289783997798321	0.3914670646679004	T	T	T
0.2970392043024176	0.9502333831295587	0.5206846846999567	T	T	T
0.3969846115978957	0.9298750597712306	0.3914868308144587	T	T	T
0.3947437524995313	0.9489433515657681	0.1938101775617905	T	T	T
0.2690523674027456	0.9705420747507907	0.2365050955067836	T	T	T
0.1434946191718373	0.1680569140642837	0.2320691733172600	T	T	T
0.1936834923099547	0.1626610530389771	0.4124047286442201	T	T	T
0.3050847641433296	0.1461027234946051	0.5172544928420590	T	T	T
0.4069741346852694	0.1727575183987321	0.3957470478323409	T	T	T
0.3963263441977022	0.1567547356572354	0.2003454465395515	T	T	T
0.2710300088361705	0.1374351115956068	0.2550884629023590	T	T	T
0.1764800946740771	0.0500304712978610	0.3104641822043083	T	T	T
0.4142867270784624	0.0512293799768746	0.3200746622991857	T	T	T
0.0679291885196334	0.8722755088545243	0.0830538001838830	T	T	T
0.0804520558453009	0.0041216588240596	0.0660420886594529	T	T	T
0.0945520396307634	0.1363635938762387	0.0533064377481555	T	T	T
0.3038524909644658	0.8709290869175074	0.1129557648992139	T	T	T
0.3149148406849630	0.9978269583135237	0.0535877883797994	T	T	T
0.3041267456993262	0.1320915257053364	0.0614298117685337	T	T	T
0.5075597479983386	0.9586567435533504	0.2849458035865748	T	T	T
0.5136732549071031	0.1376985615937564	0.2885952339220013	T	T	T
0.6385573081758755	0.5706438818089777	0.2712589373932437	T	T	T
0.6877130591313719	0.5430838000722841	0.0949189327499073	T	T	T
0.7982325021578148	0.5408182967791244	0.9831944205109210	T	T	T
0.9031803801747166	0.5721606844395647	0.1002804469157665	T	T	T
0.8972192964554235	0.5610447891379969	0.2982652093070611	T	T	T
0.7704780104630526	0.5632687742642281	0.2452719390950650	T	T	T
0.6396606459365061	0.3320113840262902	0.2448564232625558	T	T	T
0.7078294363468332	0.3709071025152861	0.0889655886814149	T	T	T
0.8126680207710965	0.3517018887607872	0.9761424011475213	T	T	T
0.9092303838282024	0.3314325894765587	0.1094386876230011	T	T	T
0.9009959756389554	0.3489437069323980	0.3051259726654830	T	T	T
0.7724702225021065	0.3456696448793227	0.2580666629193363	T	T	T
0.6942531874498836	0.4528789251475260	0.2432112423198030	T	T	T
0.9172200705118477	0.4533745993367468	0.1835920445495575	T	T	T
0.5551953825466930	0.6246417527391354	0.4034897503702757	T	T	T
0.5950761874412852	0.5006625683382649	0.4311533781140008	T	T	T
0.6064057178900338	0.3675276460434963	0.4284650590991941	T	T	T
0.8152710991799912	0.6398008645390553	0.3961522063894682	T	T	T

Structure files (CONTCAR) involved in this work:

0.8049226305540641	0.5066454845249863	0.4159182925052741	T	T	T
0.8101983308382218	0.3756389380309172	0.4454700972189197	T	T	T
0.0119239041515794	0.5466753027300324	0.2093886871249835	T	T	T
0.0170475465478571	0.3664884880718950	0.2130323369595475	T	T	T
0.8621281505038266	0.4366229993865805	0.7834551357843783	T	T	T
0.8189985752964225	0.4574160269695735	0.5989998680138997	T	T	T
0.7036974986379301	0.4441405279481185	0.5037938929398652	T	T	T
0.5872594029680981	0.4297673193466842	0.5968281107156179	T	T	T
0.6040400081024047	0.4258908111118319	0.7929663212016054	T	T	T
0.7323052258726378	0.4398150563556130	0.7451808599203349	T	T	T
0.8556734448428744	0.6747677219561937	0.7276940067461056	T	T	T
0.7784247047988330	0.6271380673947810	0.5816807791739673	T	T	T
0.6881282285454395	0.6584438094963190	0.4466759978774096	T	T	T
0.5918968373620158	0.6577471521377283	0.6080097266383385	T	T	T
0.5987440936135411	0.6508257165553966	0.8094864600720005	T	T	T
0.7255937676113127	0.6577564305285969	0.7559993884707182	T	T	T
0.8042966785908124	0.5521790390866014	0.7402614962463392	T	T	T
0.5820169789582758	0.5420469911275415	0.7026022418003061	T	T	T
0.9362270529787170	0.3817631378576233	0.9274497450396072	T	T	T
0.9203095652861439	0.5131323826044077	0.9248596762567206	T	T	T
0.8864724215324512	0.6390104421615060	0.9313504169175124	T	T	T
0.6931387277567390	0.3611760510136295	0.8952094895428934	T	T	T
0.6836986414324998	0.4958543389952393	0.9104252028786599	T	T	T
0.6961305947904606	0.6266067904965060	0.9464972876750680	T	T	T
0.4852743811100371	0.4502849994815796	0.7193018474738350	T	T	T
0.4841047965754008	0.6323128787511469	0.7183154128003018	T	T	T
0.6369535870422532	0.9436147506068047	0.2764929016718833	T	T	T
0.6847688630440019	0.9764584846876029	0.0962943390235639	T	T	T
0.7935722121093913	0.9335981492984240	0.9991366919544475	T	T	T
0.9089459816349018	0.9360114815179034	0.0940614328388513	T	T	T
0.8931415702762323	0.9327333606329348	0.2920400087559989	T	T	T
0.7662823075523419	0.9378351770211290	0.2402282214788843	T	T	T
0.6366991951245315	0.1719519030185283	0.2430574202607640	T	T	T
0.7056264075785189	0.1339703992981006	0.0846164078055708	T	T	T
0.8134138134008263	0.1557642490650046	0.9728223801905762	T	T	T
0.9155525563083836	0.1637395775018726	0.0967150819304761	T	T	T
0.8982544400383882	0.1620124082430617	0.2937815202073191	T	T	T
0.7702346347183991	0.1723472534217018	0.2459619980419071	T	T	T
0.7038499227280606	0.0572939727311257	0.2486215257335927	T	T	T
0.9154976688022864	0.0480806373923512	0.1970132475963808	T	T	T
0.5654576755480599	0.8853359988221725	0.4229438504556997	T	T	T
0.5817468002361882	0.0158532940295458	0.4239372396995247	T	T	T
0.6082582547626469	0.1443830450841996	0.4337186281483730	T	T	T
0.8076822384821996	0.8613615833888710	0.3958734171431396	T	T	T
0.8053910330072404	0.9949782751831188	0.4081199376562231	T	T	T
0.8045498368164347	0.1274644388285181	0.4276655545088044	T	T	T
0.0111805187398607	0.9536445315358496	0.2159728826854882	T	T	T
0.0165450802088429	0.1340146900062738	0.2162282815522313	T	T	T
0.8620928395441406	0.0753673335404427	0.7639007975783310	T	T	T
0.8158907421877893	0.0499514683338180	0.5854626954976020	T	T	T
0.7004335093622241	0.0551208237447561	0.4899587380668631	T	T	T
0.5920685932824608	0.0761863069160616	0.6000316644822243	T	T	T
0.6052155231782724	0.0679423125850950	0.7964510166207965	T	T	T

Structure files (CONTCAR) involved in this work:

0.7312251295573772	0.0670684004643587	0.7347251458091060	T	T	T
0.8601071900035111	0.8361134635830331	0.7412048260735435	T	T	T
0.7840340461753733	0.8685612545108172	0.5878349004911373	T	T	T
0.6860779244956182	0.8396102193477580	0.4615884578051448	T	T	T
0.5957474201576338	0.8390153565716091	0.6055741760763425	T	T	T
0.5898848198357100	0.8467751304592304	0.8042764205748167	T	T	T
0.7301341540699569	0.8508237692154024	0.7692864644938787	T	T	T
0.8073174335889387	0.9567419892002282	0.7307348734992791	T	T	T
0.5846539494426656	0.9571846163223084	0.6895667371542601	T	T	T
0.9364025070861398	0.1345539294119734	0.9032372730365714	T	T	T
0.8886958111373096	0.0163044328735222	0.9377912227196301	T	T	T
0.9072860113451725	0.8878494548722313	0.9120928373559640	T	T	T
0.6941324348817862	0.1431565374750941	0.8899294180010525	T	T	T
0.7001639735463421	0.0096932915437536	0.9060595106608044	T	T	T
0.6826390099357672	0.8786893906311098	0.9643202064488724	T	T	T
0.4871046596038497	0.0472336078942461	0.7146018711264872	T	T	T
0.4822778148534016	0.8727798216365251	0.6976295334234071	T	T	T
0.3544609980314696	0.4371167548271969	0.7121285212888518	T	T	T
0.3024795097960963	0.4288879675974675	0.8928207188367920	T	T	T
0.2019838590429944	0.4455753887903465	0.0230350339191791	T	T	T
0.1044055540152822	0.4298018648495390	0.8890103527779392	T	T	T
0.1050820207337832	0.4492249169103439	0.6911176612388443	T	T	T
0.2292476257440071	0.4713392692829784	0.7403270023722924	T	T	T
0.3591886789785768	0.6693819501440716	0.7389827393361188	T	T	T
0.3070483335808505	0.6603302753852835	0.9173964751696756	T	T	T
0.1934423208197744	0.6458715384060020	0.0179952525310110	T	T	T
0.0955701656325016	0.6729396664058928	0.8912571218510916	T	T	T
0.1096144717554910	0.6549564504447815	0.6958182443243754	T	T	T
0.2322887284942277	0.6365108797797594	0.7566141204501462	T	T	T
0.3256597810761348	0.5492508036607199	0.8112929148921123	T	T	T
0.0846719996597613	0.5512465680732375	0.8173477035628973	T	T	T
0.4300432585495061	0.3720430147112522	0.5829217239045834	T	T	T
0.4196532171399925	0.5041205086546511	0.5669467117842577	T	T	T
0.4042637382253145	0.6369865735079329	0.5585189707808034	T	T	T
0.1978084044799030	0.3708316177601685	0.6143182980766055	T	T	T
0.1894410876270953	0.4969140822007996	0.5541053593404046	T	T	T
0.2040668366270523	0.6309176486265775	0.5608629487803753	T	T	T
0.9927496994700422	0.4549769925734685	0.7858777950101198	T	T	T
0.9909435397691945	0.6430672599210601	0.7773796177215164	T	T	T
0.1427716809871284	0.5609300905539842	0.2094577592118728	T	T	T
0.1970042493825542	0.5678158532962835	0.3887507268823203	T	T	T
0.3044785860571832	0.5530164611381940	0.5047799207116613	T	T	T
0.4147569599701650	0.5706932498639889	0.3944262128853592	T	T	T
0.3973654358630492	0.5522321815731948	0.1973433112510456	T	T	T
0.2708349211071743	0.5308699204265344	0.2356174728898099	T	T	T
0.1417176749873641	0.3276278359720086	0.2400714115904713	T	T	T
0.1923594283108015	0.3418273685703395	0.4193301447628154	T	T	T
0.3085362103184837	0.3496528053724255	0.5108855950940365	T	T	T
0.4151169435246596	0.3252030703973310	0.3990629793156532	T	T	T
0.3956592784536984	0.3394758898383158	0.2039074614585288	T	T	T
0.2704062359138835	0.3565610407158843	0.2592068185386560	T	T	T
0.1777326049025440	0.4483551366423704	0.3024789978170903	T	T	T
0.4114366709349890	0.4469125900866237	0.3206409117944670	T	T	T

Structure files (CONTCAR) involved in this work:

0.0686769446586252	0.6238669103582498	0.0736754402125022	T	T	T
0.0817510855861781	0.4921427760553290	0.0623004650719332	T	T	T
0.1013232512551141	0.3609364929417098	0.0568502201946057	T	T	T
0.3089494537650218	0.6284619751083655	0.1097680607719948	T	T	T
0.3202414872453447	0.4994801960709737	0.0568975142482737	T	T	T
0.3043171904394114	0.3657695730989129	0.0654734651945523	T	T	T
0.5128779190247791	0.5305940538470741	0.2791336239202772	T	T	T
0.5144456208503307	0.3675467102079343	0.2823342177553651	T	T	T
0.4420385839226373	0.7501095371151656	0.6420265238243890	T	T	T
0.2036336754639009	0.7465409438317691	0.6507160880661431	T	T	T
0.2737687836087798	0.7497496748784757	0.0559415720578243	T	T	T
0.1095470230320573	0.7481521852821057	0.0527750030676499	T	T	T
0.0591732733700351	0.2494628980381820	0.1392617848496171	T	T	T
0.3039054456762361	0.2481351991179164	0.1533969118654914	T	T	T
0.2238254869624661	0.2491459319117802	0.5553328910238253	T	T	T
0.3894458139029825	0.2473878412864121	0.5548583430237063	T	T	T
0.5616442349499455	0.2535379072572743	0.3535194344836825	T	T	T
0.8230019253302439	0.2535154650356751	0.3813622623185968	T	T	T
0.7226054121439882	0.2522881753225009	0.9978362585066182	T	T	T
0.9023660019090404	0.2547968612189957	0.9516763170862818	T	T	T
0.9176420385603098	0.7567804094824173	0.8774433459932753	T	T	T
0.6766059117065955	0.7457656140273359	0.8928115598149037	T	T	T
0.7825094268155404	0.7491885401390691	0.4988637560738604	T	T	T
0.5805710818675783	0.7564949169144130	0.4526376185367763	T	T	T
0.8030819537473582	0.6803832007622387	0.0756293095828631	T	T	T
0.7116431757448807	0.7755948561494340	0.1184896430385127	T	T	T
0.8437539518507470	0.8025150953633511	0.0491773829629725	T	T	T
0.8431436659306991	0.7501038364674462	0.2505362042495272	T	T	T
0.7183996460494140	0.7051815092273823	0.0393869845237145	T	T	T
0.7604132513331948	0.8347703317951941	0.0480761420260661	T	T	T
0.8609986861340995	0.7232851441136899	0.9917786138190765	T	T	T
0.5070000841926088	0.6338399755925027	0.4040987268360435	T	T	T
0.9281940799990248	0.7950583070073860	0.1902215565138894	T	T	T
0.9352691445245850	0.7066342734052944	0.2126649891154586	T	T	T
0.9340296286305853	0.7643356727519631	0.3160350436473305	T	T	T
0.8247724725893305	0.7283005140463943	0.1897932583291228	T	T	T
0.9133806179257078	0.7538340805974092	0.2415687242178007	T	T	T

Figure S8(c)

Si Al O Ga H C

1.0000000000000000

20.0219993591000005 0.0000000000000000 0.0000000000000000

0.0000000000000000 19.8990001678000006 0.0000000000000000

0.0000000000000000 0.0000000000000000 13.3830003737999998

93 3 193 1 6 1

Selective dynamics

Direct

0.4228461839733048	0.0570464701696785	0.6484364076567007	T	T	T
0.3017041061233214	0.0266314690503789	0.7890858411001191	T	T	T
0.2803922657960626	0.0606738634761619	0.0124952765507144	T	T	T
0.1207842957991498	0.0640514753950139	0.0133358623653382	T	T	T
0.0681931886335980	0.0299218895927032	0.8003243621875501	T	T	T
0.1770463044524594	0.0557749761573448	0.6509349625155686	T	T	T
0.4200777542291462	0.8271127583466942	0.6699948067165838	T	T	T

Structure files (CONTCAR) involved in this work:

0.3025204586130893	0.8684238484332333	0.8093190114893799	T	T	T
0.2679095095462612	0.8284874482773812	0.0297754025796722	T	T	T
0.1128420460688014	0.8267575458908832	0.0172663854551406	T	T	T
0.0622602492754164	0.8706762469196039	0.8029965252880394	T	T	T
0.1796646966505967	0.8283992916691251	0.6731781087288864	T	T	T
0.0758911479939165	0.9431482477774052	0.1504691825117820	T	T	T
0.1969651103952595	0.9732167322057199	0.2927718705901863	T	T	T
0.2173350898246607	0.9373227912033274	0.5139248383980985	T	T	T
0.3768306260782046	0.9340619772316432	0.5156286808165650	T	T	T
0.4306601622348320	0.9696023106384556	0.3047519470904793	T	T	T
0.3214592868501682	0.9451260612021515	0.1548827571753742	T	T	T
0.0785833012410732	0.1729571323331435	0.1657599701227089	T	T	T
0.1964663346917462	0.1305235774627526	0.3074396092743380	T	T	T
0.2320235927452416	0.1730488172383717	0.5250793199525906	T	T	T
0.3866374051811897	0.1737739942427757	0.5130643267495054	T	T	T
0.4370537102170153	0.1278317186885743	0.3024071239005054	T	T	T
0.3194342847400459	0.1677609032750669	0.1710417312857911	T	T	T
0.5829709050931469	0.5555887174922411	0.3492033091488777	T	T	T
0.6947200977851431	0.5298672996829644	0.1879121103954759	T	T	T
0.7145243172674183	0.5647230787525270	0.9730610977589008	T	T	T
0.8730145064180206	0.5600454551724475	0.9773485070710038	T	T	T
0.9356355248003457	0.5284837812437211	0.1875467332279201	T	T	T
0.5781715889488169	0.3288903109921539	0.3340783080024624	T	T	T
0.7065224366561497	0.3738947725793308	0.2126071844598433	T	T	T
0.7349686305042027	0.3291723773431927	0.9932206254263289	T	T	T
0.8866391550478879	0.3279660544085506	0.9826601400944323	T	T	T
0.9376049996176379	0.3717940622998056	0.1994262034056849	T	T	T
0.9277308592565400	0.4375420457603051	0.8428974478365163	T	T	T
0.7820073710349669	0.4394759878970159	0.4810731708728597	T	T	T
0.6226321424645559	0.4317046307406400	0.4914122529125855	T	T	T
0.5681172628030031	0.4669377366136553	0.7071658222776911	T	T	T
0.6734751463612265	0.4348896183782427	0.8537840785848133	T	T	T
0.9188941652839047	0.6722340466701178	0.8292767637205452	T	T	T
0.8004357300691229	0.6323724840820842	0.6971855328478705	T	T	T
0.7707736755142421	0.6690406241760143	0.4789793975140435	T	T	T
0.6147373510699766	0.6703485997193200	0.4858242696476541	T	T	T
0.5664389183266628	0.6256327441082397	0.7042569702189169	T	T	T
0.6827381362639540	0.6813530686271435	0.8250666665280096	T	T	T
0.5754197555121841	0.9431390651544103	0.3648195793528308	T	T	T
0.6952168299148430	0.9728575362077634	0.2211442004387597	T	T	T
0.7183393026440401	0.9425726976613871	0.9989532679796990	T	T	T
0.8783804669423007	0.9339483799564957	0.9953874754153871	T	T	T
0.9313671211270785	0.9697764541042060	0.2067270143183059	T	T	T
0.8206453326942326	0.9405251542782141	0.3547077909408693	T	T	T
0.5811315495543699	0.1742180639656830	0.3357606700880203	T	T	T
0.6985787108265599	0.1307653921709463	0.2001868967809078	T	T	T
0.7318435545329560	0.1727644269751075	0.9792037226484508	T	T	T
0.8860888687310925	0.1733336329357848	0.9954230515860157	T	T	T
0.9340698806549320	0.1282634701311348	0.2070682587996659	T	T	T
0.8191513119514310	0.1689626467203443	0.3406180777245520	T	T	T
0.9241685847644080	0.0580028969249039	0.8627933897791157	T	T	T
0.8052125642279726	0.0299332003929311	0.7232582483176205	T	T	T
0.7811464355650996	0.0576027641897794	0.4973602087998349	T	T	T

Structure files (CONTCAR) involved in this work:

0.6213182384990549	0.0670608468138992	0.4949062390365232	T	T	T
0.5678228950236793	0.0323522384414629	0.7034107543808507	T	T	T
0.6779983727858306	0.0583799123934187	0.8543309236792924	T	T	T
0.9180064193745472	0.8252141961631604	0.8400113083332973	T	T	T
0.8030675100675987	0.8741530937952199	0.7055407794546471	T	T	T
0.7685854286829429	0.8304031766896275	0.4883593603497115	T	T	T
0.6133079877292341	0.8256233157012134	0.4973053512248328	T	T	T
0.5627907237850405	0.8755533821253610	0.7038027564325664	T	T	T
0.6782672376634692	0.8376062075198706	0.8374151617107058	T	T	T
0.4235385240918620	0.4453891018629770	0.6410753638182219	T	T	T
0.3033824266505428	0.4738429449601351	0.7875569599879179	T	T	T
0.2860182205575330	0.4336579884556724	0.0067748013444973	T	T	T
0.1286284448920542	0.4321522580416349	0.0045494022451518	T	T	T
0.0764177282876692	0.4725437819954854	0.7974362512114297	T	T	T
0.1819585701550769	0.4497613615888898	0.6436846483147928	T	T	T
0.4248005040987001	0.6721754777363824	0.6629450109370748	T	T	T
0.3024331890905196	0.6305373991130125	0.7995802792513326	T	T	T
0.2706040916717867	0.6725494776873374	0.0182823636716997	T	T	T
0.1163823207522222	0.6738255555317429	0.0081510572396289	T	T	T
0.0665926982450350	0.6299343167409258	0.7989316592843974	T	T	T
0.1802531927331420	0.6698644804206123	0.6626237291605949	T	T	T
0.0805849542379519	0.5538520815128397	0.1356395094208119	T	T	T
0.2019248982588017	0.5279216323139686	0.2804126975104657	T	T	T
0.2227349299614667	0.5677831185852963	0.5015848009026355	T	T	T
0.3833026748774104	0.5692538334483687	0.5046323117732768	T	T	T
0.4345525974860560	0.5274115588033451	0.2954196749239966	T	T	T
0.3287333560845260	0.5526244748004373	0.1416903243801487	T	T	T
0.0822770840468978	0.3280313340314765	0.1568169407271710	T	T	T
0.1982184938347741	0.3698981861024854	0.3026433022732088	T	T	T
0.2329748461779009	0.3296129219208736	0.5220240413998974	T	T	T
0.3874044851658635	0.3271868798603425	0.5098904590639548	T	T	T
0.4353379581926017	0.3701096470106523	0.2954841106860396	T	T	T
0.3191706972652200	0.3261798140464307	0.1659017305175290	T	T	T
0.8100124550462841	0.5642354477092443	0.3278730058603876	T	T	T
0.8299348993126310	0.3280446517148064	0.3475424333984548	T	T	T
0.7974929447548375	0.4721091654038091	0.7252233712258263	T	T	T
0.3572951772766013	0.0623470164697335	0.7191521816174036	T	T	T
0.2994501566740820	0.0658221605640476	0.8951877569015236	T	T	T
0.2003217254901787	0.0517375267609215	0.0285280790313307	T	T	T
0.1021979839261225	0.0670791151567778	0.8957826258192390	T	T	T
0.1024183104015212	0.0572165732903565	0.6981212402437239	T	T	T
0.2286783148891639	0.0315187329453838	0.7372838685865203	T	T	T
0.3580867033725486	0.8260948887787238	0.7481021735530675	T	T	T
0.3046662063018591	0.8432723207889951	0.9241926421621921	T	T	T
0.1901304537656255	0.8521198605091916	0.0211207100596670	T	T	T
0.0850578552832567	0.8320380711599714	0.9041444364146904	T	T	T
0.1023196017086502	0.8382287300135732	0.7084215579397077	T	T	T
0.2285904422129803	0.8548206365295228	0.7623225361526403	T	T	T
0.3206103984076273	0.9478657430542261	0.8041801776967785	T	T	T
0.0806782380902000	0.9496570515393342	0.8120766808215003	T	T	T
0.4311631033828188	0.1265778381172170	0.5857938406098300	T	T	T
0.4169789032462278	0.9948322454040133	0.5699610554147003	T	T	T
0.3972230914531840	0.8628192277667303	0.5662139656496497	T	T	T

Structure files (CONTCAR) involved in this work:

0.1947994366531056	0.1308283006999315	0.6121762135947344	T	T	T
0.1790842017325531	0.0030213763590635	0.5581276806349401	T	T	T
0.1931005844986002	0.8692575144540244	0.5702076353938926	T	T	T
0.9892212783641248	0.0469686345257784	0.7923974604429695	T	T	T
0.9822869846422728	0.8612192329270569	0.7872159907011955	T	T	T
0.1419949780828332	0.9392754788976941	0.2199431120989642	T	T	T
0.1985971329556457	0.9307777468823343	0.3964535435771869	T	T	T
0.2972387331950896	0.9473680013911810	0.5295069152665366	T	T	T
0.3963955296445935	0.9302945986871973	0.3983655981429539	T	T	T
0.3963402779183381	0.9452480989289628	0.2009144434830683	T	T	T
0.2701804381837326	0.9705031681293962	0.2411943388979185	T	T	T
0.1416833224380329	0.1705698109633640	0.2415473018710987	T	T	T
0.1948173103008106	0.1623234902681910	0.4187482100384849	T	T	T
0.3092452677983790	0.1481732610231868	0.5161109500450782	T	T	T
0.4140054025439734	0.1708779685006558	0.3994658477806487	T	T	T
0.3966418132426629	0.1557292144933661	0.2050178455410821	T	T	T
0.2705571860448736	0.1394721435014044	0.2590847304572941	T	T	T
0.1773661549124329	0.0512562111197341	0.3133179956512240	T	T	T
0.4185589673913842	0.0495526683044583	0.3213358684768188	T	T	T
0.0675947476913925	0.8717580764797255	0.0922233479475398	T	T	T
0.0811269252437653	0.0027284634088287	0.0674083947499198	T	T	T
0.0982651268237629	0.1350906533203231	0.0622569199399371	T	T	T
0.3037704886368188	0.8692288054395231	0.1195541434965532	T	T	T
0.3179392804929738	0.9953356990314957	0.0591426519795451	T	T	T
0.3051843846264639	0.1292037489523304	0.0664449860824353	T	T	T
0.5095438863883801	0.9526707884199891	0.2956672499119457	T	T	T
0.5169042035151152	0.1364226358047970	0.2852804101466491	T	T	T
0.6433921608446030	0.5614354135114590	0.2700822631105924	T	T	T
0.6785327503116598	0.5661755137408018	0.0814018461607439	T	T	T
0.7938821301906990	0.5464943132679924	0.9854801058495398	T	T	T
0.9072582098000217	0.5630697779533047	0.0880067321627921	T	T	T
0.9003247806419320	0.5678922118198574	0.2877054431784940	T	T	T
0.7705796201568520	0.5468361926908880	0.2182218190716680	T	T	T
0.6433364552719604	0.3358159592914079	0.2646738593888049	T	T	T
0.7245537192306117	0.3303393978275326	0.1128670131230005	T	T	T
0.8106771522476706	0.3555577253824644	0.9660243379976750	T	T	T
0.9094363362362258	0.3383822698227195	0.0970923084572986	T	T	T
0.9092931466346046	0.3351295500517658	0.2960499827374485	T	T	T
0.7698873796040892	0.3761862779807033	0.2859828768811210	T	T	T
0.6822397650389541	0.4490155410900860	0.1792193056194553	T	T	T
0.9149348501875094	0.4515801309838324	0.1990650879484464	T	T	T
0.5715973609546100	0.6272959070743674	0.4051754158039836	T	T	T
0.6001895007583659	0.4999679068584847	0.4345372557998367	T	T	T
0.5876904316020658	0.3669335049225900	0.4406812874683054	T	T	T
0.8071943366109028	0.6435110666592094	0.3790029518494045	T	T	T
0.8025249734243173	0.5029492595014918	0.4167896732194072	T	T	T
0.8322443825291966	0.3735069878580776	0.4653254053054331	T	T	T
0.0141309225211352	0.5439947182977174	0.2049082217845096	T	T	T
0.0192037925492429	0.3714496854422673	0.1967833274203638	T	T	T
0.8739146100878940	0.4290767376156810	0.7525065761965420	T	T	T
0.8105009061226075	0.4516046541535411	0.5971868498746007	T	T	T
0.7034214379041782	0.4229481353215715	0.4856370354447721	T	T	T
0.5989515298408786	0.4340290305792998	0.6064320578893906	T	T	T

Structure files (CONTCAR) involved in this work:

0.5990773667957616	0.4294786716942415	0.8042164340365725	T	T	T
0.7304252744085582	0.4286622283889228	0.7696565669168419	T	T	T
0.8643567758492844	0.6744176273973947	0.7404178054973342	T	T	T
0.8068601479804467	0.6343431100618547	0.5759549448806968	T	T	T
0.6922406684989545	0.6463550297558099	0.4805715847709116	T	T	T
0.5859169196588302	0.6582895277364113	0.5973609683714363	T	T	T
0.6059696302997672	0.6639612033731318	0.7938430639300242	T	T	T
0.7307451678873611	0.6698203143370142	0.7279761422915304	T	T	T
0.8023136435803825	0.5573201565361342	0.7416715006293831	T	T	T
0.5862022459397341	0.5466649318632739	0.7069727749555023	T	T	T
0.9362279382369694	0.3693307327619107	0.9077766324418808	T	T	T
0.9078964223318136	0.4989746277282788	0.9162237734048176	T	T	T
0.8904989396888552	0.6312366605416129	0.9252124255031582	T	T	T
0.6803993155316987	0.3760074114790272	0.9375957409780189	T	T	T
0.6779524059956054	0.5085894115121341	0.9058496605394180	T	T	T
0.7075209460921956	0.6375398119042909	0.9200747026234815	T	T	T
0.4876182202723073	0.4572058415914271	0.7120630542758379	T	T	T
0.4861529153549713	0.6350699841955103	0.7207027093166248	T	T	T
0.6406957701466987	0.9376574350775797	0.2936556512378837	T	T	T
0.6938847540298057	0.9352841926070686	0.1136880581419002	T	T	T
0.7990388146108575	0.9496022104658851	0.9906796594547203	T	T	T
0.9027903185903638	0.9288648914750366	0.1105797739061708	T	T	T
0.8956529930043400	0.9431446309522884	0.3082589927686594	T	T	T
0.7695270619959390	0.9645436079475863	0.2675781107559502	T	T	T
0.6425763975302553	0.1748536491312608	0.2575534779477483	T	T	T
0.6969892749840890	0.1542404306403187	0.0846194533829048	T	T	T
0.8094154518798766	0.1474851198707177	0.9834321880107240	T	T	T
0.9084572320332749	0.1719794266574005	0.1117305825505226	T	T	T
0.8968121768158190	0.1542987786756594	0.3071413346759038	T	T	T
0.7720087000146673	0.1419437655159342	0.2484329555089526	T	T	T
0.6775230946765627	0.0519302277236043	0.2087502426499560	T	T	T
0.9175954881380805	0.0492261952123172	0.1879765197907229	T	T	T
0.5670586282314013	0.8738447934738731	0.4280575317425598	T	T	T
0.5803922559722764	0.0059686029542785	0.4422369075936325	T	T	T
0.6036488132852026	0.1370585136963645	0.4386350908835954	T	T	T
0.8041727536620131	0.8641142344874952	0.3909618737812602	T	T	T
0.8155863257338205	0.9907757765347707	0.4499942192383598	T	T	T
0.8046186505958267	0.1248903801524339	0.4407878430247393	T	T	T
0.0109194977494033	0.9555127935264088	0.2202581667258524	T	T	T
0.0146121048668439	0.1378894888760313	0.2193288852519525	T	T	T
0.8588988520961226	0.0693591485935012	0.7927376746157131	T	T	T
0.8053233027833318	0.0628676850750598	0.6128305682425893	T	T	T
0.7004069964102135	0.0498770960740961	0.4891517920135691	T	T	T
0.5982118461312130	0.0754317493163438	0.6106562179646893	T	T	T
0.6032868694989865	0.0536358998746871	0.8077715294185717	T	T	T
0.7302427621593125	0.0356375630531289	0.7679697524576163	T	T	T
0.8554533713655330	0.8255668874139167	0.7631415516617225	T	T	T
0.8056932155259038	0.8582825768073025	0.5875624493271687	T	T	T
0.6901546072759112	0.8520468106827438	0.4913071872321837	T	T	T
0.5873710944956677	0.8278912799387259	0.6123081278563777	T	T	T
0.6013716142262985	0.8531731365120965	0.8052991505718252	T	T	T
0.7277042317714600	0.8625672753768451	0.7477280009976809	T	T	T
0.8269492659463906	0.9512613996052734	0.7229219502756076	T	T	T

Structure files (CONTCAR) involved in this work:

0.5802907195555509	0.9533038147204914	0.6782064896711829	T	T	T
0.9350297210138523	0.1251355489420221	0.9301699048987263	T	T	T
0.9174205908463626	0.9936856720624435	0.9369423091538636	T	T	T
0.8968969579745758	0.8625441332362445	0.9432550810648705	T	T	T
0.6928046200351650	0.1349768290904220	0.8889493216339948	T	T	T
0.6840482969956311	0.0091211325042471	0.9508129694093825	T	T	T
0.6948720307988716	0.8754848191548100	0.9411242179329625	T	T	T
0.4884995764064584	0.0470136115798971	0.7175833215253109	T	T	T
0.4826881147489392	0.8667859508969491	0.7204927206451466	T	T	T
0.3571680642771076	0.4429346198394392	0.7104367829595006	T	T	T
0.3025716680586361	0.4283099044168388	0.8882606377382627	T	T	T
0.2067858947388403	0.4494461688027366	0.0235322904074091	T	T	T
0.1125482902001245	0.4298306211287936	0.8853108606245306	T	T	T
0.1051881727141532	0.4535214036535866	0.6863464176623416	T	T	T
0.2300210928624166	0.4719884473869425	0.7352288300044687	T	T	T
0.3580603936426792	0.6660140845440057	0.7306139766511539	T	T	T
0.3020076692287828	0.6683654034612843	0.9066746276076643	T	T	T
0.1931089080243462	0.6470450384666759	0.0145193950463609	T	T	T
0.0921117322559319	0.6749831593997605	0.8923885055657116	T	T	T
0.1031437449622562	0.6553100065988294	0.6968584616475281	T	T	T
0.2293148021432361	0.6372667126184069	0.7468254333074471	T	T	T
0.3201964946639959	0.5514898548818523	0.8155829574667558	T	T	T
0.0860485193260711	0.5518290558151658	0.8207031416025458	T	T	T
0.4320767623426808	0.3745771576368393	0.5822258179420727	T	T	T
0.4181434794448092	0.5052060406842634	0.5587020524818542	T	T	T
0.4110377852946969	0.6381949540554456	0.5542112283868668	T	T	T
0.1957388973790491	0.3733823237501933	0.6081521543865567	T	T	T
0.1884992241364632	0.5006329578907530	0.5493696814552005	T	T	T
0.1926478771850312	0.6348286415827629	0.5543648289228853	T	T	T
0.9981015089888179	0.4535155082276690	0.7872291638149732	T	T	T
0.9862710802782275	0.6359932222125719	0.7852816180947321	T	T	T
0.1448730856536926	0.5598210060500174	0.2081790911925234	T	T	T
0.2034514987820596	0.5707570580931792	0.3838834882491338	T	T	T
0.3027281118761389	0.5639104900787120	0.5192736972570681	T	T	T
0.4022199514886305	0.5700221506636822	0.3872742255204872	T	T	T
0.4024785927802541	0.5554948815526994	0.1916914445751236	T	T	T
0.2742067444402042	0.5328617070801539	0.2271042539804496	T	T	T
0.1412325549950860	0.3312971333814654	0.2395852819413155	T	T	T
0.1955651023467686	0.3411695642910071	0.4157967691261424	T	T	T
0.3102335411344694	0.3539913965512365	0.5125741495904602	T	T	T
0.4140344099491320	0.3293086228741353	0.3957823654103079	T	T	T
0.3960125569267172	0.3391733972153173	0.1994213698407058	T	T	T
0.2711360002646586	0.3567211223514487	0.2533115315634817	T	T	T
0.1831261324888877	0.4502148666148045	0.3039613420430134	T	T	T
0.4151261124249876	0.4486292440324847	0.3102470473455082	T	T	T
0.0701108856165578	0.6230795019717394	0.0734385759969855	T	T	T
0.0848493650596981	0.4912660185341344	0.0577845460494370	T	T	T
0.1089987109613429	0.3597013904337805	0.0514520803465769	T	T	T
0.3122460507175330	0.6258666228663936	0.0949366612598135	T	T	T
0.3282167024764462	0.4954259462519731	0.0547630717859366	T	T	T
0.3047430138452422	0.3626669862664305	0.0592480706965912	T	T	T
0.5147344735099791	0.5360822590223900	0.2904147458400326	T	T	T
0.5146589972129874	0.3618431917742366	0.2750963855591467	T	T	T

Structure files (CONTCAR) involved in this work:

0.4417405395521665	0.7506479894023040	0.6443401991048925	T	T	T
0.1938361363227099	0.7495171169903592	0.6508936331450285	T	T	T
0.2736461982733687	0.7493570812282049	0.0576382876532237	T	T	T
0.1087799974606943	0.7488193510853903	0.0536773696978545	T	T	T
0.0615734336382361	0.2505041384972863	0.1377049687857873	T	T	T
0.3049518409403894	0.2468109425193908	0.1518655451944901	T	T	T
0.2280749205377576	0.2517815016745847	0.5558900332306241	T	T	T
0.3914883653341236	0.2508796630127376	0.5519109814609092	T	T	T
0.5615105579814834	0.2512098692886142	0.3609830379269838	T	T	T
0.8061949187557014	0.2460397622253111	0.3655704726572476	T	T	T
0.7273586305186285	0.2521947790248572	0.9548415443386973	T	T	T
0.8927000098413218	0.2493531601856968	0.9529763692320437	T	T	T
0.9369003142577043	0.7477141448651728	0.8662914034269781	T	T	T
0.6880174593979974	0.7587314397617742	0.8596972197378375	T	T	T
0.7763852281045903	0.7500684420148970	0.4851790758124656	T	T	T
0.6075967718673120	0.7491755367754785	0.4567702725169424	T	T	T
0.9594221004951194	0.4524145457431856	0.5636481893139118	T	T	T
0.8838239406159450	0.3875946794137209	0.5977245010919195	T	T	T
0.9162450392551276	0.3195153754632089	0.6242336636945821	T	T	T
0.9199956127504612	0.6109882336561006	0.3062619857297424	T	T	T
0.9491113522898941	0.5415765341601115	0.6483937830051588	T	T	T
0.9066792864575368	0.5389716271793246	0.5298131535092075	T	T	T
-0.0036846600411845	0.5485555038465098	0.5342525814324884	T	T	T
0.0005266805036118	0.4396613246301482	0.5991072272506037	T	T	T
0.9524208545166385	0.5257994774309863	0.5699551638342719	T	T	T

Figure S8(d)

Si Al O Ga H C

1.0000000000000000

20.0219993591000005 0.0000000000000000 0.0000000000000000

0.0000000000000000 19.8990001678000006 0.0000000000000000

0.0000000000000000 0.0000000000000000 13.3830003737999998

93 3 193 1 6 1

Selective dynamics

Direct

0.4230721518083905	0.0577199150539027	0.6484945524408524	T	T	T
0.3019721394209428	0.0274364379381448	0.7892180741002869	T	T	T
0.2803645042063462	0.0612243306268431	0.0127305868921900	T	T	T
0.1206386586345372	0.0648182625072978	0.0138254331170983	T	T	T
0.0679890685461111	0.0308148241443360	0.8008334837751454	T	T	T
0.1769328575894716	0.0566290226172651	0.6514376743948620	T	T	T
0.4197268587873596	0.8274046393716641	0.6701831703487300	T	T	T
0.3025252538530502	0.8692060013002663	0.8098114695497258	T	T	T
0.2677285095428124	0.8293433767060048	0.0300169827759307	T	T	T
0.1127307963650902	0.8274759570152116	0.0167422279887505	T	T	T
0.0621570240874237	0.8718335324116319	0.8028703741460491	T	T	T
0.1797011125757284	0.8292576096723883	0.6741844525366101	T	T	T
0.0757393681425169	0.9435782573850006	0.1508633745750244	T	T	T
0.1966918005909424	0.9737043146385459	0.2934847200196355	T	T	T
0.2173627723694643	0.9379964230172551	0.5147404080061193	T	T	T
0.3767152760660687	0.9348341078047246	0.5160253954444416	T	T	T
0.4304536903765734	0.9703699808998100	0.3053973219666040	T	T	T
0.3211610775374902	0.9457346800358759	0.1554607039155385	T	T	T
0.0785421796561985	0.1732602680702184	0.1664366414499327	T	T	T

Structure files (CONTCAR) involved in this work:

0.1965060406660357	0.1308965320310185	0.3077499424906425	T	T	T
0.2317833262534751	0.1738993649761759	0.5252016281604892	T	T	T
0.3865305009739839	0.1745661715519141	0.5132683366549020	T	T	T
0.4371637453037435	0.1285565226868347	0.3029921884538773	T	T	T
0.3195097854408869	0.1678105040337091	0.1717041651999490	T	T	T
0.5809995605206347	0.5552761019016289	0.3523900097494134	T	T	T
0.6956556797078599	0.5274747779374669	0.1929880268008814	T	T	T
0.7137966477098625	0.5659299295633384	0.9800374317660221	T	T	T
0.8728845337016692	0.5639516914233763	0.9823381567798227	T	T	T
0.9345728682004115	0.5307101326879652	0.1894827027064008	T	T	T
0.5776042657055308	0.3296654254014915	0.3382979081765336	T	T	T
0.7047980313796682	0.3732630873427553	0.2107298217332673	T	T	T
0.7322719358567594	0.3276095903448814	0.9947277715074556	T	T	T
0.8845282337161114	0.3286370323319539	0.9915989692072750	T	T	T
0.9360567663929731	0.3732193788990492	0.2044194339955868	T	T	T
0.9266600825280039	0.4398345206675301	0.8540492910748171	T	T	T
0.7784612356611820	0.4372424499226199	0.4884187230376169	T	T	T
0.6179960819139287	0.4332449064848947	0.4955338581274854	T	T	T
0.5670588449298609	0.4684259213410330	0.7113943633978791	T	T	T
0.6706833196835719	0.4367761918450372	0.8607811205528818	T	T	T
0.9184385276958291	0.6735252417915675	0.8307971275863522	T	T	T
0.8007388609231761	0.6327725385991977	0.6982934928634358	T	T	T
0.7703316579833270	0.6692348916671552	0.4790093038434661	T	T	T
0.6144977552975345	0.6710204796231346	0.4864247362115739	T	T	T
0.5655747306546518	0.6269347638734517	0.7048150609935802	T	T	T
0.6819280326800318	0.6809351391067573	0.8267380038024367	T	T	T
0.5753240302141015	0.9433042516127517	0.3651005466519178	T	T	T
0.6946615362220945	0.9733000396232360	0.2215789738208779	T	T	T
0.7187102095457011	0.9421037934984814	0.9996072975615681	T	T	T
0.8785371105314895	0.9346529896543808	0.9955926892175492	T	T	T
0.9310319802243455	0.9699034433108816	0.2063908501251743	T	T	T
0.8203578044498990	0.9433932640108925	0.3562436249772919	T	T	T
0.5812861061323350	0.1746844105714313	0.3370452183513518	T	T	T
0.6975162662636027	0.1298309297010993	0.1999474957561832	T	T	T
0.7318559203281073	0.1722592393439770	0.9794552645499101	T	T	T
0.8859627861103299	0.1743549983038409	0.9957518402884283	T	T	T
0.9345634909453839	0.1278403700723194	0.2063876021234946	T	T	T
0.8186969585350728	0.1677628887155187	0.3379821830694325	T	T	T
0.9239689035651382	0.0587219072661346	0.8634749574458201	T	T	T
0.8046285935896454	0.0298305576561924	0.7232800013417187	T	T	T
0.7813080180730468	0.0599401293534679	0.4984211461177437	T	T	T
0.6215973846699797	0.0673026044964585	0.4953486145497868	T	T	T
0.5679794300689299	0.0320639200321431	0.7039449955441525	T	T	T
0.6777417106389410	0.0570947467455449	0.8556384813317433	T	T	T
0.9184727474734672	0.8262944951139680	0.8398064285351687	T	T	T
0.8029423748402160	0.8739350003614058	0.7047025454436393	T	T	T
0.7680977168526901	0.8306050525535560	0.4868751050966345	T	T	T
0.6131624079437662	0.8260719799359577	0.4977944624173942	T	T	T
0.5627517471640866	0.8750844495197140	0.7046473033986043	T	T	T
0.6786464857429130	0.8373566509728472	0.8379507003568833	T	T	T
0.4227036735466519	0.4461227473965200	0.6433132291153834	T	T	T
0.3032424957531599	0.4746821325862445	0.7905299910474499	T	T	T
0.2857622454009853	0.4337738370484011	0.0092907422694941	T	T	T

Structure files (CONTCAR) involved in this work:

0.1283298155930930	0.4326672182899550	0.0074568525944566	T	T	T
0.0747465758941253	0.4720399416145114	0.8011542433071560	T	T	T
0.1822321370607887	0.4505190287194692	0.6475067669232925	T	T	T
0.4237505384315733	0.6725247127747113	0.6628751636951984	T	T	T
0.3016830448859609	0.6311741918550778	0.8001973726632055	T	T	T
0.2698404853248574	0.6734491801243514	0.0182568812655858	T	T	T
0.1158292918472391	0.6744426819378824	0.0077069169358048	T	T	T
0.0654430422426468	0.6299276894904434	0.7987747530213533	T	T	T
0.1795020983482498	0.6705626978223291	0.6638237490464801	T	T	T
0.0798416622543049	0.5553132330181780	0.1365136269291199	T	T	T
0.2007924273741793	0.5291673430344002	0.2812005237941956	T	T	T
0.2214063941789945	0.5684063751328015	0.5035294252979130	T	T	T
0.3820681273980745	0.5689303546385397	0.5052265527496995	T	T	T
0.4341107921930571	0.5286499003916770	0.2951242202149641	T	T	T
0.3277122088101742	0.5538477412473323	0.1427325865773418	T	T	T
0.0809711265260772	0.3283799495649308	0.1592200289159112	T	T	T
0.1975878361242586	0.3707619979181143	0.3032965510270616	T	T	T
0.2329934386939356	0.3307878755037790	0.5228129330359340	T	T	T
0.3874944781313453	0.3281204543769650	0.5115122919732537	T	T	T
0.4356490608900567	0.3709012584026627	0.2965708748401028	T	T	T
0.3190375251933821	0.3260894609592765	0.1678370577259951	T	T	T
0.8110145932843927	0.5592589526263853	0.3353894347324973	T	T	T
0.8268784320714220	0.3288480471233780	0.3459347396247501	T	T	T
0.7971017031438092	0.4715068522950833	0.7298062533776190	T	T	T
0.3575926256519585	0.0632183396482458	0.7193965995484748	T	T	T
0.2997252728941657	0.0663699906872954	0.8955636021941822	T	T	T
0.2002560378082838	0.0527197213708991	0.0286655163812513	T	T	T
0.1018558363657508	0.0679541147478992	0.8964041062033632	T	T	T
0.1023639224864269	0.0582580831454864	0.6987703631992164	T	T	T
0.2289097649500328	0.0329011615685679	0.7376210595381893	T	T	T
0.3576875946227472	0.8265471041085740	0.7482665066308641	T	T	T
0.3049849147011356	0.8443355533747320	0.9248629861083703	T	T	T
0.1900071397745918	0.8529483809048243	0.0205539698499590	T	T	T
0.0847807934747123	0.8327268645643361	0.9037388393710842	T	T	T
0.1022423136197896	0.8395191889995782	0.7082401475429428	T	T	T
0.2283130563080571	0.8559140019830269	0.7635805632646091	T	T	T
0.3207801006569244	0.9486273641175174	0.8039572512509360	T	T	T
0.0810071257776264	0.9506551156930909	0.8127408615111572	T	T	T
0.4311255824244706	0.1272348289445465	0.5856497979621896	T	T	T
0.4171866563586364	0.9954993710976056	0.5700526498214635	T	T	T
0.3970734100495368	0.8636747184865329	0.5667522523443002	T	T	T
0.1943488414215895	0.1316986810083055	0.6120063602783663	T	T	T
0.1788461212257010	0.0035241964334174	0.5590817021033899	T	T	T
0.1937372655199775	0.8696793544047435	0.5709595056222411	T	T	T
0.9889506897180096	0.0474599577778520	0.7928108382028273	T	T	T
0.9822633458002252	0.8628524947254418	0.7864613341326814	T	T	T
0.1416470997061741	0.9396945270681361	0.2208610121783758	T	T	T
0.1985561896902314	0.9314095267220126	0.3972678417256816	T	T	T
0.2972184517749415	0.9485111886476867	0.5302859265110398	T	T	T
0.3959393211027721	0.9308677924525053	0.3986340827761479	T	T	T
0.3960528913707458	0.9463312235140627	0.2014150205317424	T	T	T
0.2698382068212292	0.9711961881502503	0.2416634734038501	T	T	T
0.1420395101644950	0.1711417494605396	0.2415782086959575	T	T	T

Structure files (CONTCAR) involved in this work:

0.1947742674596961	0.1634107236112133	0.4186691907752470	T	T	T
0.3090260609790487	0.1491922259686700	0.5165930702475663	T	T	T
0.4136974628262195	0.1720244774613687	0.3995353715472438	T	T	T
0.3968134593184067	0.1560038231193080	0.2052416686891042	T	T	T
0.2707537123598810	0.1391732138235418	0.2596768566139883	T	T	T
0.1770305015534677	0.0517645276619283	0.3142311669495966	T	T	T
0.4186126338479100	0.0503315777507669	0.3225202883477842	T	T	T
0.0677145992225351	0.8724376923116701	0.0919519272278928	T	T	T
0.0811771342655082	0.0036284075742289	0.0685486613779331	T	T	T
0.0981228441320750	0.1359795547798354	0.0624939922456049	T	T	T
0.3034234610255304	0.8698083069551994	0.1203018493451044	T	T	T
0.3175504148941884	0.9957160596633884	0.0594533506422670	T	T	T
0.3053288508345760	0.1296666558685434	0.0667872593610522	T	T	T
0.5092626137411252	0.9531755850123651	0.2963889119948136	T	T	T
0.5170070324820154	0.1372004137011287	0.2860382797006664	T	T	T
0.6449885923354081	0.5550239094449934	0.2794400400080567	T	T	T
0.6820758146251741	0.5709701426160283	0.0914493222480578	T	T	T
0.7938095471271950	0.5481589445412755	0.9857641419220825	T	T	T
0.9036923128497326	0.5699549073626077	0.0954795737976429	T	T	T
0.9014282889389313	0.5654316878545045	0.2949802225858521	T	T	T
0.7716723595929535	0.5397530864542440	0.2265622114470582	T	T	T
0.6439733589176507	0.3381506854724952	0.2724900883069534	T	T	T
0.7172601500438315	0.3254934915622684	0.1133738174228931	T	T	T
0.8083971547015262	0.3558189444414555	0.9749124084962129	T	T	T
0.9053251386525963	0.3339582288775211	0.1083041315779294	T	T	T
0.9091757655743069	0.3430970635152116	0.3072078059345786	T	T	T
0.7710311323126388	0.3772634701154629	0.2775674770049438	T	T	T
0.6808698975481240	0.4478088386611848	0.1729957486696144	T	T	T
0.9151785053783008	0.4531323162088758	0.1935367337312590	T	T	T
0.5719580533249879	0.6286120895848449	0.4043451358764195	T	T	T
0.5891173238943201	0.5004590905255017	0.4420064183776888	T	T	T
0.5846465904750352	0.3670251698124531	0.4459960418623417	T	T	T
0.8059945770403468	0.6398841189320584	0.3808883926416212	T	T	T
0.8087989968840257	0.4977855518596093	0.4248232116423460	T	T	T
0.8204569782953699	0.3662843353476904	0.4682228753488316	T	T	T
0.0134341933750618	0.5455490927149730	0.2055843760933183	T	T	T
0.0178072771974610	0.3711781712449384	0.2003772224697315	T	T	T
0.8705104561583012	0.4301975091652928	0.7693263407989921	T	T	T
0.8054898589306699	0.4458557277783790	0.6039707847442601	T	T	T
0.6985576473105068	0.4300886659051065	0.4818176648682151	T	T	T
0.5985789068526477	0.4334109266314629	0.6124986889295848	T	T	T
0.5960851949679534	0.4328168665263018	0.8110425639035961	T	T	T
0.7266798552134137	0.4345366208318342	0.7757444974720031	T	T	T
0.8631221329029157	0.6764074292126897	0.7433324052968960	T	T	T
0.8071649026324245	0.6381070615234005	0.5774449358783305	T	T	T
0.6918064594401806	0.6465602846162420	0.4834782317368318	T	T	T
0.5844257646184192	0.6590824926177614	0.5973113696927189	T	T	T
0.6048545028449783	0.6657234336749989	0.7941604295917148	T	T	T
0.7299486439980938	0.6677950862260847	0.7304773194851258	T	T	T
0.8048331648965724	0.5573517082429105	0.7396661110449247	T	T	T
0.5855108213558453	0.5480358163868417	0.7083656179877188	T	T	T
0.9355175230517982	0.3733515253268048	0.9236385869802231	T	T	T
0.9130081976384119	0.5038143296247231	0.9266964450033712	T	T	T

Structure files (CONTCAR) involved in this work:

0.8896238381028017	0.6348644779570158	0.9286704513569948	T	T	T
0.6780724562285220	0.3739878147282063	0.9379914645113765	T	T	T
0.6742531886395652	0.5074660953636815	0.9215773884234643	T	T	T
0.7043489496760095	0.6370763874308977	0.9229507044926394	T	T	T
0.4863251255308630	0.4592415962611285	0.7143317673479046	T	T	T
0.4851759922593801	0.6360591938861341	0.7211589226922848	T	T	T
0.6402609177375881	0.9370725018089626	0.2933613369443231	T	T	T
0.6963656970332177	0.9342768641784590	0.1152186922026200	T	T	T
0.7992073004930975	0.9502131378677388	0.9884999730057915	T	T	T
0.9015733043977819	0.9284958248457127	0.1113415508030479	T	T	T
0.8950519411880671	0.9451173723959170	0.3086202222186614	T	T	T
0.7685055587772096	0.9686866887881996	0.2708665598551512	T	T	T
0.6430627896079957	0.1748920099656714	0.2593174100330684	T	T	T
0.6965565581284522	0.1549378689508842	0.0850867896634402	T	T	T
0.8095375785453365	0.1474182931767013	0.9850572049650379	T	T	T
0.9095469605664248	0.1722299773869581	0.1115524088960204	T	T	T
0.8966142047506586	0.1522584364399770	0.3067639742299375	T	T	T
0.7714327211343411	0.1369941014057354	0.2485457618314527	T	T	T
0.6740475169277047	0.0514775700697430	0.2059919183188448	T	T	T
0.9183991627121130	0.0491486925351484	0.1849123406913891	T	T	T
0.5666544367463011	0.8742687984174236	0.4288358026599609	T	T	T
0.5808928650892574	0.0062331208479491	0.4422542559448543	T	T	T
0.6030828579422256	0.1374553936971467	0.4402071554810749	T	T	T
0.8034275259141043	0.8670062155279991	0.3915878806657196	T	T	T
0.8171972989243500	0.9934681072454349	0.4520519315056415	T	T	T
0.8044150776562446	0.1276739563525519	0.4422158720882158	T	T	T
0.0104732414255067	0.9550685704677041	0.2202522943925699	T	T	T
0.0149960695961450	0.1377638612762282	0.2204724290278680	T	T	T
0.8583338762985914	0.0683863251353023	0.7937190644296118	T	T	T
0.8036995218016907	0.0656472914952696	0.6146999794072188	T	T	T
0.7007588502111955	0.0508335896122472	0.4881061605352693	T	T	T
0.5991071035094566	0.0748730752348203	0.6114683140266365	T	T	T
0.6031084489481635	0.0530228256460299	0.8086453107075042	T	T	T
0.7300087123646046	0.0332947244493633	0.7699014884237495	T	T	T
0.8554634506802181	0.8265705412631208	0.7639948452816729	T	T	T
0.8055248655424503	0.8550692236774711	0.5877357953421949	T	T	T
0.6898618961824345	0.8528843666672802	0.4921113096327024	T	T	T
0.5871597394100362	0.8276877905894372	0.6127806515432215	T	T	T
0.6015964908008851	0.8526332909812420	0.8058817323985165	T	T	T
0.7277647489806378	0.8631923918657438	0.7483045569726517	T	T	T
0.8268737612647290	0.9514324686759978	0.7177977770370004	T	T	T
0.5798302194832945	0.9529242808186006	0.6789664843172404	T	T	T
0.9346015742340926	0.1269644680915286	0.9285255173548772	T	T	T
0.9180834126848765	0.9951047143220170	0.9393277148316566	T	T	T
0.8978452649223103	0.8635896769397879	0.9432367374553505	T	T	T
0.6933315171063718	0.1335744041173717	0.8895846645423455	T	T	T
0.6828342860013185	0.0082826676734690	0.9527991640381590	T	T	T
0.6950775407526063	0.8749873175812904	0.9419653666141125	T	T	T
0.4887501451184116	0.0476320114975198	0.7174351819613868	T	T	T
0.4826339884908732	0.8661786922779694	0.7213810281527846	T	T	T
0.3560737202257454	0.4435177989547353	0.7123556439428165	T	T	T
0.3022436729850222	0.4288014212928539	0.8907332499227317	T	T	T
0.2065791353488896	0.4489528441124725	0.0271970664965102	T	T	T

Structure files (CONTCAR) involved in this work:

0.1132079605704798	0.4305857701384823	0.8881019104966408	T	T	T
0.1049080775748634	0.4504468459985465	0.6905340870847809	T	T	T
0.2294558964518096	0.4730012616988600	0.7390238225406121	T	T	T
0.3569126546414670	0.6664814181100941	0.7304487754122068	T	T	T
0.3012720911321851	0.6696642147465350	0.9066834790924606	T	T	T
0.1925252170976258	0.6475461071067486	0.0145158771441949	T	T	T
0.0917197472368875	0.6748581201175494	0.8919898865760307	T	T	T
0.1022406553938172	0.6557663707784668	0.6969767974231678	T	T	T
0.2284707603448398	0.6369301135919090	0.7474532067490468	T	T	T
0.3200108346246723	0.5523277427434010	0.8179777118395870	T	T	T
0.0856236230781334	0.5516969964809788	0.8190410860421938	T	T	T
0.4314727289636690	0.3748779840453167	0.5855974457475297	T	T	T
0.4165862597427839	0.5049350973544948	0.5595859846178908	T	T	T
0.4096210962782172	0.6379498582161931	0.5546431028731428	T	T	T
0.1959869104894612	0.3746181163113774	0.6094660096155082	T	T	T
0.1859981876691950	0.5023173980674431	0.5539513125398173	T	T	T
0.1924621513801653	0.6362726530245372	0.5550326611734900	T	T	T
0.9968353991776546	0.4523848216900097	0.7941011314038435	T	T	T
0.9851096945828101	0.6357493083166863	0.7869076682558195	T	T	T
0.1439319239099281	0.5617975312234846	0.2095413726256754	T	T	T
0.2012212740688832	0.5702271364932437	0.3862066700354872	T	T	T
0.3013863860308575	0.5630097260252341	0.5197524266761480	T	T	T
0.4012169452673293	0.5698245216146265	0.3880135795152663	T	T	T
0.4014510309751756	0.5571269040641985	0.1922164358166772	T	T	T
0.2732872940937247	0.5349042219164569	0.2288958111475980	T	T	T
0.1399447717873518	0.3315951628338389	0.2423858833797525	T	T	T
0.1940373148146020	0.3439916335300692	0.4179080064362566	T	T	T
0.3101177341334945	0.3549469622414496	0.5128630730267415	T	T	T
0.4145516476955468	0.3311389381492638	0.3978680158861820	T	T	T
0.3957450925691957	0.3387921369639018	0.2019109773240967	T	T	T
0.2705125873263297	0.3566343254313209	0.2550287378368590	T	T	T
0.1820150415299621	0.4510140765536095	0.3026252602836854	T	T	T
0.4155583005927764	0.4495647945778847	0.3089336425222429	T	T	T
0.0694212289705242	0.6240759683499176	0.0733811974024770	T	T	T
0.0848333832540069	0.4922381848516136	0.0597562271049549	T	T	T
0.1077411051643713	0.3605194528983141	0.0543633842176422	T	T	T
0.3114095948342189	0.6266207500981852	0.0947115865155766	T	T	T
0.3274934641883758	0.4958148463282124	0.0570954436063824	T	T	T
0.3050612605726452	0.3628166807231334	0.0612882484524677	T	T	T
0.5139905072954015	0.5390524746555789	0.2882443356292873	T	T	T
0.5149156946272202	0.3621723420702899	0.2766213746360276	T	T	T
0.4405217090666895	0.7508941442927277	0.6433242968786786	T	T	T
0.1936637662766076	0.7501513823934401	0.6532446236300004	T	T	T
0.2730281418582817	0.7501658004300722	0.0578136919067820	T	T	T
0.1086143744158164	0.7495244083609169	0.0529149587841855	T	T	T
0.0609347551936148	0.2508494312514892	0.1394666411712428	T	T	T
0.3044740845921947	0.2468836201531374	0.1534322768560433	T	T	T
0.2274438048536473	0.2528619536747962	0.5555738616439532	T	T	T
0.3911014657756307	0.2515982913378170	0.5525539872949033	T	T	T
0.5615671596750943	0.2515293967804647	0.3629345222774448	T	T	T
0.8055443986562040	0.2456426217101740	0.3543763044580961	T	T	T
0.7274842215605472	0.2512776330559395	0.9525095330804589	T	T	T
0.8915296590214785	0.2510654169778126	0.9555276260430295	T	T	T

Structure files (CONTCAR) involved in this work:

0.9384170381261088	0.7490869812171860	0.8655780173421422	T	T	T
0.6888844923549877	0.7585590922428506	0.8600763602029083	T	T	T
0.7753938550817526	0.7505006811319002	0.4769022751927984	T	T	T
0.6079705630338584	0.7497797745490838	0.4567537382796235	T	T	T
0.0221607258356861	0.3923914474116306	0.5497487024916796	T	T	T
0.8840658626005781	0.3795864952368613	0.5928436371501398	T	T	T
0.0494709932949824	0.3874183859350864	0.4891951707752270	T	T	T
0.9180943177560756	0.6100945013133071	0.3124070587354295	T	T	T
0.9479651324792731	0.4932311766267595	0.6203402244791951	T	T	T
0.9187405558045747	0.4786776828887488	0.4881833120573723	T	T	T
1.0064276312236813	0.5009219575082096	0.5143003769177432	T	T	T
0.0531939153126138	0.4081932430388295	0.6036487149916807	T	T	T
0.9594504120693895	0.4811054849255177	0.5426678177943731	T	T	T

Figure S8(e)

Si Al O Ga H C

1.0000000000000000

20.0219993591000005 0.0000000000000000 0.0000000000000000

0.0000000000000000 19.8990001678000006 0.0000000000000000

0.0000000000000000 0.0000000000000000 13.3830003737999998

93 3 193 1 6 1

Selective dynamics

Direct

0.4214705704472578	0.0565745517387330	0.6484629932742849	T	T	T
0.3006974400486662	0.0263951883657881	0.7899685783837530	T	T	T
0.2794192723609217	0.0597839562767958	0.0133935752210039	T	T	T
0.1196202586972165	0.0626045815463030	0.0128414574908832	T	T	T
0.0663275903535539	0.0285101338447469	0.7996793455418638	T	T	T
0.1759056342371125	0.0549787436110563	0.6518778719232424	T	T	T
0.4197214752188134	0.8267906900070903	0.6714020274930259	T	T	T
0.3015730130757859	0.8678390122404818	0.8100925736336038	T	T	T
0.2668316799910405	0.8277812056582120	0.0303518757854609	T	T	T
0.1118264653640229	0.8260633120987814	0.0185723157958982	T	T	T
0.0607143654666594	0.8688880877198029	0.8034949878922211	T	T	T
0.1788580653770602	0.8264632503691359	0.6745816907862552	T	T	T
0.0752309540083800	0.9424611194381736	0.1515837241383285	T	T	T
0.1962198504980059	0.9721774451302907	0.2944928503835239	T	T	T
0.2163399530464845	0.9354883379201824	0.5153036268417783	T	T	T
0.3760316994592759	0.9328808902013754	0.5161823089419587	T	T	T
0.4299926775451974	0.9682030178023723	0.3053378648912506	T	T	T
0.3204554199616671	0.9439803277717430	0.1564432839610681	T	T	T
0.0781892985501219	0.1717230223908565	0.1650880786385634	T	T	T
0.1957195040048780	0.1295781881986638	0.3080741344431421	T	T	T
0.2304929615668648	0.1725027043690762	0.5251807698397636	T	T	T
0.3854100304715194	0.1733725931938544	0.5128205369593288	T	T	T
0.4360154287119810	0.1264111403259031	0.3025888378955540	T	T	T
0.3184148088611496	0.1668517146400441	0.1721084520578847	T	T	T
0.5816300024162030	0.5557999136370599	0.3474980099553907	T	T	T
0.6927331009984489	0.5304477270939828	0.1862281638567869	T	T	T
0.7110157244698310	0.5629327168470600	0.9714950279599666	T	T	T
0.8691236511641671	0.5554257349453593	0.9707054925865348	T	T	T
0.9342545186815502	0.5259514398465039	0.1835704142960698	T	T	T
0.5756128282912049	0.3277220823986790	0.3323490192996786	T	T	T
0.7058141671463948	0.3728458704821078	0.2162325752430027	T	T	T

Structure files (CONTCAR) involved in this work:

0.7339654816590979	0.3284428772116447	0.9950640717697782	T	T	T
0.8858296248891632	0.3276380351379036	0.9779863750657859	T	T	T
0.9364400832669940	0.3702130150832598	0.1980248661730388	T	T	T
0.9243012002445895	0.4350280939587590	0.8299134207007436	T	T	T
0.7774663419322848	0.4408895479432583	0.4748547207302110	T	T	T
0.6196125020561233	0.4308889857359780	0.4889249585190502	T	T	T
0.5673189387723365	0.4651866930302582	0.7066150050878645	T	T	T
0.6738417665467361	0.4324445650796834	0.8514169936415287	T	T	T
0.9174296897975732	0.6702455160452360	0.8287740597486771	T	T	T
0.7986722394136725	0.6306219890878827	0.6989077377858042	T	T	T
0.7693520199096366	0.6667173417079133	0.4806847445031325	T	T	T
0.6131773332370257	0.6693015141561239	0.4857607268261435	T	T	T
0.5649733694350727	0.6238532692701129	0.7042548915643736	T	T	T
0.6804872415475939	0.6806465030011644	0.8258504077470418	T	T	T
0.5750045208739778	0.9425151123517663	0.3651954334114960	T	T	T
0.6952789019221477	0.9719450417626939	0.2221136673936913	T	T	T
0.7174897062680546	0.9425787124598506	0.9984845075325031	T	T	T
0.8777744938614048	0.9332620398507960	0.9962743610566014	T	T	T
0.9309480817527735	0.9690089355157590	0.2083004947430435	T	T	T
0.8201611633927900	0.9362083094873629	0.3541644929462980	T	T	T
0.5800872114944705	0.1732976309149893	0.3345966344386076	T	T	T
0.6990195588227391	0.1312242642106239	0.2017576437035070	T	T	T
0.7312079440163507	0.1713077934169087	0.9797801624255210	T	T	T
0.8858134270296829	0.1724761793195614	0.9950832203934032	T	T	T
0.9337204233851524	0.1277847382474649	0.2076826165683750	T	T	T
0.8198708132045155	0.1693905786818481	0.3433059595617844	T	T	T
0.9228478119339216	0.0570192125801233	0.8623375677713215	T	T	T
0.8046096002571126	0.0286647561492989	0.7221736538578487	T	T	T
0.7807149943316933	0.0543901195286954	0.4964737907390320	T	T	T
0.6207032343533239	0.0668432225966301	0.4947363593759351	T	T	T
0.5665424371327261	0.0326710902595210	0.7028142689286994	T	T	T
0.6775713108756607	0.0584902894186374	0.8516232648055846	T	T	T
0.9163203052067872	0.8232198666547750	0.8415731839572766	T	T	T
0.8017629703417971	0.8727230184582730	0.7067570570960766	T	T	T
0.7685062280450260	0.8280199368601657	0.4898115029915446	T	T	T
0.6130650708129505	0.8249856758511009	0.4983915741544436	T	T	T
0.5623076839304372	0.8759590951529380	0.7045002009839223	T	T	T
0.6768798824125216	0.8370609907266989	0.8386305090286933	T	T	T
0.4232759230922286	0.4446287954959803	0.6405507776348313	T	T	T
0.3049392495199262	0.4721673828147490	0.7890404510865913	T	T	T
0.2844214716031672	0.4330422164864051	0.0068519520487183	T	T	T
0.1267807452178241	0.4315152932630951	0.0049007189924039	T	T	T
0.0740201934969755	0.4720762542117476	0.7982297794573091	T	T	T
0.1825363810298782	0.4485726658352659	0.6478072919107762	T	T	T
0.4239045703600200	0.6718514008491313	0.6639017015369461	T	T	T
0.3025990833794878	0.6289417684706038	0.8008304469693878	T	T	T
0.2692950728029253	0.6713938667506548	0.0190991928794706	T	T	T
0.1151053403811959	0.6732285133623317	0.0083457496131526	T	T	T
0.0654530847997182	0.6287948384751834	0.8000704406374156	T	T	T
0.1800891132895937	0.6678294293894558	0.6646267131393211	T	T	T
0.0790520836076281	0.5534747285059123	0.1364138552263779	T	T	T
0.1994172943095941	0.5267106819320884	0.2818546709343074	T	T	T
0.2225375538564307	0.5659154741073592	0.5031710670632076	T	T	T

Structure files (CONTCAR) involved in this work:

0.3833224028615749	0.5695408232962256	0.5052579541288978	T	T	T
0.4339275683101630	0.5271725748761437	0.2956333994158045	T	T	T
0.3263216287040703	0.5515926574667365	0.1437842161310358	T	T	T
0.0816878886223023	0.3265918947930737	0.1589064545252343	T	T	T
0.1960219717385773	0.3686944767554168	0.3050206591652118	T	T	T
0.2316319862684291	0.3291167991679806	0.5243047046578655	T	T	T
0.3860758395250897	0.3267877140159753	0.5085000140537664	T	T	T
0.4332428552987801	0.3697713886543970	0.2942865664215392	T	T	T
0.3162782240616356	0.3256418804320340	0.1672281574673145	T	T	T
0.8075474159667059	0.5658249059797109	0.3211887768641866	T	T	T
0.8298669575271675	0.3267974074803971	0.3538180991073757	T	T	T
0.7941873116889444	0.4722666487916494	0.7187841837717600	T	T	T
0.3559088900998660	0.0619217775985073	0.7192008874074566	T	T	T
0.2998037418023352	0.0650560434379039	0.8965668005773981	T	T	T
0.1992385636031127	0.0502734551888151	0.0270713249830762	T	T	T
0.1001535960230654	0.0652626347689221	0.8955774980224175	T	T	T
0.1009582492476871	0.0565768634045029	0.6980941706664225	T	T	T
0.2272692434827064	0.0326414989754360	0.7396467754482855	T	T	T
0.3576489026112071	0.8258863023897837	0.7493227618589687	T	T	T
0.3039388570367276	0.8433222449802447	0.9252614204323834	T	T	T
0.1891168906616138	0.8515273115666694	0.0215549714714264	T	T	T
0.0834839727372905	0.8319025169939681	0.9058877759350329	T	T	T
0.1014959569647950	0.8360139458444795	0.7099473622451824	T	T	T
0.2277158530532714	0.8535253760597946	0.7634323959680609	T	T	T
0.3188573773404828	0.9474318386033925	0.8039057554826392	T	T	T
0.0782883465416469	0.9481881289696166	0.8103301885895410	T	T	T
0.4296011377180280	0.1261506701702642	0.5859529014013799	T	T	T
0.4155758117831563	0.9942835355269911	0.5700733668654636	T	T	T
0.3967646366276288	0.8618831793854623	0.5671893226666289	T	T	T
0.1928447115328359	0.1299433949652652	0.6115930328070870	T	T	T
0.1787437999603061	0.0012981717569753	0.5604958129962415	T	T	T
0.1920975432205541	0.8674155795685906	0.5715105849903156	T	T	T
0.9874888336462103	0.0459895263978869	0.7909606302649137	T	T	T
0.9808955848828641	0.8581817712308007	0.7878388552484312	T	T	T
0.1415621024899019	0.9389386331082222	0.2205683033687334	T	T	T
0.1969295548310978	0.9294430683764603	0.3979584295812264	T	T	T
0.2963263732437653	0.9454180091593383	0.5297579304112787	T	T	T
0.3958939480506611	0.9288529665942138	0.3990491566541257	T	T	T
0.3955976560900985	0.9438009020804341	0.2015673652845292	T	T	T
0.2696871933437087	0.9690963480081928	0.2436578467441748	T	T	T
0.1414261305874523	0.1689016823451943	0.2405491907033489	T	T	T
0.1932953259396753	0.1624384462816447	0.4187459972659564	T	T	T
0.3078255934278091	0.1481533203641822	0.5161859138952257	T	T	T
0.4128578658541024	0.1697533566838774	0.3993172577727550	T	T	T
0.3957859094417471	0.1542844455890295	0.2049511574756323	T	T	T
0.2701398971155132	0.1384257585363608	0.2608378562767460	T	T	T
0.1770060237796887	0.0502899531392945	0.3154910806420281	T	T	T
0.4176477970578722	0.0481323049602685	0.3218399410224360	T	T	T
0.0668947796556311	0.8707387256941006	0.0944185057397278	T	T	T
0.0801555019443480	0.0015083006995958	0.0676702369002653	T	T	T
0.0975127403438396	0.1338456308259425	0.0614214968949748	T	T	T
0.3024348373864176	0.8682443784184311	0.1207341900235539	T	T	T
0.3166928842156052	0.9947458000048377	0.0613575658596571	T	T	T

Structure files (CONTCAR) involved in this work:

0.3030843547223341	0.1286018331063210	0.0675922253925237	T	T	T
0.5089172438386079	0.9514427583049930	0.2962428384077549	T	T	T
0.5159060025648413	0.1346463670262814	0.2855637492781414	T	T	T
0.6423236682134230	0.5626487381829345	0.2691779102561541	T	T	T
0.6718983706434920	0.5609079047310794	0.0774707364435646	T	T	T
0.7902112398830589	0.5465482490418357	0.9884719400320180	T	T	T
0.9091417069711746	0.5523234013864469	0.0769886593878832	T	T	T
0.8968147609488831	0.5696557399689067	0.2777552615555023	T	T	T
0.7680983557765179	0.5533517907185852	0.2097822273900284	T	T	T
0.6408836040165451	0.3347696028647431	0.2632264251938791	T	T	T
0.7253047978581163	0.3315184245413373	0.1149323353572533	T	T	T
0.8092816644860481	0.3539420527599950	0.9651025883209542	T	T	T
0.9121188262608894	0.3420678962334606	0.0898506442783845	T	T	T
0.9058573545824300	0.3314703135911563	0.2913901797197411	T	T	T
0.7671610747642685	0.3718316220030185	0.2933606368544928	T	T	T
0.6836752486205182	0.4490170171762268	0.1860134557814226	T	T	T
0.9139278947216237	0.4497952261354961	0.2046092444037732	T	T	T
0.5696612961173068	0.6270549653395354	0.4045037309937004	T	T	T
0.5984161494784457	0.4994344955071165	0.4319947680666544	T	T	T
0.5838251332024591	0.3665363562562739	0.4385784257053929	T	T	T
0.8063578145502712	0.6422481650347177	0.3807464530435211	T	T	T
0.7964641121744863	0.4988349528029149	0.3993513684975664	T	T	T
0.8317441314209855	0.3761308451079935	0.4707882027732428	T	T	T
0.0119314860405112	0.5436642454615306	0.2042951650688372	T	T	T
0.0180881569897270	0.3693007596813972	0.1988424795644227	T	T	T
0.8740421434735371	0.4264655777746098	0.7313612082670433	T	T	T
0.8048912105655582	0.4662702052057766	0.5870144670650128	T	T	T
0.7002006103185771	0.4203644751824098	0.4837907375819382	T	T	T
0.5967948487152592	0.4337858064499384	0.6040818537207123	T	T	T
0.5998395219625063	0.4260253674254830	0.8009916006633315	T	T	T
0.7317175111219449	0.4246505938523220	0.7682916291806882	T	T	T
0.8631369881594617	0.6728988057867091	0.7395411948867199	T	T	T
0.8035855713620348	0.6305328383489663	0.5776642614069055	T	T	T
0.6904841061891988	0.6449891203554554	0.4793816410876660	T	T	T
0.5844451740942468	0.6558102282972991	0.5969684818906068	T	T	T
0.6040351246584795	0.6632442545085176	0.7930957346725868	T	T	T
0.7295837718727285	0.6692917566986432	0.7301068061615460	T	T	T
0.7997309719225634	0.5562214025943181	0.7467505826089949	T	T	T
0.5851385049579448	0.5449733774837718	0.7086678000696625	T	T	T
0.9312102460819310	0.3667610076845207	0.8946134881204166	T	T	T
0.8949916718658186	0.4941015404464199	0.9001866919803805	T	T	T
0.8888357529945603	0.6273186383819798	0.9228465235059471	T	T	T
0.6799075374969160	0.3753838887683081	0.9382385707529863	T	T	T
0.6776928690316797	0.5073371687958924	0.8995047752901654	T	T	T
0.7037144727667132	0.6366760350832269	0.9215331078259016	T	T	T
0.4870178906390488	0.4547427250607659	0.7128928038207986	T	T	T
0.4846716818568189	0.6329680616668910	0.7204729873194148	T	T	T
0.6401113115249236	0.9369850800645404	0.2938079506331815	T	T	T
0.6907115250607352	0.9380651935382329	0.1123045088838650	T	T	T
0.7983632201579441	0.9489267578957477	0.9932296611077005	T	T	T
0.9032116873912174	0.9287799405123827	0.1109861084643097	T	T	T
0.8954933007670413	0.9406953645329997	0.3091564892980155	T	T	T
0.7697457854197060	0.9582723349416684	0.2650262525206772	T	T	T

Structure files (CONTCAR) involved in this work:

0.6406465098339493	0.1747074618952421	0.2548491704644585	T	T	T
0.6967295457986904	0.1497329787705852	0.0842091783777416	T	T	T
0.8090663228592380	0.1470811351265825	0.9831074006286956	T	T	T
0.9084456536403390	0.1705172642079885	0.1111465250846373	T	T	T
0.8971083022665688	0.1559422369005676	0.3069260196378075	T	T	T
0.7716698948809796	0.1482972450951454	0.2487819013630800	T	T	T
0.6814076354681892	0.0520830208431771	0.2173413561953525	T	T	T
0.9162833710363562	0.0485762781899029	0.1917432368842110	T	T	T
0.5670724766299539	0.8734873331866736	0.4291581917347699	T	T	T
0.5798939711050236	0.0057490258336541	0.4418318485838043	T	T	T
0.6042541969580393	0.1365995059661422	0.4370321082797277	T	T	T
0.8050623150748366	0.8597735162408014	0.3916556922881285	T	T	T
0.8122452329409414	0.9862439765081685	0.4490984675287927	T	T	T
0.8054535813169417	0.1199281031576014	0.4373646072402463	T	T	T
0.0106254067739748	0.9554667488938869	0.2217868568373605	T	T	T
0.0143733586407918	0.1366849364563046	0.2190582968127214	T	T	T
0.8573617719103889	0.0684456885111624	0.7927880022726769	T	T	T
0.8073416744922824	0.0598305264941539	0.6107430695708670	T	T	T
0.6997076504405748	0.0492584516694331	0.4918806504984561	T	T	T
0.5960621800991256	0.0759433510297693	0.6096480698218388	T	T	T
0.6023746606555908	0.0545763622277874	0.8066116589126525	T	T	T
0.7289218567047231	0.0364368966167077	0.7635374732401099	T	T	T
0.8536474117421341	0.8239962602651913	0.7648985029633508	T	T	T
0.8050451660353933	0.8572531202199283	0.5887019871510160	T	T	T
0.6901919273791010	0.8504282159246387	0.4909641255280836	T	T	T
0.5875477187213182	0.8280752088964616	0.6136373715899917	T	T	T
0.6002369953990424	0.8542502751820598	0.8068877636440902	T	T	T
0.7261784956199672	0.8612339998221455	0.7482463663457930	T	T	T
0.8255370227864938	0.9497818902601398	0.7252596205783154	T	T	T
0.5796322767683760	0.9536384891906474	0.6780453131907639	T	T	T
0.9343826411362296	0.1242437172108731	0.9291984073929741	T	T	T
0.9163576484193100	0.9928717297435899	0.9367625375086267	T	T	T
0.8960448453323296	0.8617437135514637	0.9442871349102742	T	T	T
0.6928930488743453	0.1346820181441857	0.8877659486056576	T	T	T
0.6842727451959268	0.0083152724459857	0.9467365463726156	T	T	T
0.6947415939402954	0.8745232750962892	0.9422960971889996	T	T	T
0.4871284892169370	0.0466485668902779	0.7176193236941927	T	T	T
0.4821800939097642	0.8671980369164012	0.7209537541627186	T	T	T
0.3570356562740275	0.4406356111878074	0.7098680703083128	T	T	T
0.3058011096956736	0.4269900152651736	0.8901508100378150	T	T	T
0.2051242140332716	0.4506643562223707	0.0168217995154983	T	T	T
0.1062076769813381	0.4273185099004549	0.8875395377796168	T	T	T
0.1067726656195789	0.4537944630051953	0.6905000103740150	T	T	T
0.2309511333551528	0.4695582308082899	0.7394868325681750	T	T	T
0.3571802346854518	0.6660395704345035	0.7317253885992170	T	T	T
0.3021474643779397	0.6659723838332057	0.9085838899928143	T	T	T
0.1917929780367247	0.6462968507924393	0.0140497903779950	T	T	T
0.0905427716859099	0.6749335859380701	0.8928725753700819	T	T	T
0.1030743349641365	0.6532938815391968	0.6985032676999369	T	T	T
0.2292063519608073	0.6350516415548588	0.7488244512967610	T	T	T
0.3220997734933053	0.5500937143706378	0.8151220752587200	T	T	T
0.0843333428015276	0.5509514964986549	0.8249878352473872	T	T	T
0.4315985822103802	0.3750691014359746	0.5782830762760314	T	T	T

Structure files (CONTCAR) involved in this work:

0.4183736720739099	0.5063597169250191	0.5613725498071642	T	T	T
0.4096407128155519	0.6391855409269015	0.5544335978833487	T	T	T
0.1944597002253320	0.3712218803901013	0.6127577254085901	T	T	T
0.1910853136403029	0.4979652738334612	0.5523510850097985	T	T	T
0.1925618180402248	0.6327496055227915	0.5564665992097007	T	T	T
0.9955625288242809	0.4554927122509928	0.7833725010069034	T	T	T
0.9854396229763787	0.6356893315350860	0.7850667223369631	T	T	T
0.1428062829823189	0.5599131355993200	0.2100277882858829	T	T	T
0.2010542692244241	0.5682157492696002	0.3863137133127169	T	T	T
0.3028094933880816	0.5633835994436683	0.5176481689327851	T	T	T
0.4033630320227115	0.5700516092416394	0.3883725268094719	T	T	T
0.4002396663181109	0.5547659842601405	0.1929782146791945	T	T	T
0.2720308139026865	0.5315072251121582	0.2293540842035879	T	T	T
0.1394614662326193	0.3282565403781640	0.2436489737616360	T	T	T
0.1934725955189610	0.3421513815336534	0.4193153328974830	T	T	T
0.3088400177632929	0.3532647789397486	0.5140924790985514	T	T	T
0.4110695440624986	0.3280762488708612	0.3934743075490169	T	T	T
0.3932749934172466	0.3409014741779897	0.1975214506650216	T	T	T
0.2691755039817842	0.3548990185243827	0.2567166933223717	T	T	T
0.1799258544485232	0.4487496432630910	0.3022469158360357	T	T	T
0.4149449871203269	0.4484460986397095	0.3121620998870311	T	T	T
0.0688680894136982	0.6224658271772485	0.0736246785638385	T	T	T
0.0837017349816972	0.4903315114039613	0.0598793701270552	T	T	T
0.1102515565369828	0.3593720536253898	0.0554668525047899	T	T	T
0.3096280524830117	0.6248910766937144	0.0975691471619563	T	T	T
0.3261280332016571	0.4942985314687027	0.0571356193596901	T	T	T
0.2991989691215842	0.3617833700965379	0.0612872647800376	T	T	T
0.5139574991854192	0.5361580330286363	0.2873479423126603	T	T	T
0.5121840602733376	0.3598889011621501	0.2724105538136527	T	T	T
0.4420359619154385	0.7502830478120609	0.6471243175925429	T	T	T
0.1936917808403207	0.7476139866902309	0.6530566178973610	T	T	T
0.2724864913388702	0.7485156775581918	0.0572041998640503	T	T	T
0.1079514197974378	0.7481057359467082	0.0546183230528736	T	T	T
0.0612702122670575	0.2492619338759035	0.1369845775729391	T	T	T
0.3039786784388033	0.2459365494124179	0.1535278608808591	T	T	T
0.2261332058915101	0.2510317453479904	0.5571986763558825	T	T	T
0.3907512190986104	0.2506029449088246	0.5511019140363035	T	T	T
0.5596283429918431	0.2500317888079908	0.3601189993752267	T	T	T
0.8084634862304806	0.2449241511445063	0.3789202623281596	T	T	T
0.7252470993836418	0.2511012144503584	0.9591058851147899	T	T	T
0.8926423108132893	0.2484709082964871	0.9529375367199370	T	T	T
0.9337780127219676	0.7455559569735987	0.8688374556712679	T	T	T
0.6850600020128461	0.7580386750712003	0.8607610546435094	T	T	T
0.7755453022533014	0.7476348202539576	0.4898418206818071	T	T	T
0.6061137140256379	0.7484542643980820	0.4587156201019734	T	T	T
0.0463770370149285	0.2966423733005992	0.6239060882952726	T	T	T
0.8906940127967637	0.4195008234281516	0.5805193290109948	T	T	T
0.0430525320174038	0.2493459463862703	0.6416553185321423	T	T	T
0.9204693323850641	0.6093050366745739	0.3019247744191781	T	T	T
1.0064219219921575	0.4700534302087450	0.5828457217086176	T	T	T
0.9693007521351620	0.4702790628611439	0.4591061004919584	T	T	T
0.0050287489447477	0.3940567494722430	0.5100912148253794	T	T	T
0.0930526559492467	0.3081437041083304	0.6360421181464291	T	T	T

Structure files (CONTCAR) involved in this work:

0.9787525955579919 0.4409895653130460 0.5272001029881679 T T T

Figure S10 Zn-IS

Si Al O Zn H C

1.0000000000000000

20.0219999999999985 0.0000000000000000 0.0000000000000000

0.0000000000000000 19.8990000000000009 0.0000000000000000

0.0000000000000000 0.0000000000000000 13.3829999999999991

93 3 194 2 9 2

Selective dynamics

Direct

0.4234991897022539 0.0583938196313458 0.6481323394826523 T T T

0.3070361241286315 0.0281466516205854 0.7939389107775693 T T T

0.2828354971289225 0.0563283037072397 0.0163627094989635 T T T

0.1240204909623361 0.0604100460243812 0.0114087842124727 T T T

0.0687557576119014 0.0308837539171770 0.7999741573508842 T T T

0.1825696011344304 0.0590904369014516 0.6635832913323981 T T T

0.4194061352478943 0.8257775849163974 0.6672171861233097 T T T

0.3055696908975749 0.8694082552323568 0.8081336444656820 T T T

0.2670799845112292 0.8293696501705490 0.0248917365180913 T T T

0.1125643099812695 0.8259313812356632 0.0100413018913911 T T T

0.0659341972582264 0.8736342828205580 0.7967037673654155 T T T

0.1841210376318038 0.8277956574305914 0.6724187618692640 T T T

0.0784535700864085 0.9393032896915383 0.1489444310253276 T T T

0.1956037775397707 0.9694265870008041 0.2949870692707362 T T T

0.2195455225162820 0.9395092709086422 0.5163733256886149 T T T

0.3789273267986230 0.9348448513644281 0.5126027571863347 T T T

0.4348548176360147 0.9670429217604695 0.3006148433835419 T T T

0.3204655478051889 0.9381702305599190 0.1647323567487717 T T T

0.0836549278416738 0.1700619622576513 0.1664516418856391 T T T

0.1966912779421235 0.1284944040247452 0.3096749747661429 T T T

0.2348539410563804 0.1700749796122170 0.5255577416191620 T T T

0.3898051735705890 0.1730150317060387 0.5080941178130822 T T T

0.4366541041420021 0.1254239965953709 0.2946364517918593 T T T

0.3166017288974912 0.1693440261283720 0.1713164677026984 T T T

0.5762870376391972 0.5537462368000077 0.3513889714570674 T T T

0.6893007094512456 0.5255900268036855 0.1954684876810721 T T T

0.7120480865890292 0.5694796981798751 0.9805893690591448 T T T

0.8705493012204938 0.5729559724402477 0.9810760005616650 T T T

0.8079281352627598 0.5482023906631690 0.3404728807413056 T T T

0.5729784468777505 0.327788332282698 0.3288449922033452 T T T

0.6943629145944896 0.3715927347832840 0.1906406497781618 T T T

0.7304999984624672 0.3263355371889008 0.9803640426244180 T T T

0.8852189239308234 0.3258395042915971 0.9978110435441910 T T T

0.9446109447986152 0.3756536994914809 0.1917391382133189 T T T

0.9181483857681533 0.4439883871224400 0.8601207828519822 T T T

0.7997485620620038 0.4716225295083322 0.7180828861014473 T T T

0.7712550425283941 0.4349655729059233 0.4942197827561655 T T T

0.6131765687355671 0.4270234027799916 0.4896806131483934 T T T

0.5654236347486168 0.4679858221195766 0.7043935031391173 T T T

0.6749913785907250 0.4467882216068866 0.8541411702465134 T T T

0.9196951384251274 0.6775316399087465 0.8250466594241480 T T T

0.7698671142502884 0.6668187388253294 0.4616239934679354 T T T

0.6137909612827646 0.6712410550923374 0.4830976898872645 T T T

Structure files (CONTCAR) involved in this work:

0.5604840455478115	0.6264759450059734	0.6959303368739936	T	T	T
0.6725715296142746	0.6749963383721688	0.8217434621363445	T	T	T
0.5796223423082280	0.9440308462990469	0.3540848951865274	T	T	T
0.6992425498237798	0.9729348291057767	0.2090253881501157	T	T	T
0.7217918724252094	0.9375325197151897	0.9877593120276054	T	T	T
0.8824753876585445	0.9334734086525485	0.9918103672605304	T	T	T
0.9342743890461739	0.9677866426176371	0.2021723583727137	T	T	T
0.8225774306884179	0.9448295835110044	0.3482813949214144	T	T	T
0.5790749097372161	0.1724881764684341	0.3239642492826829	T	T	T
0.6990367527881914	0.1319315641206101	0.1875939128894805	T	T	T
0.7331585639365439	0.1708393050206221	0.9672612507455352	T	T	T
0.8877843208797922	0.1731922419795472	0.9830488659362560	T	T	T
0.9376771462581740	0.1253875139527947	0.1950924225401018	T	T	T
0.8217672514532387	0.1733594222533282	0.3240714588110651	T	T	T
0.9238500618036449	0.0552278037110325	0.8531941845835491	T	T	T
0.8050136958643402	0.0268162131981328	0.7026071448672659	T	T	T
0.7816293907531401	0.0661707379697265	0.4858986096960705	T	T	T
0.6210846154134763	0.0690552427763888	0.4867294023200283	T	T	T
0.5681910444639258	0.0316462165501002	0.6956278424373641	T	T	T
0.6817926648088485	0.0538277459130504	0.8411431227601551	T	T	T
0.9241494493267255	0.8297849525426993	0.8315479492784326	T	T	T
0.8041565511936002	0.8696435102298912	0.6903537706575638	T	T	T
0.7710890720194821	0.8247856042061389	0.4742014376660304	T	T	T
0.6154024544711708	0.8250574065037815	0.4866826515039983	T	T	T
0.5642773429345487	0.8746716147255480	0.6939912973160983	T	T	T
0.6801779485560107	0.8339089474318501	0.8264151895422457	T	T	T
0.4214863390877003	0.4416229779939770	0.6475278086355867	T	T	T
0.3042450172926192	0.4691898056791826	0.7921662476601367	T	T	T
0.2787000197524704	0.4400782478951955	0.0148420588070399	T	T	T
0.1203411412086243	0.4356935748782624	0.0159101507420312	T	T	T
0.0628167538779349	0.4675124267027823	0.8025747262781021	T	T	T
0.1775345038027715	0.4399123010289812	0.6645071210610157	T	T	T
0.4159201624350210	0.6723985017936501	0.6618185272586018	T	T	T
0.3029707593333436	0.6278152381416635	0.8038398875663817	T	T	T
0.2671763224691542	0.6693287769499295	0.0210139867857729	T	T	T
0.1133228734871763	0.6718552095255685	0.0037590376805490	T	T	T
0.0619628170571522	0.6265507603074317	0.7923359655986216	T	T	T
0.1816934739011529	0.6693522603075194	0.6684573093358049	T	T	T
0.0760925865971332	0.5590449527426709	0.1475121035484716	T	T	T
0.1930546779997772	0.5266620197059613	0.2923324260070987	T	T	T
0.2154000300357834	0.5578048877420286	0.5166251840096875	T	T	T
0.3742700635354519	0.5636040260349601	0.5122343158262099	T	T	T
0.4291605476083566	0.5284510419500160	0.3004441299084600	T	T	T
0.3185139914552508	0.5584935495118110	0.1603306401625386	T	T	T
0.0866050924374007	0.3220712530150869	0.1641069353377090	T	T	T
0.1984013040577740	0.3680761364468702	0.3049618614085109	T	T	T
0.2343762205226921	0.3296951481944218	0.5248146426724148	T	T	T
0.3888886967901878	0.3272210664134556	0.5068098274273487	T	T	T
0.4325518057971927	0.3712688818661160	0.2906221769820920	T	T	T
0.3156488758188912	0.3272400839719198	0.1669197959017162	T	T	T
0.9208624101352880	0.5288691165871038	0.1882649454158952	T	T	T
0.8230267401970768	0.3371896151464583	0.3241393451239753	T	T	T
0.7986905310601731	0.6340981172252417	0.6918550393871916	T	T	T

Structure files (CONTCAR) involved in this work:

0.3585120577885303	0.0665066822250549	0.7198120381230118	T	T	T
0.3158891498351011	0.0582566098385050	0.9057323955654791	T	T	T
0.2030700977289513	0.0430108670886232	0.0079484773697649	T	T	T
0.0940861660862094	0.0693036121723073	0.9000381433019671	T	T	T
0.1059339663654451	0.0622413344993659	0.7027561143725503	T	T	T
0.2304904464319273	0.0398924572525697	0.7576078961214588	T	T	T
0.3616085143638311	0.8246023342170720	0.7522765592627833	T	T	T
0.3080697019584671	0.8521894006580059	0.9261987780059434	T	T	T
0.1894365164086328	0.8524394379113737	0.0132153085557956	T	T	T
0.0843135277998596	0.8319851958228857	0.8973780340487215	T	T	T
0.1064531903497830	0.8413344327639178	0.7026335570103865	T	T	T
0.2313908853075199	0.8515503443781377	0.7652234043318539	T	T	T
0.3231373422221169	0.9481094263022645	0.7902939155952465	T	T	T
0.0875156210220453	0.9515969131380536	0.8108530489895382	T	T	T
0.4333411198250395	0.1266829402113104	0.5833277694633237	T	T	T
0.4156176993784700	0.9951637089850562	0.5724057797257051	T	T	T
0.3919539791450327	0.8635952289732313	0.5678866690000172	T	T	T
0.2030486444747141	0.1325328923194020	0.6215878533699388	T	T	T
0.1879693483683100	0.0026427288082245	0.5765004462931996	T	T	T
0.2028498996103751	0.8688316872768593	0.5714839627999604	T	T	T
0.9891652400977957	0.0412155479038379	0.7842839859755898	T	T	T
0.9861527978263499	0.8682752894033120	0.7760566308254995	T	T	T
0.1440303287667953	0.9323340535624136	0.2195130358757023	T	T	T
0.1864868279936800	0.9373552026487201	0.4055865718082682	T	T	T
0.2995064877047312	0.9503227286253121	0.5080762888898800	T	T	T
0.4096549875379288	0.9293143239231469	0.4013041811350523	T	T	T
0.3967828509616682	0.9348334397605487	0.2047448490628833	T	T	T
0.2719397975872748	0.9576086011245100	0.2580038677692043	T	T	T
0.1404834493273934	0.1721632484675608	0.2525218558304580	T	T	T
0.1934001350415022	0.1480554425678079	0.4267884280067309	T	T	T
0.3123660655638187	0.1479675002922104	0.5109807964146286	T	T	T
0.4178657524809058	0.1670857165792579	0.3950937169084426	T	T	T
0.3944844816291955	0.1564576579023091	0.2010389124199833	T	T	T
0.2706267646006437	0.1456710745639337	0.2657146652006401	T	T	T
0.1795182457522356	0.0493673045810344	0.2947609423547130	T	T	T
0.4174762918459726	0.0467387265549722	0.3095652758444441	T	T	T
0.0679944217169645	0.8692332817887836	0.0881526660190093	T	T	T
0.0854543065191557	0.9997790454012835	0.0683777978259709	T	T	T
0.1118800483613921	0.1304770220179809	0.0695308933143399	T	T	T
0.2998868066164659	0.8647825768941144	0.1219913544483896	T	T	T
0.3159536150758347	0.9945361463807103	0.0775546261623315	T	T	T
0.2972183671392693	0.1274345683359689	0.0714014424931529	T	T	T
0.5141743587736007	0.9547300028994389	0.2842075957628790	T	T	T
0.5162875865079214	0.1326291681356820	0.2729906893434172	T	T	T
0.6365520026009771	0.5591465085137785	0.2720095194664920	T	T	T
0.6960795420261923	0.5744116166899701	0.0993071387302403	T	T	T
0.7913395334242226	0.5610742688375955	0.9567772343128391	T	T	T
0.8836209836023432	0.5779335361419805	0.0992615897849911	T	T	T
0.8836305811860907	0.5284877856285131	0.3078192089114072	T	T	T
0.7611598420368203	0.5232784642379806	0.2509898721157465	T	T	T
0.6412753109832833	0.3369366559441583	0.2669967280040335	T	T	T
0.6898108985934247	0.3308559836835404	0.0848974344297670	T	T	T
0.8076153768046427	0.3500822023422658	0.9975644884965641	T	T	T

Structure files (CONTCAR) involved in this work:

0.9124612333757374	0.3218339980739804	0.1130282451009849	T	T	T
0.9067267771722834	0.3698817178146929	0.3014119153844078	T	T	T
0.7680530108803945	0.3692452665484926	0.2371129204514940	T	T	T
0.6695360402981264	0.4488539440543013	0.1677533329050451	T	T	T
0.9372467144158997	0.4494863044948680	0.1470104219985497	T	T	T
0.5691424072570139	0.6253220996864548	0.4084628594436037	T	T	T
0.5891270428532601	0.4955900491327823	0.4345291472609334	T	T	T
0.5781047684073745	0.3620158230176702	0.4393124105137062	T	T	T
0.8002445389932576	0.6282843136183525	0.3637875233506243	T	T	T
0.7871632244076245	0.5112494864565356	0.4478823585627418	T	T	T
0.8199120209657702	0.3830774966633480	0.4375895529066801	T	T	T
0.0057934007094037	0.5612905728484188	0.2162459992441440	T	T	T
0.0225626447486539	0.3580878788751408	0.2145576420742267	T	T	T
0.8534094136743259	0.4325786185650048	0.7878269823246309	T	T	T
0.7918205745495172	0.4337135788383897	0.6110762882923276	T	T	T
0.6934645379672032	0.4186580118909586	0.4769333823129995	T	T	T
0.5936659097609550	0.4288328984551308	0.6065901498127262	T	T	T
0.6016958073645791	0.4390984584112785	0.8037527462556719	T	T	T
0.7269709943042137	0.4734864564904323	0.7694388000446321	T	T	T
0.8595743455125470	0.6813453335414981	0.7471126093352554	T	T	T
0.8135837524941384	0.6412519797124980	0.5588080180138576	T	T	T
0.6918381061885951	0.6470714430399807	0.4793323776481181	T	T	T
0.5852382150665523	0.6645242663789932	0.5953215938306082	T	T	T
0.5939595223783102	0.6632903638703261	0.7919065540332912	T	T	T
0.7187835412120055	0.6469330818472044	0.7323615084598172	T	T	T
0.8255821764184021	0.5481121805070041	0.6941841572505791	T	T	T
0.5810174492107555	0.5475825544331554	0.6908886765766430	T	T	T
0.9284738753260097	0.3779649188516340	0.9303715345706027	T	T	T
0.9105824177573648	0.5102681963659050	0.9293362786023138	T	T	T
0.8977468702886124	0.6416423202670274	0.9292465006642583	T	T	T
0.6969779551716703	0.3740162205511993	0.8961690517743380	T	T	T
0.6721592061682912	0.5031293079940600	0.9413839926934192	T	T	T
0.6854377281452277	0.6374718910355237	0.9281264382096401	T	T	T
0.4860517895643158	0.4534393135751738	0.7182781967378949	T	T	T
0.4796256042523887	0.6315192522610599	0.7054698287783753	T	T	T
0.6451623682792131	0.9391123070607660	0.2836626932348866	T	T	T
0.6967464384319040	0.9338914142202576	0.1028047039879954	T	T	T
0.8025344126273651	0.9438358694646191	0.9816856301251077	T	T	T
0.9042236976728505	0.9257916604330141	0.1080947889949740	T	T	T
0.8985584566004732	0.9452011345291625	0.3056676565115087	T	T	T
0.7733760713404818	0.9641687462033435	0.2562339387214005	T	T	T
0.6416945667717975	0.1727944854268288	0.2476810652860471	T	T	T
0.6952792078672591	0.1552461411274767	0.0717979688970290	T	T	T
0.8107775446899115	0.1471353597389139	0.9778530167150666	T	T	T
0.9154599243424588	0.1665936908149507	0.0961754187701021	T	T	T
0.8980373064167272	0.1521081870859431	0.2926290148842829	T	T	T
0.7722609688056137	0.1475024853191562	0.2339872944299177	T	T	T
0.6825566991260804	0.0520525900960167	0.1952059363193119	T	T	T
0.9217063976874682	0.0463932598081814	0.1778635368188721	T	T	T
0.5714885812249535	0.8740762090782991	0.4157187834881894	T	T	T
0.5842059343406046	0.0057594829776519	0.4332754046396951	T	T	T
0.6004465161169181	0.1379061150018843	0.4294216855089782	T	T	T
0.8078839022052302	0.8695314698239724	0.3895519219730102	T	T	T

Structure files (CONTCAR) involved in this work:

0.8155002568751918	0.9991700807525236	0.4377316554584829	T	T	T
0.8029766835839530	0.1336650507112875	0.4271371291365708	T	T	T
0.0133001882791215	0.9518594456905544	0.2181678090975790	T	T	T
0.0175530670372292	0.1346593153735423	0.2126618795213083	T	T	T
0.8585841718447237	0.0561527344708837	0.7819495265760368	T	T	T
0.8071424604919908	0.0716616007689670	0.6011606397553969	T	T	T
0.7010091215414820	0.0568440465463697	0.4816505980163786	T	T	T
0.5965578297276084	0.0755263069335855	0.6020110259724778	T	T	T
0.6059187167086465	0.0513313030422355	0.7987421116787495	T	T	T
0.7307147758180734	0.0304629267289545	0.7507234661761319	T	T	T
0.8593394379102299	0.8339226220416959	0.7600388471310028	T	T	T
0.8072525568300922	0.8333906989113848	0.5818487552453990	T	T	T
0.6934684803497155	0.8480635805879893	0.4825135502082536	T	T	T
0.5889751840419223	0.8282472162895580	0.6011410295135858	T	T	T
0.6039563584457872	0.8533141185690379	0.7949343306027716	T	T	T
0.7301157192738530	0.8609414441170394	0.7385888350354600	T	T	T
0.8218432893530977	0.9488090343933936	0.6770261587315884	T	T	T
0.5791426430494295	0.9528341532803232	0.6676204248780117	T	T	T
0.9324155268331813	0.1280046566553673	0.9069831096176599	T	T	T
0.9189027244430547	0.9976724844031526	0.9396064784587933	T	T	T
0.9067032380331391	0.8647561097459372	0.9379775730937049	T	T	T
0.6982620553214007	0.1299285493749409	0.8764408564269780	T	T	T
0.6889316289568900	0.0035956505228479	0.9361092086988573	T	T	T
0.6981489015290179	0.8692992870534034	0.9322400731591074	T	T	T
0.4895952585016882	0.0471234446442869	0.7157987876673029	T	T	T
0.4847776053580826	0.8634238192586650	0.7123116826165700	T	T	T
0.3557601404370457	0.4311901859387992	0.7174707616434188	T	T	T
0.3102863237631717	0.4374456064835380	0.9034010691628823	T	T	T
0.1988726941252868	0.4563269294994285	0.0124799464083724	T	T	T
0.0893428804330172	0.4331707949358476	0.9051487461954910	T	T	T
0.1021741206760195	0.4344651679888404	0.7083371515450865	T	T	T
0.2277335107251270	0.4587434366869430	0.7556187110251504	T	T	T
0.3570395889282263	0.6730359497584659	0.7449405419369212	T	T	T
0.3069082385932735	0.6488144427175460	0.9203760234792764	T	T	T
0.1898622982756713	0.6450947632454948	0.0090351396732550	T	T	T
0.0855722776669931	0.6681904461810014	0.8909389562793352	T	T	T
0.1037224674622752	0.6555337267034591	0.6967858967757914	T	T	T
0.2282155765473728	0.6418178798858249	0.7599927568939445	T	T	T
0.3219525079993568	0.5489366374534479	0.7916140028245249	T	T	T
0.0789349031206922	0.5475549767740321	0.8081007680322023	T	T	T
0.4334422417514044	0.3751956444393991	0.5788037616042343	T	T	T
0.4140931287718865	0.5062684816674683	0.5741142179447322	T	T	T
0.3873605283014416	0.6370964531698809	0.5608062167962927	T	T	T
0.1983687345563406	0.3680591576432812	0.6168610103163279	T	T	T
0.1798801612284082	0.4987407682336827	0.5805005092109899	T	T	T
0.1994209345629973	0.6310259752338775	0.5644619691819228	T	T	T
0.9837505783894028	0.4528372052736179	0.7891586797688267	T	T	T
0.9828080049878047	0.6369918868757073	0.7738193313106878	T	T	T
0.1384081980571772	0.5662476128148164	0.2235602398716922	T	T	T
0.1848055974239200	0.5560271959881919	0.4043360582718900	T	T	T
0.2952948493510866	0.5449398259492523	0.5140225015459146	T	T	T
0.4014164728036449	0.5667034250040516	0.3988331872171281	T	T	T
0.3941815068787936	0.5613008949282542	0.2025420270809497	T	T	T

Structure files (CONTCAR) involved in this work:

0.2679486958617778	0.5409612875598552	0.2521703999506470	T	T	T
0.1458452426746412	0.3206820750043421	0.2467106793929957	T	T	T
0.1959743460966293	0.3498730218314696	0.4224205227061517	T	T	T
0.3117537499164627	0.3530377655331214	0.5148543679076973	T	T	T
0.4132097657296377	0.3298718993024707	0.3913518404689654	T	T	T
0.3936757350331163	0.3409105797942419	0.1936615627538197	T	T	T
0.2731048038314910	0.3535045200985795	0.2633600367763206	T	T	T
0.1778745632795891	0.4464952991278696	0.2871272432622432	T	T	T
0.4109345605589126	0.4490817457693310	0.3077759380578997	T	T	T
0.0687203162643245	0.6247758571305524	0.0774537590126181	T	T	T
0.0795919452317633	0.4909429667246507	0.0831971391352783	T	T	T
0.1117207041339935	0.3620594614700639	0.0651695495309857	T	T	T
0.3002372975348739	0.6318482115193076	0.1159470378210521	T	T	T
0.3144726399894261	0.5009635164820627	0.0748724334619488	T	T	T
0.2927284032578695	0.3679845347007391	0.0675656186297044	T	T	T
0.5088018453451724	0.5383465186332405	0.2891661078107206	T	T	T
0.5119015108280991	0.3638382652210482	0.2682390380767901	T	T	T
0.4372206514602024	0.7490648687948753	0.6360424075682739	T	T	T
0.1948825392576447	0.7485989189611496	0.6495226907306797	T	T	T
0.2714710342033511	0.7490703458517713	0.0407961348952868	T	T	T
0.1080925509946698	0.7480200401789019	0.0455947382313061	T	T	T
0.0677427256467848	0.2462665111426487	0.1309610801806362	T	T	T
0.3033187885627602	0.2480249683517902	0.1465505501732734	T	T	T
0.2289593698217770	0.2499850542467801	0.5449326699677129	T	T	T
0.3953495152005672	0.2503298298474538	0.5455740881374330	T	T	T
0.5563789757898401	0.2490699562574042	0.3463158440838213	T	T	T
0.8171451118421986	0.2523777662324805	0.3411289416221137	T	T	T
0.7281350937884523	0.2497995271288488	0.9389438194795504	T	T	T
0.8926126173836501	0.2513395116138946	0.9490400369243128	T	T	T
0.9456313724825184	0.7528924386496921	0.8534593759653286	T	T	T
0.6869183236643441	0.7540734476666576	0.8414621293528004	T	T	T
0.7779815293866992	0.7464979783790282	0.4413884241072612	T	T	T
0.6079478634942813	0.7486523990465331	0.4461833552969683	T	T	T
0.9371499725421037	0.5016919908176214	0.5084586954298367	T	T	T
0.9833215136477194	0.6673844219591091	0.3068655916140214	T	T	T
0.9149013138808920	0.4397329501094344	0.4115042548543615	T	T	T
0.8727675553249823	0.5559124024085900	0.5570755306947510	T	T	T
1.0006287272359642	0.6075253954998817	0.2562969502243586	T	T	T
0.9816897186636692	0.6198486738044465	0.4423343850064183	T	T	T
0.9492835595579331	0.7043403985123041	0.4441493060634103	T	T	T
0.0382958837927622	0.6899948756410875	0.4371004763164822	T	T	T
0.9917583345076419	0.7105629859093774	0.2750506381325248	T	T	T
0.0259029060041854	0.3753924341306233	0.4417440723076199	T	T	T
0.0505430803765900	0.4590861255172111	0.4031607535461541	T	T	T
0.0326684796677543	0.4429213428344574	0.5316264885158580	T	T	T
0.1052426150508079	0.4070948181080064	0.4732265768201762	T	T	T
0.9887797810063118	0.6713662199173069	0.4147860798292330	T	T	T
0.0530698924966285	0.4213404011239673	0.4630061237795085	T	T	T

Figure S10 Zn-TS

Si Al O Zn H C

1.0000000000000000

20.0219999999999985 0.0000000000000000 0.0000000000000000

0.0000000000000000 19.8990000000000009 0.0000000000000000

Structure files (CONTCAR) involved in this work:

0.0000000000000000 0.0000000000000000 13.3829999999999991
93 3 194 2 9 2

Selective dynamics

Direct

0.4235247021940495	0.0585573746220215	0.6475213678869507	T	T	T
0.3070162412743044	0.0278580173550194	0.7930279318657105	T	T	T
0.2829636187228702	0.0564085083149476	0.0154722608034457	T	T	T
0.1242934609267792	0.0599623695785987	0.0107214795618165	T	T	T
0.0690044946833516	0.0308040899251123	0.7996440786516332	T	T	T
0.1824161185901984	0.0587787074915674	0.6623691125916880	T	T	T
0.4192212376788038	0.8257647071306167	0.6667285130405589	T	T	T
0.3056917241746694	0.8693259556141891	0.8079019449020746	T	T	T
0.2669235729942931	0.8294173563788458	0.0248308889599134	T	T	T
0.1123885180318060	0.8258481722599309	0.0102726712182347	T	T	T
0.0660068640882529	0.8736398948679632	0.7969167910197469	T	T	T
0.1841155666793111	0.8280373218925011	0.6720320582393147	T	T	T
0.0780762607403280	0.9394255745296999	0.1482071763972004	T	T	T
0.1955438274004826	0.9695092608676980	0.2939035491364126	T	T	T
0.2194363342236766	0.9396168971813632	0.5154557078192343	T	T	T
0.3788357479900518	0.9350807776506693	0.5123415548600857	T	T	T
0.4347912462296860	0.9672523780933084	0.3003836227575041	T	T	T
0.3207617500438744	0.9386427126441368	0.1635136183271073	T	T	T
0.0836404120772285	0.1699344058697245	0.1657150299582234	T	T	T
0.1961910485207201	0.1283319228776628	0.3094437273393230	T	T	T
0.2342542195602876	0.17010990925558615	0.5252068080879003	T	T	T
0.3891361254933697	0.1732471267481006	0.5080268744779690	T	T	T
0.4364074525117018	0.1258706818746833	0.2946101552843705	T	T	T
0.3161441480866656	0.1693572675747821	0.1711297697991123	T	T	T
0.5767282687851698	0.5541074131791293	0.3516878244947819	T	T	T
0.6899850357793109	0.5262782484946458	0.1974426408225824	T	T	T
0.7127989348779585	0.5694118920874016	0.9811251046527620	T	T	T
0.8709799407802837	0.5728151479911887	0.9820250913829257	T	T	T
0.8100935884682738	0.5479201229336118	0.3436257501441012	T	T	T
0.5730418708399827	0.3281513606855994	0.3295720076359311	T	T	T
0.6938136099405456	0.3721899043391797	0.1904466330064793	T	T	T
0.7305059858328095	0.3265501722034561	0.9794814474491644	T	T	T
0.8851721762261704	0.3248387298555449	0.9927772400848581	T	T	T
0.9437981466069385	0.3733444767375083	0.1870487497147434	T	T	T
0.9182875009316717	0.4444242724770114	0.8595987074907905	T	T	T
0.7993202484153972	0.4719754440416032	0.7183944250677875	T	T	T
0.7747008358949955	0.4357840017396113	0.4947295555751198	T	T	T
0.6164332293521174	0.4275709898996883	0.4894906583616009	T	T	T
0.5660887963369050	0.4682322989034795	0.7037467156323393	T	T	T
0.6747471156708215	0.4467502126118542	0.8540775082815345	T	T	T
0.9197624089071389	0.6775455153089867	0.8266642631319203	T	T	T
0.7705384018446281	0.6671658637436375	0.4624530329928502	T	T	T
0.6144361967352311	0.6711183413209142	0.4836929056553339	T	T	T
0.5602541480336195	0.6268574323619032	0.6962767737056692	T	T	T
0.6710272470183560	0.6752051015766647	0.8239426508422181	T	T	T
0.5795069576134534	0.9438457230646211	0.3544243529245819	T	T	T
0.6993653198211953	0.9731289799670813	0.2102087922823302	T	T	T
0.7218365633257026	0.9379597916707142	0.9884206087039231	T	T	T
0.8824391662416187	0.9334747536616933	0.9919415642708668	T	T	T

Structure files (CONTCAR) involved in this work:

0.9338303154723417	0.9687454046304589	0.2025058436280612	T	T	T
0.8229236710691251	0.9449317844075583	0.3494905562478366	T	T	T
0.5789675021013841	0.1729472569412479	0.3247869327834666	T	T	T
0.6986669164064239	0.1319833086611349	0.1882938164977276	T	T	T
0.7326016157618415	0.1706497519167064	0.9677004087062958	T	T	T
0.8870557493594207	0.1727415871992042	0.9814528707151136	T	T	T
0.9369288843873995	0.1266834681885091	0.1945077864164355	T	T	T
0.8210365479311628	0.1738332312116398	0.3247598425708311	T	T	T
0.9240298978510544	0.0545520880533479	0.8528445535432992	T	T	T
0.8044252132929312	0.0263681205302297	0.7031550480152458	T	T	T
0.7817455671207424	0.0658040651495765	0.4864995155065954	T	T	T
0.6212187910650476	0.0688713702105318	0.4867300105055626	T	T	T
0.5682006969296490	0.0315985337016276	0.6956754525169027	T	T	T
0.6812680665729359	0.0538656596449346	0.8421068187316537	T	T	T
0.9242299892586141	0.8298959224810104	0.8321684533411735	T	T	T
0.8037170502085994	0.8691617563522122	0.6909901810479802	T	T	T
0.7710027205075278	0.8248423931233616	0.4746540407047158	T	T	T
0.6155416205695439	0.8250551326460106	0.4870385202029217	T	T	T
0.5640590571340186	0.8745943105835612	0.6941044693282413	T	T	T
0.6795374057854517	0.8339243568673629	0.8277556920952578	T	T	T
0.4212954577573332	0.4418606835131042	0.6464944364122833	T	T	T
0.3037581051863329	0.4695528500547436	0.7914385646275549	T	T	T
0.2783730083573900	0.4401317703318897	0.0142891757572003	T	T	T
0.1202450459867578	0.4358456493930269	0.0145766182679010	T	T	T
0.0626761498386248	0.4684735156030405	0.8013337547833962	T	T	T
0.1769566593414750	0.4401463222036471	0.6628053479440043	T	T	T
0.4155207218852037	0.6725562097419002	0.6608078856887194	T	T	T
0.3026523736014075	0.6281507934632697	0.8034731033237674	T	T	T
0.2669852785510505	0.6694754194210500	0.0208050065582467	T	T	T
0.1130884582759744	0.6718430171481068	0.0036356103873880	T	T	T
0.0617063450932090	0.6273723697677112	0.7918496585088697	T	T	T
0.1813537081380318	0.6697199257155299	0.6680804614791974	T	T	T
0.0756769004321754	0.5587178827638930	0.1464900932202327	T	T	T
0.1929133042563765	0.5270210632380719	0.2910099141384275	T	T	T
0.2146281449350798	0.5577110484953687	0.5156252995681325	T	T	T
0.3734163290007184	0.5637171571413885	0.5119788517056802	T	T	T
0.4285714358422985	0.5281695905132009	0.3008818167721301	T	T	T
0.3188614964720915	0.5582446879747617	0.1591630349759466	T	T	T
0.0866250343366609	0.3219914256448259	0.1616986285304294	T	T	T
0.1969348164585365	0.3685069989171363	0.3053449572667202	T	T	T
0.2323366011326541	0.3298970179354797	0.5238628857258831	T	T	T
0.3870582517557877	0.3271966938131298	0.5063037839432629	T	T	T
0.4316951994340240	0.3710778691840813	0.2911656834160808	T	T	T
0.3146685477812487	0.3274016559387801	0.1677656901796138	T	T	T
0.9205049657189331	0.5269738854834339	0.1883309735800280	T	T	T
0.8224311902905522	0.3366915791486867	0.3236486541037449	T	T	T
0.7970501590408318	0.6352855169531533	0.6942475177726909	T	T	T
0.3583909313506330	0.0663113250018247	0.7189253985433086	T	T	T
0.3152184435730525	0.0590152826223715	0.9043012562403254	T	T	T
0.2032851067009980	0.0422078269840969	0.0078873194758471	T	T	T
0.0947188396993551	0.0696233977778688	0.8992034702602606	T	T	T
0.1059081102286743	0.0618367433567791	0.7020117862634490	T	T	T
0.2304959158435032	0.0383381996781725	0.7556817634244775	T	T	T

Structure files (CONTCAR) involved in this work:

0.3614977954391089	0.8242771288158451	0.7518617762612304	T	T	T
0.3078807704307547	0.8518353400768436	0.9258846342416868	T	T	T
0.1892553477202616	0.8524483703749491	0.0133348266786864	T	T	T
0.0842983517627473	0.8318428000404416	0.8974969691401290	T	T	T
0.1064833671551621	0.8413529880242798	0.7027690696496236	T	T	T
0.2314943486012993	0.8518990789976573	0.7646562059843846	T	T	T
0.3239317715432236	0.9479432641181565	0.7907453412733162	T	T	T
0.0877210260789803	0.9515519906475102	0.8111905123928477	T	T	T
0.4330517973880071	0.1270162057866860	0.5829737802017438	T	T	T
0.4160210082892973	0.9953310982687105	0.5716748377290070	T	T	T
0.3918222278626821	0.8638066521559039	0.5675833851818123	T	T	T
0.2029227923942437	0.1325683846214298	0.6216523636561090	T	T	T
0.1872036755974451	0.0030765225030821	0.5740781242154643	T	T	T
0.2025158242401218	0.8691939351207251	0.5711149664494808	T	T	T
0.9893933475360929	0.0409454363112599	0.7839713500606587	T	T	T
0.9861551339298782	0.8683924217398076	0.7765018745386472	T	T	T
0.1437364842863438	0.9325594830367807	0.2186433060526591	T	T	T
0.1873482272958104	0.9364968246824965	0.4040930581265586	T	T	T
0.2994437961753226	0.9507949086672275	0.5087803310571243	T	T	T
0.4090265368983127	0.9294451231326656	0.4007286947282993	T	T	T
0.3968841828695310	0.9351941240821260	0.2042547145001956	T	T	T
0.2718076568194754	0.9588465098301769	0.2559233100469960	T	T	T
0.1399644058146751	0.1721344662784298	0.2525890374867461	T	T	T
0.1929307400164203	0.1478228288364330	0.4265656501254927	T	T	T
0.3117868760470085	0.1480166295936446	0.5108285370542923	T	T	T
0.4172293672555564	0.1674589028618079	0.3950085023416727	T	T	T
0.3940770246021643	0.1566729445328946	0.2009515993372733	T	T	T
0.2701694801269378	0.1451201112478635	0.2652668455762507	T	T	T
0.1786951563433695	0.0492637204916721	0.2950046063401424	T	T	T
0.4177511669547851	0.0470212960838551	0.3094128313508924	T	T	T
0.0676034253785174	0.8689498111252963	0.0883893864399437	T	T	T
0.0851975940923330	0.9991547559498727	0.0664010769431870	T	T	T
0.1123486626233303	0.1296146609384183	0.0698417035636002	T	T	T
0.2999755285481674	0.8651041142179178	0.1215058597285000	T	T	T
0.3170085243509664	0.9945687844685100	0.0755723441911349	T	T	T
0.2970667366667351	0.1274689621497048	0.0709706132548472	T	T	T
0.5141103622961836	0.9545764955080657	0.2844537598549891	T	T	T
0.5160316486240127	0.1335978072463068	0.2733044641137273	T	T	T
0.6352407888935092	0.5611347134143067	0.2695755675438508	T	T	T
0.6992702898063433	0.5740221652609073	0.1004697684377201	T	T	T
0.7919155833018711	0.5625866868079916	0.9546154283662152	T	T	T
0.8827570855794946	0.5769724618398309	0.1005738339191584	T	T	T
0.8845466681413111	0.5260884635389728	0.3084184556751255	T	T	T
0.7601550795757780	0.5234760640470320	0.2574547642252315	T	T	T
0.6400762681275382	0.3367337775582939	0.2647614909100453	T	T	T
0.6901518698641432	0.3322398735269813	0.0840342158670931	T	T	T
0.8078740517383143	0.3502176506734978	0.9947894264428483	T	T	T
0.9139974955389344	0.3197495953377905	0.1063738883957635	T	T	T
0.9055597029729823	0.3639948962972628	0.2944840190966895	T	T	T
0.7669668209619491	0.3694534655667164	0.2381818814407545	T	T	T
0.6694937743929459	0.4497933099702213	0.1692288539924086	T	T	T
0.9355823170722954	0.4478835969780178	0.1447690840680915	T	T	T
0.5690340342219523	0.6252514121891563	0.4099313508266236	T	T	T

Structure files (CONTCAR) involved in this work:

0.5927594393994577	0.4960724278842995	0.4338073250114052	T	T	T
0.5806121519575828	0.3628068523061075	0.4394661316190328	T	T	T
0.8033156436969385	0.6283164878380398	0.3665633765632750	T	T	T
0.7910431353117588	0.5127431490041519	0.4528282936469147	T	T	T
0.8242490473529595	0.3853056114108170	0.4360101806100672	T	T	T
0.0055151664404203	0.5601941334496433	0.2154125303331905	T	T	T
0.0221909475307109	0.3579232609679577	0.2105190680194239	T	T	T
0.8530350570103498	0.4336955189033741	0.7885275800788191	T	T	T
0.7943210748468827	0.4331347770526379	0.6118924488880702	T	T	T
0.6968745472753768	0.4187948554779744	0.4765221704975296	T	T	T
0.5965766262306385	0.4299673545634169	0.6064580163148363	T	T	T
0.6011304469297554	0.4397424208100268	0.8044339542285024	T	T	T
0.7260475246588169	0.4731304069099482	0.7680562689179521	T	T	T
0.8584193097276505	0.6810946535858140	0.7508663766497806	T	T	T
0.8132072268668299	0.6437632984211406	0.5618902046676468	T	T	T
0.6924459713787998	0.6465869344952051	0.4784313705147988	T	T	T
0.5864144246684186	0.6648400019688564	0.5963512007613994	T	T	T
0.5925172522784022	0.6637389433858482	0.7932552117833560	T	T	T
0.7171627962125321	0.6475743055657099	0.7341818805515613	T	T	T
0.8241774556140647	0.5490749729109714	0.6956273969295464	T	T	T
0.5809289989327648	0.5480358785203248	0.6915819554665704	T	T	T
0.9290226787927484	0.3767661410110622	0.9258022652484713	T	T	T
0.9108426308175972	0.5096320594272695	0.9309556375596846	T	T	T
0.8999100867804364	0.6412857944154001	0.9314891806913138	T	T	T
0.6965525836126689	0.3736136822204827	0.8948210851066385	T	T	T
0.6734240619114765	0.5025907360473649	0.9422091611819353	T	T	T
0.6839195366361963	0.6369451192551232	0.9297564945469302	T	T	T
0.4867571746239501	0.4527997720997883	0.7156163516735189	T	T	T
0.4793099868761024	0.6315990928277352	0.7039586506045373	T	T	T
0.6450715717033224	0.9388121899281643	0.2840348301287751	T	T	T
0.6979094542682909	0.9341029022742381	0.1039072470785035	T	T	T
0.8025715933487946	0.9438773777304297	0.9803867774638314	T	T	T
0.9034906734331573	0.9267486082238167	0.1085786035044105	T	T	T
0.8987322722604512	0.9454547397499243	0.3061738795381834	T	T	T
0.7733054295651427	0.9647860340328440	0.2582056860008362	T	T	T
0.6415140320598878	0.1731945192339795	0.2483169927788224	T	T	T
0.6949077623531786	0.1550966739906199	0.0723932553924490	T	T	T
0.8101034900120541	0.1463083828108299	0.9774482086378765	T	T	T
0.9148856476559910	0.1670708560283750	0.0946538903718087	T	T	T
0.8976909823662167	0.1551902497352904	0.2914354758725223	T	T	T
0.7719916916881584	0.1473823833363591	0.2344132256196322	T	T	T
0.6820388831104753	0.0521140517334139	0.1963209635017896	T	T	T
0.9204490787260187	0.0474731155004527	0.1796129928591472	T	T	T
0.5713439779523246	0.8738787267951151	0.4161192071274625	T	T	T
0.5840231595192069	0.0056294072818006	0.4335820617913518	T	T	T
0.6002755479363953	0.1377761587824655	0.4298520653600125	T	T	T
0.8083843513626859	0.8695605880896108	0.3905493024374967	T	T	T
0.8161659218109045	0.9986376716831546	0.4398518801080756	T	T	T
0.8039003796898018	0.1327415716047403	0.4272232573143249	T	T	T
0.0130211448378815	0.9529628687869280	0.2172228951876285	T	T	T
0.0169547197148357	0.1353651118226039	0.2114503745371851	T	T	T
0.8586799805452743	0.0550558659101075	0.7818711634697945	T	T	T
0.8061017071761519	0.0717572179882351	0.6022605859217175	T	T	T

Structure files (CONTCAR) involved in this work:

0.7011039431363139	0.0565782248240073	0.4805484103434132	T	T	T
0.5972938895064386	0.0752980393053184	0.6023886950205519	T	T	T
0.6055591053591127	0.0508815543472971	0.7992759602868944	T	T	T
0.7304770101261796	0.0301182014545805	0.7522929278579410	T	T	T
0.8593821084230913	0.8341841788263072	0.7607436547106547	T	T	T
0.8067898076983453	0.8324620209721821	0.5827832261971629	T	T	T
0.6934712178206658	0.8485969797394803	0.4827951934872432	T	T	T
0.5890717734875007	0.8281330661521472	0.6015015839644129	T	T	T
0.6035205151428834	0.8534283367400224	0.7953048789683652	T	T	T
0.7299294359662448	0.8598895372955914	0.7398307895345619	T	T	T
0.8206912170835570	0.9483793854446573	0.6765887100393397	T	T	T
0.5787768111000701	0.9527518876658312	0.6675626240980080	T	T	T
0.9321542930158498	0.1273739638461823	0.9063809156931526	T	T	T
0.9194928784219906	0.9971771466105082	0.9394948243679502	T	T	T
0.9068941409882253	0.8644844163096126	0.9389676520676198	T	T	T
0.6972552286924950	0.1301935730738126	0.8767534613741711	T	T	T
0.6886195570160606	0.0041804272971409	0.9377349121787485	T	T	T
0.6973564999186150	0.8699706243620040	0.9330790417902981	T	T	T
0.4896347974562456	0.0475031417998955	0.7152848673142429	T	T	T
0.4845743163724997	0.8632490390441969	0.7121183106121485	T	T	T
0.3559048668254962	0.4318841744884064	0.7173410226352336	T	T	T
0.3089298816704921	0.4366941520744396	0.9021306215679701	T	T	T
0.1986461009534075	0.4571074976781341	0.0123015846943135	T	T	T
0.0895501591743805	0.4338328845397794	0.9034378730574727	T	T	T
0.1013826349629133	0.4352477634556517	0.7064563854240499	T	T	T
0.2273891947974064	0.4602714117119334	0.7530031834037396	T	T	T
0.3567181630401626	0.6731663033276961	0.7441522024239476	T	T	T
0.3065822069349527	0.6496646245141533	0.9197441146618812	T	T	T
0.1896664453445753	0.6450598005679953	0.0089454289545991	T	T	T
0.0853211352093740	0.6685942666808445	0.8907130156188272	T	T	T
0.1031984827735558	0.6568496115719898	0.6964226838767240	T	T	T
0.2278127280765518	0.6419660528298423	0.7595358985115273	T	T	T
0.3217500730475368	0.5492133319279354	0.7923627168510339	T	T	T
0.0792255755904079	0.5483781956834585	0.8065865310105383	T	T	T
0.4318729012468006	0.3753780042308889	0.5775902928407493	T	T	T
0.4140071756983448	0.5067218519315919	0.5734822503120849	T	T	T
0.3865921667194238	0.6373796099833358	0.5599301572437928	T	T	T
0.1975584379281184	0.3675927814300159	0.6176443899401174	T	T	T
0.1780782427538608	0.4976517497703845	0.5765267823209803	T	T	T
0.1982736182091096	0.6305491569861792	0.5644709367132509	T	T	T
0.9834390447657458	0.4545394298090477	0.7878449594843783	T	T	T
0.9823949691252652	0.6373431362860598	0.7731843949778149	T	T	T
0.1382635035895356	0.5664314760814743	0.2220429266442981	T	T	T
0.1852886263199585	0.5573530032805399	0.4025959761732990	T	T	T
0.2945253258464964	0.5445825914219620	0.5155655080477805	T	T	T
0.3994748069396600	0.5668237919630366	0.3980729808685188	T	T	T
0.3944798511807741	0.5608036633784298	0.2020042332135195	T	T	T
0.2678532110533773	0.5403293784325578	0.2503632747236944	T	T	T
0.1451736846110940	0.3212037359199451	0.2454070073012986	T	T	T
0.1925336448375732	0.3511625831490341	0.4230491514501259	T	T	T
0.3098795326280399	0.3530213713029409	0.5129717113552898	T	T	T
0.4118845791735137	0.3292018245646512	0.3911152253536026	T	T	T
0.3928568697798552	0.3409624126400534	0.1939640265934546	T	T	T

Structure files (CONTCAR) involved in this work:

0.2719751893435694	0.3534533921632749	0.2644713956761907	T	T	T
0.1767294639963029	0.4470270537852965	0.2871470129352255	T	T	T
0.4099559618343034	0.4488838070421575	0.3083118985500224	T	T	T
0.0681599149049730	0.6245043399271911	0.0765238916354846	T	T	T
0.0789695060993742	0.4905789983965649	0.0821367142442044	T	T	T
0.1121093266394638	0.3618332109173303	0.0626810420690001	T	T	T
0.3005563785230015	0.6316957430469852	0.1151567948024880	T	T	T
0.3150705647447892	0.5010767758140473	0.0730393322559984	T	T	T
0.2919776604767370	0.3683613792734532	0.0682665198010669	T	T	T
0.5083747975476133	0.5375373523442106	0.2923103830108545	T	T	T
0.5112015049334914	0.3639364719402148	0.2703302531129821	T	T	T
0.4370022915602974	0.7491340513539699	0.6350317023937003	T	T	T
0.1950881065493162	0.7488522710655240	0.6486602908938871	T	T	T
0.2712121260846010	0.7491446062455236	0.0413460805484371	T	T	T
0.1079719526166058	0.7479175872859457	0.0458077329542224	T	T	T
0.0686944282135667	0.2459659837183764	0.1286650592258438	T	T	T
0.3024654933341978	0.2481354276693689	0.1470190892515890	T	T	T
0.2274537625826970	0.2500607174024839	0.5434456124277338	T	T	T
0.3937790299768497	0.2505172357655774	0.5459793215429671	T	T	T
0.5565929548808501	0.2494988846341312	0.3483101456567853	T	T	T
0.8136188549336607	0.2523683812474198	0.3444619665989863	T	T	T
0.7277723352570952	0.2496584566672567	0.9397246880583088	T	T	T
0.8910224749117794	0.2502571064441189	0.9439960227638012	T	T	T
0.9458032505835042	0.7529973341077564	0.8539093157782228	T	T	T
0.6855983316923304	0.7541515540679710	0.8445839265039848	T	T	T
0.7774517252270859	0.7467857023882142	0.4407546937166831	T	T	T
0.6086215075118697	0.7485369392608542	0.4467012671286457	T	T	T
0.9373511943196705	0.5074500583501194	0.5063622792296861	T	T	T
0.9850789831304924	0.6661116605228717	0.3090520373723948	T	T	T
0.9220729580469178	0.4321610612299271	0.4093753764401395	T	T	T
0.8757459042283788	0.5607036846308611	0.5653061727604503	T	T	T
0.0007045983818878	0.6056831589441648	0.2568286095015508	T	T	T
0.9823318356227272	0.6186617604032568	0.4445402065460981	T	T	T
0.9505726011791362	0.7033067502714340	0.4459927122804672	T	T	T
0.0394926918498798	0.6883709822826761	0.4400615919522254	T	T	T
0.9928836848373259	0.7094591011600857	0.2774345622675319	T	T	T
0.0197511099266311	0.3634015222346593	0.4492840105748112	T	T	T
0.0551502980547242	0.4360460874435483	0.3905050175847359	T	T	T
0.9853462321636404	0.4685223926816595	0.4975718948436954	T	T	T
0.0567844859373228	0.4256051502082007	0.5226309267900227	T	T	T
0.9899952134853298	0.6701236621614902	0.4169862627420550	T	T	T
0.0263332845865697	0.4182571439437497	0.4550612293482230	T	T	T

Figure S10 Zn-FS

Si Al O Zn H C

1.0000000000000000

20.0219999999999985 0.0000000000000000 0.0000000000000000

0.0000000000000000 19.8990000000000009 0.0000000000000000

0.0000000000000000 0.0000000000000000 13.3829999999999991

93 3 194 2 9 2

Selective dynamics

Direct

0.4231628931501809 0.0589849561123131 0.6466527540527077 T T T

0.3067268520606149 0.0278797377244879 0.7922615711953571 T T T

Structure files (CONTCAR) involved in this work:

0.2826844479973022	0.0565078739662473	0.0143784044009321	T	T	T
0.1240128384120596	0.0589807610550730	0.0099207265563490	T	T	T
0.0690918452148706	0.0303966727605049	0.7993387610181545	T	T	T
0.1820094681677245	0.0585597531348064	0.6613625332110631	T	T	T
0.4187642440802570	0.8258808791513759	0.6673675053470636	T	T	T
0.3050421498067747	0.8695360668242229	0.8079607241996245	T	T	T
0.2662215813254813	0.8294979561988612	0.0257658723953358	T	T	T
0.1116408780903515	0.8253669048514187	0.0123815318198123	T	T	T
0.0660813597983582	0.8734573978524441	0.7984146803903797	T	T	T
0.1834815530834412	0.8283956902608361	0.6715818165697813	T	T	T
0.0770422513358501	0.9393157090629968	0.1476308162542538	T	T	T
0.1949433380093538	0.9701029733745773	0.2926456773774763	T	T	T
0.2190372553212980	0.9397876849016755	0.5144170819997623	T	T	T
0.3787056299079438	0.9351378007384862	0.5122732242976433	T	T	T
0.4343837375049034	0.9679867312154959	0.3005602894000672	T	T	T
0.3207305294672434	0.9393860429326826	0.1623500625074353	T	T	T
0.0826043373296847	0.1701297268867966	0.1648438064404556	T	T	T
0.1947222456019968	0.1288692644538093	0.3089652935635347	T	T	T
0.2330185382348373	0.1700747471137543	0.5250153142153794	T	T	T
0.3875939290675288	0.1735829774155526	0.5080948560213193	T	T	T
0.4350754077363205	0.1267043439249482	0.2950054029853567	T	T	T
0.3150301387202272	0.1697264967257481	0.1703181107304662	T	T	T
0.5769374183738493	0.5554098252469730	0.3506886580800391	T	T	T
0.6896298223304573	0.5272493037509338	0.1987482703047830	T	T	T
0.7140407467909097	0.5683974746905215	0.9809980581511881	T	T	T
0.8719064757540240	0.5721269367195893	0.9829262259323157	T	T	T
0.8105638136860632	0.5503427404833274	0.3442404718358946	T	T	T
0.5728085185437642	0.3287407016309081	0.3296021142015872	T	T	T
0.6935426967468050	0.3733975088381534	0.1916294708048761	T	T	T
0.7312707526644775	0.3271131121820246	0.9782041334134431	T	T	T
0.8859528156253412	0.3241765603485936	0.9858845849762649	T	T	T
0.9419892448306745	0.3695173934374080	0.1848315429448200	T	T	T
0.9187135863993502	0.4451950008332215	0.8574334641886869	T	T	T
0.7983175057879600	0.4727685514174188	0.7176383160255581	T	T	T
0.7786792361594445	0.4360222306295930	0.4937538270760090	T	T	T
0.6208112196970601	0.4292025609486890	0.4868973481132392	T	T	T
0.5678916182286654	0.4690062139045870	0.7006617340413025	T	T	T
0.6743764938638810	0.4459546077774613	0.8535962808673887	T	T	T
0.9199549697821316	0.6774413212575531	0.8285343126583000	T	T	T
0.7669937440988991	0.6694176881724836	0.4631800781512906	T	T	T
0.6120438455146988	0.6722135537839198	0.4841075059469713	T	T	T
0.5586074917381200	0.6274920117758520	0.6961607553689246	T	T	T
0.6686371690777519	0.6752791600520498	0.8264236323471159	T	T	T
0.5789398738372619	0.9441437769025847	0.3548358737225084	T	T	T
0.6987680283795263	0.9735157343104905	0.2117408329308357	T	T	T
0.7214593376797656	0.9388504129856670	0.9895675934502137	T	T	T
0.8818185138479824	0.9341931693803184	0.9921260618284296	T	T	T
0.9327566547505375	0.9707859610825238	0.2031143166596530	T	T	T
0.8227323332517342	0.9453718974695108	0.3505260138599885	T	T	T
0.5781105691463352	0.1737685788372290	0.3261109477367073	T	T	T
0.6971488129254483	0.1320067845155361	0.1895605218336506	T	T	T
0.7316402747425030	0.1704921267807336	0.9681208848190543	T	T	T
0.8858841236271432	0.1724350588113443	0.9779805058354457	T	T	T

Structure files (CONTCAR) involved in this work:

0.9346882289834187	0.1294345156330439	0.1937353307585775	T	T	T
0.8187938943826903	0.1752360134775935	0.3266449334528463	T	T	T
0.9240831041391214	0.0536944339412783	0.8517622223014382	T	T	T
0.8029854569949055	0.0253526459843262	0.7041360300867680	T	T	T
0.7820768516172592	0.0654229487716023	0.4873668086099901	T	T	T
0.6215506445654669	0.0689763401550822	0.4867770905426486	T	T	T
0.5678592776903121	0.0317463042112355	0.6956061667115482	T	T	T
0.6799117677232567	0.0540646961522827	0.8436949296435189	T	T	T
0.9238137436785049	0.8300095443364106	0.8333705263488025	T	T	T
0.8027119347904541	0.8676253472394544	0.6915888672786248	T	T	T
0.7689547789605312	0.8263184576427302	0.4749856726214380	T	T	T
0.6141960882685399	0.8261483636561116	0.4879350668072022	T	T	T
0.5632441461189658	0.8747659550740926	0.6952473749323023	T	T	T
0.6784814929259362	0.8332888702294288	0.8303199052104088	T	T	T
0.4218277467843606	0.4422563295283095	0.6432371631124680	T	T	T
0.3039804140888804	0.4695224765535111	0.7894814808290866	T	T	T
0.2779417120456801	0.4405131772744405	0.0118302292096545	T	T	T
0.1204194128368176	0.4357419824828365	0.0122535501580245	T	T	T
0.0625653508385205	0.4699003599310700	0.8002013470218986	T	T	T
0.1761624959905700	0.4406321707050446	0.6603047393890724	T	T	T
0.4144480217486156	0.6727320978496998	0.6598642928694346	T	T	T
0.3015909849704305	0.6282562826031632	0.8025230720321745	T	T	T
0.2669016280275831	0.6696680345555436	0.0205845657109010	T	T	T
0.1129672161555501	0.6714542457578474	0.0039960381842080	T	T	T
0.0618245805356995	0.6285780287468004	0.7917050157840009	T	T	T
0.1807990686688411	0.6701946344157133	0.6669234621657224	T	T	T
0.0755644311913985	0.5575260060533437	0.1452884284725932	T	T	T
0.1933333765120347	0.5270610413085842	0.2892812490689075	T	T	T
0.2140602766249223	0.5583624983509829	0.5141934653613178	T	T	T
0.3726627318540058	0.5644274003192473	0.5105539074057487	T	T	T
0.4277882529285942	0.5274315472528269	0.3009039848522495	T	T	T
0.3194387630027067	0.5579718408253491	0.1572246251338355	T	T	T
0.0867759163582818	0.3220199193099423	0.1572663015671565	T	T	T
0.1961140243011237	0.3682155402762146	0.3035577105991486	T	T	T
0.2305268508500290	0.3297324561500545	0.5226762892210687	T	T	T
0.3848518778646657	0.3270793946764177	0.5053401792775087	T	T	T
0.4298914246424737	0.3705693411367000	0.2911993782750928	T	T	T
0.3138160747749073	0.3276493530664460	0.1660463507852521	T	T	T
0.9196424627729719	0.5254996196030665	0.1909748352577665	T	T	T
0.8223970336444528	0.3355047335841677	0.3239947030596567	T	T	T
0.7952094807665063	0.6371141513503209	0.6967161712806630	T	T	T
0.3580125431986606	0.0662671478551628	0.7180669278102401	T	T	T
0.3144633315241913	0.0599839618781933	0.9029693989196222	T	T	T
0.2030852015591635	0.0416181246384890	0.0072982866737521	T	T	T
0.0947198565113322	0.0699751240143864	0.8983564835947577	T	T	T
0.1055719039961420	0.0609816531136273	0.7011763226686286	T	T	T
0.2302837468015857	0.0373946739626085	0.7540449124792949	T	T	T
0.3607197515573329	0.8242399896800718	0.7520193425861348	T	T	T
0.3061603728740451	0.8516414448593034	0.9257783469482973	T	T	T
0.1883529521197860	0.8524033658953595	0.0166544417221367	T	T	T
0.0843695475594098	0.8317951704338836	0.8991547772777426	T	T	T
0.1059505722798342	0.8408444369477820	0.7038601525565713	T	T	T
0.2310495592703954	0.8527677774403943	0.7635648278626620	T	T	T

Structure files (CONTCAR) involved in this work:

0.3241371965906119	0.9480304370190723	0.7916325817275583	T	T	T
0.0882793237256236	0.9512822215218870	0.8119671820463448	T	T	T
0.4323043316102615	0.1274899312414924	0.5821523961042677	T	T	T
0.4159076339018076	0.9956056211296953	0.5710109694902057	T	T	T
0.3921993136506861	0.8640827110246507	0.5678814252195151	T	T	T
0.2018398319577729	0.1327635684710974	0.6217627797201852	T	T	T
0.1869004917339788	0.0037524883630933	0.5718431338114633	T	T	T
0.2008058688838069	0.8697854972983149	0.5704433681004578	T	T	T
0.9894692186592378	0.0399895286378740	0.7830716117758278	T	T	T
0.9861066337991363	0.8685532368927597	0.7788502430707492	T	T	T
0.1425928882679656	0.9330410002045121	0.2183911366759532	T	T	T
0.1878594085074227	0.9364631640728007	0.4025832893212936	T	T	T
0.2991957139539020	0.9502585674759071	0.5093055307269977	T	T	T
0.4085305310365434	0.9295880752831919	0.4004081112282175	T	T	T
0.3966271985295698	0.9363444841448982	0.2040417338134077	T	T	T
0.2710597904196198	0.9602626418728176	0.2534967756364658	T	T	T
0.1379721001792471	0.1724952633500388	0.2531277475349769	T	T	T
0.1918854022425610	0.1477012663842039	0.4263215796075415	T	T	T
0.3105177784420698	0.1477174311650224	0.5111615038222632	T	T	T
0.4151366052230496	0.1684216507072458	0.3948136979375887	T	T	T
0.3928082127527227	0.1568183748887037	0.2008654228979511	T	T	T
0.2684273017647636	0.1462732285831278	0.2641871003142440	T	T	T
0.1776229546127214	0.0497021333697323	0.2944052772620063	T	T	T
0.4172301251297659	0.0476802906171351	0.3103249326567240	T	T	T
0.0661355008573303	0.8676991808871585	0.0907724986868080	T	T	T
0.0850639745964586	0.9968749646615186	0.0626332403034617	T	T	T
0.1116019426632207	0.1274802172327896	0.0714482020646121	T	T	T
0.3004017898797089	0.8654234500803645	0.1213599960822889	T	T	T
0.3175670108311215	0.9945480298850711	0.0732577715932198	T	T	T
0.2963376115232918	0.1273610535622353	0.0704859522974590	T	T	T
0.5137662119492443	0.9556106864110863	0.2846789256574693	T	T	T
0.5146580967658356	0.1354093410645413	0.2745983438933370	T	T	T
0.6331373505213203	0.5648627068421617	0.2651268067409591	T	T	T
0.7029120772229451	0.5731130831388241	0.1008468694275611	T	T	T
0.7929947120860911	0.5640588080464898	0.9520025039210722	T	T	T
0.8825130718971737	0.5752567936551636	0.1014995755837470	T	T	T
0.8854028722680539	0.5330896965580805	0.3106756016139249	T	T	T
0.7578652579263577	0.5232699416857038	0.2640202704844904	T	T	T
0.6380592697299334	0.3358843381394504	0.2605892923670097	T	T	T
0.6932271594415053	0.3348458294477538	0.0841370662372135	T	T	T
0.8089493240601481	0.3510588495245460	0.9883083982454173	T	T	T
0.9158863290783253	0.3182471413224288	0.0977660598999348	T	T	T
0.9051805905845230	0.3512972113317872	0.2889568375283867	T	T	T
0.7652831699677992	0.3716856244398680	0.2439205055386720	T	T	T
0.6680712184492279	0.4508960078008270	0.1719586126471171	T	T	T
0.9294289494549884	0.4453203878823956	0.1496027129699018	T	T	T
0.5672197148098763	0.6262040542250672	0.4096564257735644	T	T	T
0.5984965501308798	0.4982587293315291	0.4314584096518115	T	T	T
0.5832335978471107	0.3652921364083745	0.4377387079068176	T	T	T
0.8007518323575882	0.6301814637406937	0.3688173876318629	T	T	T
0.7951354778372214	0.5145215705848384	0.4560077765323282	T	T	T
0.8308628173746671	0.3871876179395655	0.4357750804981588	T	T	T
0.0056870401166724	0.5579757815426941	0.2144699041170316	T	T	T

Structure files (CONTCAR) involved in this work:

0.0219018175848910	0.3585651501001100	0.2023267001717564	T	T	T
0.8529796775719191	0.4359823013829991	0.7873211419669918	T	T	T
0.7959252697635308	0.4328141447549759	0.6115425598096145	T	T	T
0.7013531765380994	0.4188261354558280	0.4717447270352566	T	T	T
0.6022423642948110	0.4323441891138085	0.6045261543721553	T	T	T
0.6006809329872239	0.4412940734577476	0.8036496513910159	T	T	T
0.7250085182121128	0.4718264433210994	0.7663181592554176	T	T	T
0.8575914448128991	0.6804528761984290	0.7545543134133689	T	T	T
0.8103302983399511	0.6477362153414181	0.5633886997215853	T	T	T
0.6898162466350213	0.6466771018531441	0.4801797787714999	T	T	T
0.5835958858210822	0.6666893778221930	0.5965072879603223	T	T	T
0.5904399075273007	0.6639428847836978	0.7938861679407827	T	T	T
0.7153274252189832	0.6503698502649051	0.7355367157459922	T	T	T
0.8202618355407425	0.5504193410806418	0.6937916927605825	T	T	T
0.5808583154156423	0.5492206317173742	0.6895696314959385	T	T	T
0.9302851170643415	0.3756472142478601	0.9184136770314570	T	T	T
0.9115136726749179	0.5085017960232925	0.9322936560461272	T	T	T
0.9023333235568481	0.6403918972432909	0.9335383806182720	T	T	T
0.6949694705149608	0.3721841930559331	0.8930375359735382	T	T	T
0.6757581358116926	0.5005736513116120	0.9434329316946792	T	T	T
0.6818132396172668	0.6345466360600629	0.9300205288651101	T	T	T
0.4888760256802617	0.4518362347779648	0.7090790154976719	T	T	T
0.4775950979751091	0.6309744119312577	0.7037640728395290	T	T	T
0.6446168746972788	0.9380276931693577	0.2847348097620446	T	T	T
0.6986085836547425	0.9343786492243423	0.1054868626855177	T	T	T
0.8020918159033001	0.9453312014525466	0.9798860155982524	T	T	T
0.9025114042364715	0.9288474352615376	0.1089773534091156	T	T	T
0.8983282994985082	0.9454198354909535	0.3063609824921413	T	T	T
0.7726357807932003	0.9666503092704644	0.2605641403895554	T	T	T
0.6396397512801923	0.1737942686734695	0.2477735024565435	T	T	T
0.6948927369963958	0.1545797241344450	0.0733725817427545	T	T	T
0.8090697490840228	0.1453991365627676	0.9748937695702711	T	T	T
0.9134438823799296	0.1673751647344601	0.0913766098117968	T	T	T
0.8955258826672865	0.1612810941973436	0.2885162939196806	T	T	T
0.7700555371808875	0.1470451355738902	0.2371089545153054	T	T	T
0.6799104920758918	0.0521913285993696	0.1979959690610816	T	T	T
0.9178984226176851	0.0497353302204625	0.1837450858046335	T	T	T
0.5694993020238192	0.8744689766355104	0.4170108670019306	T	T	T
0.5841787761880836	0.0057601006423833	0.4340092881437530	T	T	T
0.6000007885372872	0.1377703276187375	0.4302568244739888	T	T	T
0.8072772639844017	0.8699906235672720	0.3908003165106612	T	T	T
0.8167942063379068	0.9978703728681859	0.4425162624112858	T	T	T
0.8061933692529689	0.1315599988235170	0.4282244064526780	T	T	T
0.0122257450905095	0.9556466331185619	0.2158802804400345	T	T	T
0.0147967763502949	0.1377141814236571	0.2103328634948284	T	T	T
0.8585464847598633	0.0528503918614369	0.7814876951877070	T	T	T
0.8046392159543704	0.0712715745754382	0.6038826048776924	T	T	T
0.7014269608257396	0.0569658417331160	0.4789878364994808	T	T	T
0.5983119603839991	0.0750586499387353	0.6028403025588103	T	T	T
0.6045019823232846	0.0503139431743831	0.8000054168339484	T	T	T
0.7296434013920191	0.0299196728031074	0.7548376803415767	T	T	T
0.8599145506519926	0.8339648199292425	0.7599820015706376	T	T	T
0.8055101034854393	0.8315160523155701	0.5828430981912807	T	T	T

Structure files (CONTCAR) involved in this work:

0.6917979233456950	0.8511381115737783	0.4841977138158970	T	T	T
0.5878827536702230	0.8281726882631529	0.6024907670216841	T	T	T
0.6031264022145966	0.8540656961325170	0.7962615149136889	T	T	T
0.7296856711995395	0.8556326645679174	0.7414455838700095	T	T	T
0.8174810107448407	0.9471681449804661	0.6767700303030666	T	T	T
0.5775853281939599	0.9527737154742346	0.6676490192444838	T	T	T
0.9316148389690102	0.1268328893790071	0.9040816799294762	T	T	T
0.9201181518631663	0.9968902311294157	0.9392692675180644	T	T	T
0.9052192464200645	0.8645164205432725	0.9398562276633722	T	T	T
0.6949014662354687	0.1307584361268161	0.8776246480585791	T	T	T
0.6872745869765804	0.0049446255014827	0.9400283064075731	T	T	T
0.6970533383213861	0.8709693598398091	0.9339396292403609	T	T	T
0.4894014202540528	0.0484820678724477	0.7142065994712057	T	T	T
0.4838991814893128	0.8630791357216236	0.7139838670177148	T	T	T
0.3575066525886066	0.4330044962882217	0.7163522210293435	T	T	T
0.3086558965432589	0.4359432377064611	0.8997942360686654	T	T	T
0.1983821418767762	0.4585686128122624	0.0081297724201744	T	T	T
0.0880691637363962	0.4341847529915857	0.9019205750512930	T	T	T
0.1007136397020979	0.4370288750053606	0.7048632593030932	T	T	T
0.2279886329468788	0.4598786225586250	0.7492418323890668	T	T	T
0.3551051282007380	0.6733220876039284	0.7422193439455896	T	T	T
0.3055949174644385	0.6508273115407818	0.9183293799980438	T	T	T
0.1896067235546517	0.6448176895214269	0.0098438401174780	T	T	T
0.0857569336177405	0.6694943444703095	0.8905454306948393	T	T	T
0.1025322185367825	0.6579911969822562	0.6955373455080323	T	T	T
0.2267201641261758	0.6414303476768913	0.7582699805278847	T	T	T
0.3210550935362642	0.5493903195040597	0.7925591289740862	T	T	T
0.0796647626762184	0.5496213043041196	0.8063887090886886	T	T	T
0.4308573999762972	0.3757936069133765	0.5739295391948538	T	T	T
0.4140894860574701	0.5075469137639623	0.5710597850507187	T	T	T
0.3861606395348779	0.6381462577342398	0.5581363277202742	T	T	T
0.1948975902048764	0.3675796231065606	0.6155166908658255	T	T	T
0.1770082136325961	0.4982167557106378	0.5741643655371297	T	T	T
0.1970417805091587	0.6311300712874987	0.5629505571737806	T	T	T
0.9829807694137264	0.4576560298828947	0.7840204144943375	T	T	T
0.9824259478130677	0.6381797920299517	0.7729880070430757	T	T	T
0.1384820343562282	0.5660102316600961	0.2200286687291029	T	T	T
0.1859898602269643	0.5581615896216434	0.4004976097184722	T	T	T
0.2939060503701772	0.5451366432620751	0.5163731259262437	T	T	T
0.3973341829044743	0.5675169803425939	0.3959251076242339	T	T	T
0.3951829737374583	0.5592159913650339	0.2001870248439917	T	T	T
0.2682374501065998	0.5403640784181244	0.2482428571862507	T	T	T
0.1441598333696306	0.3216571093436510	0.2429351876270553	T	T	T
0.1916141571546447	0.3501113612659626	0.4209333911054343	T	T	T
0.3080063569627504	0.3535012489177772	0.5136645643917346	T	T	T
0.4085726275967112	0.3277663018425446	0.3895633088737842	T	T	T
0.3920283543995532	0.3416304774014104	0.1922985333230627	T	T	T
0.2712161808842057	0.3527311317992000	0.2632019132212488	T	T	T
0.1775988930365155	0.4471385976705675	0.2859676963732536	T	T	T
0.4084336039114173	0.4483847373400444	0.3097928385515417	T	T	T
0.0676702200940120	0.6231413652310944	0.0748954170558339	T	T	T
0.0786577772929499	0.4892299065808005	0.0813024119141667	T	T	T
0.1145970461687640	0.3612105721177408	0.0588463416445091	T	T	T

Structure files (CONTCAR) involved in this work:

0.3018558492158395	0.6317766966942262	0.1137304593115399	T	T	T
0.3149164838950833	0.5014645958921103	0.0701906240139557	T	T	T
0.2906990008026852	0.3690464695906037	0.0671408359720129	T	T	T
0.5078666578301296	0.5356592902974305	0.2955394639055573	T	T	T
0.5096056658334387	0.3634899583589975	0.2724841436165939	T	T	T
0.4365859008846338	0.7492888242675376	0.6353460585557962	T	T	T
0.1952086591001017	0.7492780613731670	0.6480684588463164	T	T	T
0.2706221470434728	0.7492251674643324	0.0422971621808566	T	T	T
0.1074435512351449	0.7472501387816243	0.0472208507277105	T	T	T
0.0699907736709117	0.2456776023582108	0.1241979516202802	T	T	T
0.3019825592676551	0.2483912846865300	0.1446892189458293	T	T	T
0.2262350456143068	0.2499984478817697	0.5431333949718633	T	T	T
0.3916778485869530	0.2507819963766573	0.5465608333115350	T	T	T
0.5570674781104712	0.2503813639770431	0.3521401981885577	T	T	T
0.8060069744146408	0.2526573014454040	0.3504984186285376	T	T	T
0.7273195513980355	0.2496541592229803	0.9414691932452958	T	T	T
0.8895454752670532	0.2492941253487723	0.9373958191596774	T	T	T
0.9452850777992636	0.7531438949146974	0.8556024319979655	T	T	T
0.6823147868938020	0.7537945734244690	0.8515929343346731	T	T	T
0.7729145217847138	0.7484832586485788	0.4394176908969097	T	T	T
0.6080946780606163	0.7496496539480559	0.4468334762438984	T	T	T
0.9361830739526432	0.5096867693355349	0.5210815897604802	T	T	T
0.9879968984033821	0.6645114322594996	0.3099627821796496	T	T	T
0.9329037485352850	0.4131782082634435	0.4302129242831421	T	T	T
0.8655626419879490	0.5635257579308798	0.5583699678482913	T	T	T
0.0014235457593018	0.6027085472781116	0.2568829185706643	T	T	T
0.9848478392976183	0.6181649339622087	0.4464732640195466	T	T	T
0.9521613543055462	0.7022796399606348	0.4458313595934363	T	T	T
0.0412841572779147	0.6879610856698504	0.4414257788131704	T	T	T
0.9949704181533793	0.7078190120948195	0.2776765049169742	T	T	T
1.0473218121813446	0.3552086263538402	0.4180967040472320	T	T	T
0.0477123030843920	0.4389210200699770	0.3703198968401510	T	T	T
0.9664691213805617	0.4988815483356456	0.5759200092284268	T	T	T
0.0516184823240734	0.4255671263667575	0.5020368189249097	T	T	T
0.9920796339595072	0.6693511403270473	0.4176962450893572	T	T	T
1.0303022682173104	0.4067317176782637	0.4318900619007220	T	T	T

Figure S10 Ga-IS

Si Al O Ga H C

1.0000000000000000

20.0219999999999985 0.0000000000000000 0.0000000000000000

0.0000000000000000 19.8990000000000009 0.0000000000000000

0.0000000000000000 0.0000000000000000 13.3829999999999991

93 3 193 1 10 2

Selective dynamics

Direct

0.4218904926815678	0.0580784327121771	0.6483674519103902	T	T	T
0.3020928374189639	0.0275936466564866	0.7905718785742857	T	T	T
0.2800084127865840	0.0598595685794682	0.0142149900569832	T	T	T
0.1199163156334771	0.0633925368086919	0.0126051156247718	T	T	T
0.0664862583101500	0.0297476903114489	0.7989050322213752	T	T	T
0.1773139738325343	0.0567936976794408	0.6541272767171161	T	T	T
0.4199060666745488	0.8273975621457785	0.6718815705035939	T	T	T
0.3025872576341873	0.8690391242734775	0.8104619753648097	T	T	T

Structure files (CONTCAR) involved in this work:

0.2670125705227641	0.8288894560746409	0.0299898595916506	T	T	T
0.1119630392289832	0.8268596030897806	0.0169197552128312	T	T	T
0.0614991832723283	0.8703617127383672	0.8020190925251670	T	T	T
0.1802024970652717	0.8275782319166216	0.6755090578634274	T	T	T
0.0758165366662951	0.9425723181806047	0.1513568758930205	T	T	T
0.1957246065291598	0.9720666302661797	0.2947701301102708	T	T	T
0.2171303809424102	0.9370520282555812	0.5159873269773322	T	T	T
0.3771444723379392	0.9338931220550644	0.5160360696433280	T	T	T
0.4313578461350996	0.9689426113291245	0.3048881215572566	T	T	T
0.3203416234770994	0.9435302904199815	0.1589108420558693	T	T	T
0.0790119455014203	0.1727498506880799	0.1649935727223961	T	T	T
0.1958561741797572	0.1299363708398295	0.3075071340122005	T	T	T
0.2312187832586262	0.1728542027806719	0.5244961513568931	T	T	T
0.3858595363594683	0.1741140028989072	0.5112771436165552	T	T	T
0.4369873149158238	0.1271447207891292	0.3014880845662436	T	T	T
0.3187839851009165	0.1674889720728551	0.1724479948950482	T	T	T
0.5832075848468530	0.5565855528104384	0.3462680436259136	T	T	T
0.6956592876543313	0.5304566759870789	0.1865817296748412	T	T	T
0.7127899663533371	0.5646908061313511	0.9720498766942495	T	T	T
0.8714019702455880	0.5590931230417781	0.9742994600845752	T	T	T
0.9338235953041373	0.5291799826220092	0.1867215617806524	T	T	T
0.5773634676217223	0.3287240828981117	0.3290099482876200	T	T	T
0.7056092599971057	0.3739943737745688	0.2102809370768918	T	T	T
0.7352960275183875	0.3291546280805775	0.9905331679716030	T	T	T
0.8865346951432889	0.3278541506335934	0.9799792750678106	T	T	T
0.9361800503071537	0.3717979052241185	0.1975198910825068	T	T	T
0.9257719011868496	0.4364774367720525	0.8375624287074137	T	T	T
0.7802472664365425	0.4410190685364541	0.4771938252585166	T	T	T
0.6205508127727728	0.4326763612551094	0.4887751580781537	T	T	T
0.5662965811072612	0.4658814626504609	0.7048834505571024	T	T	T
0.6727278954499261	0.4347527583964959	0.8511573614633088	T	T	T
0.9179548848642146	0.6722023622873625	0.8275019637842491	T	T	T
0.7998252727944882	0.6328839321954279	0.6960123448962976	T	T	T
0.7679753636986998	0.6684063720080106	0.4789007653570387	T	T	T
0.6118512860064549	0.6708849605070725	0.4850126812116543	T	T	T
0.5637514757077414	0.6245689522393391	0.7022897441558985	T	T	T
0.6809278418346666	0.6809881662888241	0.8230537697745205	T	T	T
0.5757650520165223	0.9436024844648808	0.3636189141701561	T	T	T
0.6949868646756894	0.9722908038875939	0.2192124945565840	T	T	T
0.7184782563180870	0.9425261232098915	0.9971143400114016	T	T	T
0.8785847209905849	0.9342576479677246	0.9948134581989730	T	T	T
0.9317403786361832	0.9692225322018593	0.2067888177277560	T	T	T
0.8198022078774965	0.9386342729038273	0.3519371617995470	T	T	T
0.5811398063271948	0.1742251216990051	0.3332667869223073	T	T	T
0.6986277427109155	0.1304457034855893	0.1983010490882254	T	T	T
0.7323244534093440	0.1720969624862468	0.9776495508434626	T	T	T
0.8867521840788964	0.1731509112302131	0.9934451053510096	T	T	T
0.9348305672477298	0.1280494547048677	0.2058675936892480	T	T	T
0.8194133053473330	0.1685240752568122	0.3386835344707639	T	T	T
0.9232576000641207	0.0578822476217220	0.8605416013630354	T	T	T
0.8048370092608699	0.0294087898254357	0.7206535273733997	T	T	T
0.7812115745810111	0.0563172575454610	0.4951553084835343	T	T	T
0.6211917281321303	0.0679692335694033	0.4936284261402816	T	T	T

Structure files (CONTCAR) involved in this work:

0.5668221638235026	0.0338208816469476	0.7020001911594904	T	T	T
0.6781992860091433	0.0584778517500476	0.8507824219584315	T	T	T
0.9171907152742937	0.8249085957253280	0.8388071217126623	T	T	T
0.8025136328739152	0.8735464655515536	0.7037478567825273	T	T	T
0.7676923745348296	0.8298163951827576	0.4872335050132376	T	T	T
0.6123316353565051	0.8263309681678216	0.4974467913107027	T	T	T
0.5621974182313846	0.8770943050213886	0.7037657839576347	T	T	T
0.6777993472164112	0.8376290103147296	0.8360598854910489	T	T	T
0.4214926060800591	0.4444017667835723	0.6411762026254944	T	T	T
0.3053328641092629	0.4720653733977638	0.7908457955379402	T	T	T
0.2836409458994434	0.4349332500137820	0.0100470263422091	T	T	T
0.1262003553350429	0.4326152510109816	0.0035913914259572	T	T	T
0.0733531207414555	0.4719923660705777	0.7960606600427054	T	T	T
0.1837109895321370	0.4485475333854435	0.6502787490768398	T	T	T
0.4233707101712313	0.6728489276723943	0.6646447505731221	T	T	T
0.3028456538734083	0.6291207899251196	0.8003596101963414	T	T	T
0.2689132685109520	0.6717662513023254	0.0193053700599323	T	T	T
0.1147316514040845	0.6738236345693021	0.0074353422952018	T	T	T
0.0652569369676987	0.6292690894739205	0.7985269604473717	T	T	T
0.1805193812961291	0.6688088362827342	0.6648668412707660	T	T	T
0.0785206888829298	0.5542069147994932	0.1349081175503700	T	T	T
0.1980629946599168	0.5282749285539927	0.2822498440594181	T	T	T
0.2213671285932832	0.5671254231668604	0.5024712005643275	T	T	T
0.3830289512722114	0.5706225351988937	0.5041846050506495	T	T	T
0.4365883573530052	0.5284991762746327	0.2950707101855981	T	T	T
0.3259110432074353	0.5542291187068472	0.1486948389289174	T	T	T
0.0818074321163389	0.3273753195029298	0.1578771582427765	T	T	T
0.1955833617442235	0.3693999119039298	0.3049510279289576	T	T	T
0.2317983478603383	0.3303592113727894	0.5232136430502405	T	T	T
0.3861088435350851	0.3275604359510073	0.5062422007017359	T	T	T
0.4342940379250223	0.3709877442017365	0.2929541635177507	T	T	T
0.3160413177666952	0.3262638363616462	0.1684655716095230	T	T	T
0.8117442124490095	0.5655965242100142	0.3234267062067930	T	T	T
0.8277131714804589	0.3273212119088740	0.3474266659321639	T	T	T
0.7961342821917412	0.4735777647631739	0.7225485127517464	T	T	T
0.3563294586612608	0.0640375839973692	0.7190534981813845	T	T	T
0.3030256566760589	0.0644438885329862	0.8984705093805492	T	T	T
0.1996294954729503	0.0507096404372722	0.0238372977104002	T	T	T
0.0985502830644048	0.0662222404924115	0.8962451033067449	T	T	T
0.1019789130566726	0.0585081167319761	0.6986326902546174	T	T	T
0.2278800516466004	0.0347528250831014	0.7432324891645220	T	T	T
0.3580545484541271	0.8259508955201843	0.7502363024407660	T	T	T
0.3052267173058968	0.8461922602206418	0.9263760641873729	T	T	T
0.1892618882250273	0.8522647577953414	0.0201503930275058	T	T	T
0.0837594076753176	0.8327420124112771	0.9041489358713518	T	T	T
0.1023959166946577	0.8372609188250446	0.7086314038041741	T	T	T
0.2282706303696137	0.8542205127465482	0.7655241988540855	T	T	T
0.3204326102531657	0.9483347766444139	0.8008372579289204	T	T	T
0.0796019740012065	0.9494671751871908	0.8090976853731791	T	T	T
0.4301318641723055	0.1271938866306079	0.5847859680815551	T	T	T
0.4160383589112345	0.9950977006911819	0.5712864199763561	T	T	T
0.3964042078731891	0.8628879258600897	0.5682612180411043	T	T	T
0.1952457144232535	0.1312995796504781	0.6134156953938851	T	T	T

Structure files (CONTCAR) involved in this work:

0.1805567661366958	0.0024679985065662	0.5636130261187277	T	T	T
0.1947072615488299	0.8684892737411514	0.5728129526334361	T	T	T
0.9874389553861530	0.0460513530151750	0.7885600732305658	T	T	T
0.9816726723889276	0.8603088908677766	0.7854337879630473	T	T	T
0.1422168429478484	0.9374638006687867	0.2201954949848272	T	T	T
0.1943104811541421	0.9314203966782080	0.3999982833233263	T	T	T
0.2973346276518381	0.9471566843834091	0.5254762822377830	T	T	T
0.3993196584758649	0.9294339007256336	0.3999357589206493	T	T	T
0.3958402476767203	0.9434037247502798	0.2025709642950934	T	T	T
0.2702489924459214	0.9672989377737767	0.2477781086804375	T	T	T
0.1421374073414402	0.1708080756133513	0.2408441896466780	T	T	T
0.1927321608646171	0.1603106796423293	0.4195928883022758	T	T	T
0.3085055395475058	0.1484124626648307	0.5140128563078900	T	T	T
0.4139685935608953	0.1705496234187258	0.3981518511098643	T	T	T
0.3963557298731862	0.1548741798442074	0.2041701349848643	T	T	T
0.2706947223750831	0.1395376942784796	0.2618421991718025	T	T	T
0.1764015342144413	0.0506753688636918	0.3104145369661365	T	T	T
0.4184891309276601	0.0488559702361046	0.3208646821911740	T	T	T
0.0669190749518590	0.8715788748007206	0.0924308253443386	T	T	T
0.0811128785475306	0.0025661529634173	0.0691498379863565	T	T	T
0.0988364783122436	0.1346961699864502	0.0618154604138379	T	T	T
0.3019535685866542	0.8680809623603698	0.1221672468179917	T	T	T
0.3157806134787463	0.9949175987652834	0.0647671822786002	T	T	T
0.3028587773693470	0.1288663283057495	0.0685226123886132	T	T	T
0.5103585192379234	0.9530667060178651	0.2933820096401026	T	T	T
0.5168461045717623	0.1357601644692869	0.2841031537729625	T	T	T
0.6460747107604398	0.5616160246394948	0.2716202002371397	T	T	T
0.6767661063682467	0.5661678281010099	0.0804161077559259	T	T	T
0.7921229896918683	0.5473030380594053	0.9850413130849978	T	T	T
0.9080168512629725	0.5606525448673012	0.0829308252823678	T	T	T
0.8997306241386660	0.5687956888850388	0.2845110260301965	T	T	T
0.7718194392896471	0.5476891994980480	0.2135376782455735	T	T	T
0.6410334905458523	0.3348524231472235	0.2564245801903143	T	T	T
0.7267977135103952	0.3319909876363433	0.1104669866069332	T	T	T
0.8106780540338880	0.3552467431205716	0.9611624950222766	T	T	T
0.9086240318702121	0.3379384228216393	0.0947461026803570	T	T	T
0.9063722245161311	0.3364161390915033	0.2945972387882363	T	T	T
0.7663307019350065	0.3749277133632570	0.2886940906437312	T	T	T
0.6825110425223959	0.4495889892005620	0.1783124054395281	T	T	T
0.9147531157794194	0.4513433530597802	0.1953444016155733	T	T	T
0.5708630139885055	0.6285673030366349	0.4009702541814518	T	T	T
0.5968779084955648	0.5010851384167994	0.4335004279972292	T	T	T
0.5887644506183036	0.3676356109277381	0.4345148206764878	T	T	T
0.8022324000805072	0.6431471643372245	0.3779106434062526	T	T	T
0.8026989707236923	0.5011378689159965	0.4086594795976249	T	T	T
0.8279963424454360	0.3717281904428359	0.4677142310113097	T	T	T
0.0129043407187935	0.5442208737944468	0.2054173612145052	T	T	T
0.0177887655749593	0.3697222804782296	0.1968169795751652	T	T	T
0.8713255248121284	0.4253573605592156	0.7464041808284753	T	T	T
0.8104656449200185	0.4553650469696590	0.5930868307756892	T	T	T
0.7016589528840524	0.4265387404923885	0.4865653496308869	T	T	T
0.5957198476047735	0.4326125050490121	0.6033495787769091	T	T	T
0.598430787754897	0.4289077966183402	0.8015047869173400	T	T	T

Structure files (CONTCAR) involved in this work:

0.7291988251991695	0.4295084184942424	0.7657509642743894	T	T	T
0.8635883012641912	0.6754913299172256	0.7382749684495761	T	T	T
0.8054360701672190	0.6336777153436898	0.5748499939952313	T	T	T
0.6892758711031289	0.6469121244731885	0.4847433838425600	T	T	T
0.5801118218617681	0.6575269175788970	0.5944787537223120	T	T	T
0.6046770379631136	0.6628949642903575	0.7902702684478480	T	T	T
0.7300436123280380	0.6701278515395748	0.7271512303048046	T	T	T
0.8020820418584781	0.5580777168536804	0.7419937060768282	T	T	T
0.5841484161602580	0.5456922837512088	0.7036100679351371	T	T	T
0.9356436002000774	0.3691129871257186	0.9040073865456030	T	T	T
0.9021276998902584	0.4975251352147248	0.9087356454334133	T	T	T
0.8894272189512948	0.6302142421159578	0.9222397293291416	T	T	T
0.6804825662419374	0.3751182797775814	0.9337771459501479	T	T	T
0.6769498706684537	0.5078914359913013	0.9047983583301817	T	T	T
0.7049287773819283	0.6372338955112083	0.9184741824359501	T	T	T
0.4859861415777377	0.4555690031857120	0.7116624614619314	T	T	T
0.4837296946865349	0.6337000043309664	0.7219925196695889	T	T	T
0.6412521232232041	0.9370844088091906	0.2930785575904268	T	T	T
0.6916000120084429	0.9361275786895885	0.1108148969635217	T	T	T
0.7992233106326837	0.9501338879202968	0.9928343073339144	T	T	T
0.9045527967217896	0.9289249270895985	0.1091950525702734	T	T	T
0.8952643964758062	0.9415161598035442	0.3071701245040955	T	T	T
0.7698595607307924	0.9625454855247665	0.2631455073435123	T	T	T
0.6422297458270985	0.1747701651753046	0.2544048378910672	T	T	T
0.6967600812224937	0.1523469911444305	0.0820471709975367	T	T	T
0.8099725271527204	0.1473401901759425	0.9829509443559427	T	T	T
0.9102048771383433	0.1710111993599970	0.1091719966926847	T	T	T
0.8971669073750679	0.1557302139381570	0.3046423483078929	T	T	T
0.7721431832564984	0.1428788230332700	0.2457509158281320	T	T	T
0.6780849819119275	0.0516722823540250	0.2094014959391965	T	T	T
0.9178830467412705	0.0488351871240759	0.1893577587019981	T	T	T
0.5665896710208166	0.8749743306339272	0.4281062316376683	T	T	T
0.5807023249609172	0.0069828924963367	0.4399808391383654	T	T	T
0.6045881305700694	0.1378531031576061	0.4363493457066709	T	T	T
0.8029402238887065	0.8623953684683932	0.3886061995328462	T	T	T
0.8134102243067377	0.9886410559388810	0.4472581802573516	T	T	T
0.8055921778890910	0.1226162939915544	0.4371102775481753	T	T	T
0.0112333567878755	0.9551492389595669	0.2218816169669892	T	T	T
0.0152789800789369	0.1375042745283945	0.2190740988493101	T	T	T
0.8572750796613247	0.0690795287909262	0.7918908734671916	T	T	T
0.8073637734061162	0.0614967033009161	0.6097305928057822	T	T	T
0.7002573069525914	0.0505678651801689	0.4902475729850990	T	T	T
0.5966842546098980	0.0767361535745265	0.6086552268355663	T	T	T
0.6029595117340288	0.0551077932725059	0.8058916776115772	T	T	T
0.7291082509252103	0.0360607329755232	0.7623274106643826	T	T	T
0.8549121674712907	0.8250468483863074	0.7613707477571113	T	T	T
0.8055812006127954	0.8585491659200905	0.5854513462552765	T	T	T
0.6894079106556905	0.8519753822234094	0.4908941534624621	T	T	T
0.5867533443907845	0.8290944817099175	0.6126473159667076	T	T	T
0.6012297223281691	0.8560317875324687	0.8055210722206102	T	T	T
0.7270767769362221	0.8612255187719211	0.7452837595713387	T	T	T
0.8261026475815788	0.9506155463487100	0.7225574531182034	T	T	T
0.5789134062505165	0.9547500084072071	0.6765388009761129	T	T	T

Structure files (CONTCAR) involved in this work:

0.9351171972830985	0.1254013473707410	0.9265761594753246	T	T	T
0.9170189640783823	0.9941990334927114	0.9359445321349789	T	T	T
0.8962285577821554	0.8630701554629858	0.9414118599258768	T	T	T
0.6943109585112576	0.1346758834719836	0.8861014149944620	T	T	T
0.6847443269319853	0.0083655162055596	0.9461256857369469	T	T	T
0.6968961355742640	0.8746836191026800	0.9394750451236150	T	T	T
0.4876470902397366	0.0486621463368456	0.7175250125152519	T	T	T
0.4822868402751407	0.8677835543809919	0.7217070177277981	T	T	T
0.3560494141839460	0.4377225006035944	0.7119948176662695	T	T	T
0.3079508934875589	0.4299485629635651	0.8946016524371759	T	T	T
0.2042923134130321	0.4528948435325250	0.0152783953385234	T	T	T
0.1054712034949628	0.4280415623830030	0.8864329113030897	T	T	T
0.1068462489188827	0.4531152392737827	0.6890873608903141	T	T	T
0.2303207893835624	0.4691050026510889	0.7445928820615813	T	T	T
0.3565490657205859	0.6684902633390223	0.7325420729013047	T	T	T
0.3021053536183923	0.6641195019412078	0.9094342038185872	T	T	T
0.1913586361671714	0.6468940396137287	0.0141827195660531	T	T	T
0.0906182347439839	0.6748503653965028	0.8916782935135403	T	T	T
0.1031241786998481	0.6544122735205846	0.6972734421902930	T	T	T
0.2291900486674953	0.6349864671194977	0.7486616471956654	T	T	T
0.3240141774331844	0.5505081210622507	0.8107285364245767	T	T	T
0.0833617212997331	0.5511427912983496	0.8217668167098382	T	T	T
0.4310114091545709	0.3758380132122745	0.5770244561321201	T	T	T
0.4135638485885982	0.5068296526520545	0.5640416592245004	T	T	T
0.4082732788219205	0.6397459759259790	0.5558498322093767	T	T	T
0.1980351244281661	0.3723332334279769	0.6140662346531255	T	T	T
0.1935175562274807	0.4997020125437324	0.5569378541831105	T	T	T
0.1926781958249962	0.6345225803629019	0.5560156980497354	T	T	T
0.9949586089725723	0.4544308809599110	0.7813379462959472	T	T	T
0.9853714984826523	0.6369544638303464	0.7824904964815502	T	T	T
0.1430704837345363	0.5612839240681839	0.2074296011803973	T	T	T
0.1930441077322202	0.5677855008193849	0.3884719111078170	T	T	T
0.3020032235638231	0.5664903616312480	0.5059817349904564	T	T	T
0.4094216534951406	0.5709066035642717	0.3903554770532424	T	T	T
0.4005839774427851	0.5576681768452643	0.1951127293074010	T	T	T
0.2726409402984556	0.5369811162307692	0.2374032734328918	T	T	T
0.1391365885468897	0.3289165832666607	0.2434223499971820	T	T	T
0.1912774465957584	0.3453572302454014	0.4203988090335612	T	T	T
0.3089594334062660	0.3539882956277224	0.5089344648355347	T	T	T
0.4127166770099804	0.3290814822196759	0.3920842941049710	T	T	T
0.3932585449575992	0.3423286878144187	0.1969439074560231	T	T	T
0.2693081614371651	0.3538244827333081	0.2597027993882075	T	T	T
0.1802500139411183	0.4495180731966668	0.2975333506300440	T	T	T
0.4166843287090138	0.4498828559501593	0.3105491675273891	T	T	T
0.0680996540806821	0.6233925237375144	0.0725768050958725	T	T	T
0.0826762006738321	0.4912954768913346	0.0581215417957904	T	T	T
0.1108930544580830	0.3604886696932569	0.0550097648143666	T	T	T
0.3088909083261349	0.6266719520134919	0.0999162684353147	T	T	T
0.3240305198208084	0.4953198093171438	0.0646522216493743	T	T	T
0.2968432500711058	0.3631842579852373	0.0639326571038055	T	T	T
0.5165939003220896	0.5368889244092844	0.2830565865507753	T	T	T
0.5132140854918396	0.3610945535776354	0.2711219540476000	T	T	T
0.4422655960444702	0.7510189170138939	0.6467363763010082	T	T	T

Structure files (CONTCAR) involved in this work:

0.1945325464801320	0.7485490468174559	0.6542012518906347	T	T	T
0.2724290557765860	0.7493641722939707	0.0546487197595271	T	T	T
0.1077994403061115	0.7489097397950836	0.0529194253094317	T	T	T
0.0616588790053692	0.2500041480827198	0.1358341934967224	T	T	T
0.3046731538517922	0.2465655948784942	0.1532976140335993	T	T	T
0.2270059351975049	0.2518241775658469	0.5531387027844479	T	T	T
0.3905451123941350	0.2514564731915805	0.5491842090553677	T	T	T
0.5612587198320638	0.2512418929370571	0.3579947341442968	T	T	T
0.8059166911530299	0.2450368214868758	0.3670981524792934	T	T	T
0.7273683455254579	0.2516964159156215	0.9545902469136015	T	T	T
0.8928861217445078	0.2491749052804521	0.9509060586891790	T	T	T
0.9354698239714512	0.7474919273830626	0.8662580151873503	T	T	T
0.6847720741239400	0.7584473706080355	0.8578243785475712	T	T	T
0.7750485008053778	0.7494947952257230	0.4860598316069760	T	T	T
0.6053144007286032	0.7499632797900304	0.4571624233616297	T	T	T
0.9833661640890605	0.6409613291567756	0.3749070946929665	T	T	T
0.8784436651517580	0.3878056911931602	0.5978506339849755	T	T	T
0.9372362328377019	0.3384612201136968	0.6057171601507649	T	T	T
0.9323026730827237	0.5998166455845794	0.3255479260502082	T	T	T
0.9902175536216170	0.6315387762442284	0.5321564604013207	T	T	T
0.9314727878568140	0.6911976640731948	0.4838741683959211	T	T	T
0.0191127751140131	0.7097690547316712	0.4804485203220785	T	T	T
1.0282208543901106	0.6255248256893576	0.3585449773551794	T	T	T
0.9406618480966150	0.4587783674108030	0.4542374784756827	T	T	T
0.0055982007915858	0.5180659079034037	0.4681066187491437	T	T	T
0.9559413134280964	0.4996366175019433	0.5741694549410054	T	T	T
1.0142616378344251	0.4382285473274418	0.5271314695049831	T	T	T
0.9814587666795896	0.6698236783818551	0.4743309407395034	T	T	T
0.9786121839708620	0.4776626045175166	0.5066882728852795	T	T	T

Figure S10 Ga-TS

Si Al O Ga H C

1.0000000000000000

20.0219999999999985 0.0000000000000000 0.0000000000000000

0.0000000000000000 19.8990000000000009 0.0000000000000000

0.0000000000000000 0.0000000000000000 13.3829999999999991

93 3 193 1 10 2

Selective dynamics

Direct

0.4217213175552045	0.0572682262932821	0.6475733297733702	T	T	T
0.3010491241212284	0.0268317302946554	0.7893277220416670	T	T	T
0.2796556080356864	0.0604776914823235	0.0125289716062042	T	T	T
0.1199483663308637	0.0631757870742186	0.0118776798588476	T	T	T
0.0672309121884154	0.0295738304162490	0.7988730509552632	T	T	T
0.1765751994466780	0.0558762480765670	0.6510278713357595	T	T	T
0.4197597100403510	0.8272082424577262	0.6707679774014407	T	T	T
0.3017880737399702	0.8684146013159759	0.8095933698155422	T	T	T
0.2667816288065412	0.8283035639201765	0.0298259082628708	T	T	T
0.1116606577300224	0.8263198957087535	0.0176660072943202	T	T	T
0.0617372994627813	0.8704643916289496	0.8027732861708048	T	T	T
0.1792337986767195	0.8277755237873768	0.6734583739671398	T	T	T
0.0753398418558046	0.9428715400595645	0.1501391252562716	T	T	T
0.1960863151012057	0.9728910996440704	0.2930493608508070	T	T	T
0.2168784111046778	0.9367565804721844	0.5139897062368318	T	T	T

Structure files (CONTCAR) involved in this work:

0.3766474897380438	0.9335863168568899	0.5151944747212480	T	T	T
0.4303292920583729	0.9692980656506478	0.3041361377645159	T	T	T
0.3205179206512269	0.9447823788595728	0.1554535037770755	T	T	T
0.0781737968132245	0.1727668842924029	0.1640964812172678	T	T	T
0.1954017056816356	0.1302535796648498	0.3070930658619967	T	T	T
0.2307288340638823	0.1730586666835599	0.5240110111689029	T	T	T
0.3852980553291945	0.1738833270786884	0.5116356745583774	T	T	T
0.4362497601083153	0.1275393129834139	0.3013933919995091	T	T	T
0.3182882812769634	0.1676019712779550	0.1713038464739674	T	T	T
0.5828714248547410	0.5549053314460448	0.3507433050658175	T	T	T
0.6967899539505134	0.5288986757786093	0.1907473325111651	T	T	T
0.7138918734678155	0.5657981031350828	0.9770842745416178	T	T	T
0.8723415530291920	0.5622247125192079	0.9815333686063653	T	T	T
0.9323518543260060	0.5295958432723790	0.1905326756178542	T	T	T
0.5757212223533975	0.3299857174900354	0.3331846428091277	T	T	T
0.7037567446446872	0.3742907902073166	0.2070402486196129	T	T	T
0.7310083530802858	0.3269281050529563	0.9915309854686496	T	T	T
0.8829676580320389	0.3273964461790654	0.9797380028080543	T	T	T
0.9373574732022180	0.3720161193835058	0.1926480242693105	T	T	T
0.9280270708883931	0.4414249188472280	0.8470050914179440	T	T	T
0.7791742228447064	0.4390916458220801	0.4839154232971086	T	T	T
0.6212566066916887	0.4304771815790511	0.4906967875143314	T	T	T
0.5690529623456594	0.4672205394065470	0.7050724792724576	T	T	T
0.6699600555471997	0.4364693309831207	0.8609977961746680	T	T	T
0.9182943754583210	0.6728395091579604	0.8301606617530373	T	T	T
0.7996256504833649	0.6361285667709231	0.6940472869800917	T	T	T
0.7688034155180413	0.6713265894503675	0.4762482837630131	T	T	T
0.6133238042315816	0.6715202852268646	0.4854718390997639	T	T	T
0.5650490518174724	0.6256784666039266	0.7022159706117552	T	T	T
0.6815391690364172	0.6813719608158847	0.8239100752826471	T	T	T
0.5749131917124565	0.9436788074176996	0.3640414555252499	T	T	T
0.6939197314399540	0.9733175445543459	0.2198401536396522	T	T	T
0.7174995893227385	0.9420911997826152	0.9984454802122148	T	T	T
0.8776423020562515	0.9344563220350739	0.9946010944576125	T	T	T
0.9312491930628451	0.9707328186967509	0.2051560457931772	T	T	T
0.8197896916662112	0.9428319832480092	0.3519003106510976	T	T	T
0.5799554450830475	0.1748998883783171	0.3337237813690290	T	T	T
0.6971303889471723	0.1308508261100259	0.1988344298398649	T	T	T
0.7309196309418927	0.1712562349300837	0.9772035358679065	T	T	T
0.8849409061512509	0.1733553672940822	0.9923351600464659	T	T	T
0.9332667756063914	0.1292888710651068	0.2044918136660709	T	T	T
0.8180615827914187	0.1705199086840855	0.3383208782305031	T	T	T
0.9231291460211887	0.0581189335831543	0.8605731845202710	T	T	T
0.8043582428024024	0.0297972256849559	0.7208372171627301	T	T	T
0.7805271818947285	0.0600673828015308	0.4952544960724060	T	T	T
0.6205347985065139	0.0683089964268780	0.4932027382097326	T	T	T
0.5668091857454670	0.0324881742971508	0.7011462065198047	T	T	T
0.6771108203311735	0.0570376979755591	0.8519936236841849	T	T	T
0.9174085880391623	0.8256474454976580	0.8388558031118716	T	T	T
0.8025442681038881	0.8738361469114302	0.7038779563401628	T	T	T
0.7668216613374433	0.8325111424170258	0.4859152613629596	T	T	T
0.6121539329912492	0.8265171179177037	0.4968958668710997	T	T	T
0.5621008202744768	0.8760450685344221	0.7029904563942100	T	T	T

Structure files (CONTCAR) involved in this work:

0.6776618413033710	0.8373693600873251	0.8370642656389540	T	T	T
0.4231197789983634	0.4452728333498506	0.6391181044208145	T	T	T
0.3048195906147638	0.4734395845744982	0.7888269127135881	T	T	T
0.2854185423768351	0.4343688341724893	0.0075971327959697	T	T	T
0.1289476129428012	0.4328963281757749	0.0048363969486329	T	T	T
0.0760338835911328	0.4730107184652393	0.7978120724908115	T	T	T
0.1826774404426068	0.4494202014444642	0.6460986539553787	T	T	T
0.4240580031800354	0.6722840633928797	0.6638608737290970	T	T	T
0.3017285109915694	0.6301197865226965	0.7993718456375299	T	T	T
0.2693138286668308	0.6722332223550742	0.0182917287199453	T	T	T
0.1151952339901729	0.6734495757905938	0.0082521201958570	T	T	T
0.0656971928310791	0.6301008799200771	0.7995003888029889	T	T	T
0.1793105561736779	0.6692657766636466	0.6627931486822078	T	T	T
0.0782041710913089	0.5535767291269970	0.1356852200331042	T	T	T
0.1997068067625898	0.5282218392288573	0.2800306555266420	T	T	T
0.2214935038936821	0.5676029386965094	0.5017167907955631	T	T	T
0.3824283778310491	0.5705038352443358	0.5041818863551198	T	T	T
0.4345698195423208	0.5280684430649339	0.2960528909990558	T	T	T
0.3278682347052933	0.5529663054846935	0.1430951334685803	T	T	T
0.0829256870083325	0.3275486390761538	0.1549410458781283	T	T	T
0.1959706865987849	0.3697632772336819	0.3037837280189520	T	T	T
0.2314635080700700	0.3299393242393561	0.5225754914174663	T	T	T
0.3857101414244127	0.3272851976047465	0.5074590001953262	T	T	T
0.4334224131764954	0.3708948660029032	0.2939659803336446	T	T	T
0.3165384005937520	0.3262782774656764	0.1666666436934305	T	T	T
0.8118652250690781	0.5631450380990820	0.3344403299468374	T	T	T
0.8285968209802921	0.3297913121778640	0.3371878115098061	T	T	T
0.7929804181980642	0.4750474590103526	0.7253941939303831	T	T	T
0.3563544443365556	0.0622937573358162	0.7186729264930413	T	T	T
0.2999132691907089	0.0657508831388002	0.8956956746127326	T	T	T
0.1995305060635249	0.0509329381189222	0.0265443371669552	T	T	T
0.1007290554272896	0.0667974565494211	0.8946300156717847	T	T	T
0.1015933546662332	0.0571994210489110	0.6969667040768907	T	T	T
0.2277396346399305	0.0325910701534422	0.7386176295369579	T	T	T
0.3575321211292807	0.8263094830733066	0.7484324253102325	T	T	T
0.3038425008219897	0.8434963920166594	0.9245863739227933	T	T	T
0.1889790141294842	0.8517016221064987	0.0208970950813182	T	T	T
0.0836539840764047	0.8322723971948566	0.9046928510822624	T	T	T
0.1018256199221717	0.8372038940083192	0.7087207446153880	T	T	T
0.2279288228045351	0.8543895105098683	0.7626320607214553	T	T	T
0.3194319555645726	0.9479259811610503	0.8039363746038535	T	T	T
0.0805420845381211	0.9493957801014590	0.8105407094567444	T	T	T
0.4294931685255438	0.1268954285508425	0.5851155707091523	T	T	T
0.4160325743103275	0.9949362532516173	0.5692928926057560	T	T	T
0.3971884963463321	0.8626344763781639	0.5665794216577349	T	T	T
0.1940602053640046	0.1307957670852699	0.6115445147845698	T	T	T
0.1794017840197196	0.0025981546047294	0.5589903933450251	T	T	T
0.1925649986359025	0.8687126132873978	0.5704561546238738	T	T	T
0.9881494292519410	0.0460954363345402	0.7903877801506627	T	T	T
0.9818019297774174	0.8615636009423043	0.7862545543557693	T	T	T
0.1415261820803269	0.9390497436157867	0.2194982745911133	T	T	T
0.1970949159598409	0.9304747146692699	0.3968060187655122	T	T	T
0.2969076172118369	0.9462633628325493	0.5281412118368485	T	T	T

Structure files (CONTCAR) involved in this work:

0.3968721062710354	0.9297166613127048	0.3981710585820114	T	T	T
0.3955781111191244	0.9445302992544218	0.2008350290398367	T	T	T
0.2696218169872697	0.9699694367021695	0.2424228829832452	T	T	T
0.1411045466938019	0.1701107803702133	0.2401474358610618	T	T	T
0.1928450085658308	0.1623121769483439	0.4181912677175640	T	T	T
0.3079100239452632	0.1481954021184854	0.5139389221154931	T	T	T
0.4134157152154396	0.1706291864929573	0.3984877492737600	T	T	T
0.3956441231059422	0.1553012325796128	0.2041234377175004	T	T	T
0.2698426182949619	0.1392610935136429	0.2598879414302597	T	T	T
0.1764547644821226	0.0509635286392073	0.3131583615352309	T	T	T
0.4179182430978662	0.0492242148574099	0.3206388365330454	T	T	T
0.0666766055055578	0.8710390873121225	0.0933642060945930	T	T	T
0.0806880494780720	0.0014751062607611	0.0656162258397257	T	T	T
0.0974305464144722	0.1339276966055291	0.0613781513050623	T	T	T
0.3024001696047475	0.8690463638278472	0.1198588292844110	T	T	T
0.3170136768468180	0.9953821016334710	0.0601966067851222	T	T	T
0.3032879582420783	0.1292564348545646	0.0668030160227812	T	T	T
0.5093484783588720	0.9530517316194266	0.2940878847147108	T	T	T
0.5160040640328714	0.1364632420272407	0.2836225018240942	T	T	T
0.6447527397271757	0.5577663930487653	0.2741541621832879	T	T	T
0.6839883946228811	0.5727037999487595	0.0890526870250399	T	T	T
0.7933938372537825	0.5459361893001894	0.9815537614916500	T	T	T
0.9024414836478594	0.5680465034380840	0.0943554895811348	T	T	T
0.9009505399707933	0.5615386173750859	0.2966144932381988	T	T	T
0.7725210067330212	0.5397402872487996	0.2264874580363661	T	T	T
0.6418484214828404	0.3393929118350374	0.2667634375546899	T	T	T
0.7179646898857438	0.3261791053134057	0.1105411785741239	T	T	T
0.8066467433330587	0.3548869606759550	0.9666756013265523	T	T	T
0.9079389767456377	0.3355833710338338	0.0934309334491005	T	T	T
0.9096491554308853	0.3374329420726915	0.2917100786357031	T	T	T
0.7696654183294508	0.3774385380719988	0.2745666708599543	T	T	T
0.6810316489598726	0.4493166781674184	0.1698333828246236	T	T	T
0.9148727273297123	0.4512407355999878	0.1871307230862002	T	T	T
0.5718641714792830	0.6277052938324132	0.4037095726664125	T	T	T
0.5975240981084889	0.5002150681944497	0.4388399539268700	T	T	T
0.5825634119307197	0.3675054641143926	0.4409067035559595	T	T	T
0.8034736343087785	0.6444297544204121	0.3763304794975538	T	T	T
0.7994274348322010	0.5079258998560932	0.4326483547195770	T	T	T
0.8330672650530194	0.3784180554124891	0.4521236021706165	T	T	T
0.0118537277985171	0.5444442387489173	0.2049825326098532	T	T	T
0.0188285313016963	0.3712632844743364	0.1897658432865635	T	T	T
0.8735628896838181	0.4379435433863896	0.7547691570249213	T	T	T
0.8014849557014292	0.4395257279965330	0.6038126441240788	T	T	T
0.7014321172980599	0.4189210311717315	0.4761025589175676	T	T	T
0.6035309986411449	0.4320346019055260	0.6084131950626179	T	T	T
0.5973141741737104	0.4326896015502677	0.8060557928666945	T	T	T
0.7295103722150700	0.4333772607064860	0.7810875593051326	T	T	T
0.8637367231936903	0.6754142669258970	0.7415414750629234	T	T	T
0.8080991261970517	0.6413115036380757	0.5737749672635298	T	T	T
0.6907928302449955	0.6475871688147197	0.4849279812170448	T	T	T
0.5820075121482438	0.6603411107736692	0.5957933195521720	T	T	T
0.6051985183298743	0.6629371760717639	0.7920064831102731	T	T	T
0.7301914384994218	0.6733719157495638	0.7268014296884275	T	T	T

Structure files (CONTCAR) involved in this work:

0.7987773645052846	0.5598940203980277	0.7330619345385291	T	T	T
0.5864394374154408	0.5470714927114613	0.7011349630512496	T	T	T
0.9313629703314177	0.3700790626706636	0.9045402613567860	T	T	T
0.9107994928357226	0.5010895869207214	0.9241007683407345	T	T	T
0.8896469881544747	0.6324230763559291	0.9264356649535150	T	T	T
0.6754092892288740	0.3731485414709095	0.9373050702251995	T	T	T
0.6723410235040943	0.5073858813790931	0.9211502264771072	T	T	T
0.7063894493883431	0.6362083999858990	0.9174482366115556	T	T	T
0.4887866228747796	0.4568120277367454	0.7065087678853229	T	T	T
0.4848473115321569	0.6339213269475535	0.7214419802931334	T	T	T
0.6406213759410929	0.9375032244496126	0.2938298123645571	T	T	T
0.6915586765048229	0.9356441415066244	0.1125275806395595	T	T	T
0.7981912734808905	0.9498407737454146	0.9923697571052593	T	T	T
0.9036061877062573	0.9292674737148219	0.1089646844061412	T	T	T
0.8949958356618768	0.9443356723328516	0.3063236532508331	T	T	T
0.7690394737273232	0.9660802104062954	0.2638312801723592	T	T	T
0.6412598808494563	0.1757157632523536	0.2552559668777338	T	T	T
0.6960782273708875	0.1533934319981180	0.0828423060328831	T	T	T
0.8085507352945349	0.1461991342423853	0.9822583233926501	T	T	T
0.9082436800529158	0.1727952528412013	0.1083784432974785	T	T	T
0.8954611545435727	0.1553757935665621	0.3041418186485235	T	T	T
0.7704212932486436	0.1418790739785604	0.2477646237151897	T	T	T
0.6752918929844188	0.0522520339094806	0.2081803189733042	T	T	T
0.9172734203224305	0.0501028269956763	0.1856302651096255	T	T	T
0.5656581624962532	0.8748828039190545	0.4281884260956074	T	T	T
0.579942237222526	0.0070520749654155	0.4404295850963272	T	T	T
0.6024612511237093	0.1382556641268849	0.4370660444831330	T	T	T
0.8023679049457199	0.8671261697391098	0.3894850137866680	T	T	T
0.8151539605400762	0.9940835104642483	0.4459158316316519	T	T	T
0.8039645030574383	0.1282159518108143	0.4405383737113495	T	T	T
0.0107355981781827	0.9565893948722716	0.2200997045328678	T	T	T
0.0136747190548717	0.1390824418227205	0.2181447221589144	T	T	T
0.8578167082085314	0.0693475922872153	0.7905405855089891	T	T	T
0.8046826483724189	0.0634211345674556	0.6108845721031575	T	T	T
0.6998056575249582	0.0521214209702286	0.4870000479574211	T	T	T
0.5974067554573489	0.0761014250175664	0.6090563580924768	T	T	T
0.6023320949107960	0.0527332016275741	0.8058540101253144	T	T	T
0.7292435959572912	0.0347780121913075	0.7652289276581205	T	T	T
0.8555754691519099	0.8255274002138056	0.7606539350397229	T	T	T
0.8047946955329656	0.8582769144325603	0.5857623743155785	T	T	T
0.6885301763213186	0.8544007021341902	0.4914483769898900	T	T	T
0.5862048974361846	0.8276364328083664	0.6120193344903099	T	T	T
0.6012680019277059	0.8550165348068539	0.8046054914596307	T	T	T
0.7276230771123454	0.8612664248547173	0.7472915803170128	T	T	T
0.8262032495321984	0.9511115135365414	0.7207742653483389	T	T	T
0.5789016592372810	0.9535505045837356	0.6747366689752015	T	T	T
0.9342919985036553	0.1257267990970951	0.9268255963340838	T	T	T
0.9159274949219054	0.9944283744913905	0.9356984363256147	T	T	T
0.8955656860313093	0.8632906843789806	0.9413965414029908	T	T	T
0.6920883376046439	0.1333912506903606	0.8870293339734993	T	T	T
0.6830383069436262	0.0077916808324044	0.9483268180157788	T	T	T
0.6953737844831199	0.8744828009972353	0.9408946618631610	T	T	T
0.4876381495735632	0.0474990930800043	0.7161742448774377	T	T	T

Structure files (CONTCAR) involved in this work:

0.4821563920197097	0.8671899372718184	0.7213266868727312	T	T	T
0.3586189458573480	0.4420837267654689	0.7121254701801739	T	T	T
0.3047935805331815	0.4285091046330911	0.8901524228010379	T	T	T
0.2066223361419692	0.4536314928041756	0.0205420943365062	T	T	T
0.1108567080339721	0.4298604425152916	0.8865795385529889	T	T	T
0.1066038273826517	0.4542197094777931	0.6888233118106536	T	T	T
0.2314439555970524	0.4710556339200988	0.7371767673982079	T	T	T
0.3569588328104432	0.6667102102534339	0.7309015452163092	T	T	T
0.3000919919093775	0.6680781222881924	0.9063172539449657	T	T	T
0.1918661101941448	0.6465793137922554	0.0158727015869542	T	T	T
0.0918218083731851	0.6756531088334559	0.8921174530216548	T	T	T
0.1020884305326355	0.6555486768892135	0.6971913986098844	T	T	T
0.2287510574035608	0.6356858823491363	0.7456471373834900	T	T	T
0.3211971470646284	0.5514830476000804	0.8155125157794979	T	T	T
0.0853188955834140	0.5522826121622346	0.8223726119116249	T	T	T
0.4307466870437860	0.3749813870154235	0.5787852819036537	T	T	T
0.4155424338348348	0.5057428352712504	0.5584629346392851	T	T	T
0.4103329388403856	0.6389751582473086	0.5547255085738206	T	T	T
0.1959257439904649	0.3727904740359718	0.6110201949688738	T	T	T
0.1902968485101020	0.4996979014811915	0.5510865908293525	T	T	T
0.1901068822736712	0.6343225617143041	0.5539886894998822	T	T	T
0.9975532643123356	0.4541358858481460	0.7887333787354504	T	T	T
0.9854311801213036	0.6364146540219541	0.7860179101545091	T	T	T
0.1420484452697199	0.5610767322444227	0.2095273852988820	T	T	T
0.1998147124392454	0.5698076090318761	0.3847575333515095	T	T	T
0.3016899147056314	0.5666319333626864	0.5162127545322293	T	T	T
0.4028947450623325	0.5714016449593275	0.3875278538394679	T	T	T
0.4015918294349692	0.5563601313798617	0.1931285649183741	T	T	T
0.2723370692344373	0.5345175499567212	0.2280214220273047	T	T	T
0.1388038595191372	0.3301416391122740	0.2424607059735789	T	T	T
0.1925228156466671	0.3431864357053534	0.4179956393885477	T	T	T
0.3086493384046891	0.3541263305863766	0.5106982185477906	T	T	T
0.4120042658560968	0.3288675231376588	0.3931128258350465	T	T	T
0.3934840686914714	0.3414297421287016	0.1975173176929326	T	T	T
0.2690922860146992	0.3554083493612982	0.2558499436760628	T	T	T
0.1810869817872600	0.4501348626676897	0.3007674617057041	T	T	T
0.4143432092902440	0.4494813973464470	0.3114562401739159	T	T	T
0.0683227713681360	0.6221857797497700	0.0716394303405558	T	T	T
0.0837129451116695	0.4900313738231869	0.0600044766848392	T	T	T
0.1136919091461998	0.3594995652908328	0.0523181985310285	T	T	T
0.3115298499793850	0.6256274211234490	0.0943591798705161	T	T	T
0.3285167358382502	0.4945600229104880	0.0580520844801259	T	T	T
0.2997523529646048	0.3625693346066164	0.0606868332422610	T	T	T
0.5148958214002128	0.5358993241532796	0.2904433721514919	T	T	T
0.5125542004936116	0.3620305100069916	0.2724005181313359	T	T	T
0.4417830800695551	0.7506896132688419	0.6461425586369307	T	T	T
0.1936090211779416	0.7488646085170378	0.6511574055543675	T	T	T
0.2725588766768509	0.7491280344786545	0.0573634600112433	T	T	T
0.1076121458045777	0.7483911459115148	0.0541343844085030	T	T	T
0.0622721614411043	0.2502328389519752	0.1342190564388238	T	T	T
0.3039519255499104	0.2466840181643503	0.1526193325348084	T	T	T
0.2268524402516964	0.2517629405364514	0.5546345075098819	T	T	T
0.3899187785281703	0.2511000091087181	0.5500378376347241	T	T	T

Structure files (CONTCAR) involved in this work:

0.5602015255951479	0.2518697568902681	0.3585184137019765	T	T	T
0.8054417403210237	0.2482060296325997	0.3602105966071941	T	T	T
0.7260349749292134	0.2503675696518619	0.9508939677285447	T	T	T
0.8895314246533548	0.2491575884413037	0.9479051622190416	T	T	T
0.9365405006369985	0.7484547043933779	0.8664091340949744	T	T	T
0.6849071791876613	0.7584170424224091	0.8606844823728512	T	T	T
0.7734821263807922	0.7524908554797092	0.4780529551002070	T	T	T
0.6069211224120911	0.7502767795959707	0.4551768054429225	T	T	T
0.9836659494382317	0.6388065787510474	0.3783616150085577	T	T	T
0.8832359436521158	0.3866401326194200	0.6265620184142870	T	T	T
0.8924643621040297	0.3111082291420246	0.6491181370455077	T	T	T
0.9337951691128206	0.5948400127378760	0.3340931351446374	T	T	T
0.9890179265940118	0.6283366284061176	0.5354741573033106	T	T	T
0.9277728565361272	0.6853108774186965	0.4864596602241372	T	T	T
0.0143566549499537	0.7085590535381734	0.4862301138535025	T	T	T
0.0290358165669765	0.6237600893085087	0.3644124238347690	T	T	T
0.8907839896981237	0.4045655782062584	0.4816499580307192	T	T	T
0.9423276912525600	0.4566446755693671	0.4439198851509359	T	T	T
0.9434141349316196	0.4850805121802684	0.5660078750361013	T	T	T
0.9934963531427978	0.4130867510939645	0.5299284276063611	T	T	T
0.9789498780741441	0.6667214612056636	0.4782357438091310	T	T	T
0.9450959597529722	0.4382858719318002	0.5219510628318969	T	T	T

Figure S10 Ga-FS

Si Al O Ga H C

1.0000000000000000

20.0219999999999985 0.0000000000000000 0.0000000000000000

0.0000000000000000 19.8990000000000009 0.0000000000000000

0.0000000000000000 0.0000000000000000 13.3829999999999991

93 3 193 1 10 2

Selective dynamics

Direct

0.4218196515172738	0.0575587840191864	0.6481850629482352	T	T	T
0.3014076842225049	0.0271273702991047	0.7899218951383322	T	T	T
0.2795579891714520	0.0601165548363807	0.0132043385039851	T	T	T
0.1196239397495784	0.0630938597383307	0.0123305460970748	T	T	T
0.0667127278157427	0.0295102491599100	0.7986514257819262	T	T	T
0.1768551787218748	0.0560333665052511	0.6521584212271765	T	T	T
0.4198001400764003	0.8271922906845087	0.6713472242844606	T	T	T
0.3020612057808225	0.8686881040651294	0.8101165010746177	T	T	T
0.2669254598356492	0.8283993834834016	0.0299783528934094	T	T	T
0.1118471001216884	0.8265326661790093	0.0171225408910869	T	T	T
0.0614740163726928	0.8702985865313323	0.8021716866187006	T	T	T
0.1796532197803526	0.8276196739475689	0.6745524332547628	T	T	T
0.0754726315416611	0.9425502752521145	0.1510317011511361	T	T	T
0.1960592531680564	0.9724358513035503	0.2939726622672081	T	T	T
0.2171377223084818	0.9366166156062725	0.5149905946756769	T	T	T
0.3769528735532359	0.9337209724340318	0.5158024405736086	T	T	T
0.4306779854671975	0.9690782822414555	0.3045259373913549	T	T	T
0.3204382827922065	0.9442396209424923	0.1566713121467614	T	T	T
0.0786004359995391	0.1723393672248539	0.1646820206202175	T	T	T
0.1958199941646612	0.1299319719949708	0.3074647150309118	T	T	T
0.2309386786807071	0.1729939156736835	0.5241831616781611	T	T	T
0.3855693753612520	0.1738676423337492	0.5115698975398185	T	T	T

Structure files (CONTCAR) involved in this work:

0.4367944667364150	0.1272719091685532	0.3015782692134146	T	T	T
0.3186486140870116	0.1672472190270815	0.1719849024769784	T	T	T
0.5836654623927811	0.5548118432774910	0.3492696033415685	T	T	T
0.6958993647295352	0.5292043152166060	0.1883040813613428	T	T	T
0.7145044419594851	0.5650116052783460	0.9743576938098872	T	T	T
0.8728933262623306	0.5629284344828729	0.9830618257280163	T	T	T
0.9329409920895249	0.5310483758644581	0.1909903709960706	T	T	T
0.5760639170049409	0.3290802991132211	0.3316312714297447	T	T	T
0.7009486734363007	0.3736778272239125	0.2019839750396417	T	T	T
0.7320194896558648	0.3266607879172991	0.9866794404818915	T	T	T
0.8837846963644710	0.3268369956354499	0.9836616565370776	T	T	T
0.9358753683495450	0.3728663138640154	0.1954895940816012	T	T	T
0.9286873070123054	0.4405903928111681	0.8542100670878683	T	T	T
0.7823176361438700	0.4421926494100666	0.4877499827344315	T	T	T
0.6239335943342784	0.4305345297268011	0.4901614236092066	T	T	T
0.5681052721599013	0.4669894652627066	0.7035538171117939	T	T	T
0.6708944922964988	0.4357339525407158	0.8543195115106250	T	T	T
0.9181154044822222	0.6719556021103691	0.8286487819017644	T	T	T
0.7999645368899364	0.6326007046526536	0.6942963057573992	T	T	T
0.7681371549709530	0.6696015355800184	0.4778928348973963	T	T	T
0.6123958456987938	0.6710402753713156	0.4855480389797032	T	T	T
0.5641970914412410	0.6253827943282856	0.7019754843140891	T	T	T
0.6816623451238228	0.6801961843322166	0.8222099906045589	T	T	T
0.5751670609468748	0.9432593443550285	0.3638356278508167	T	T	T
0.6939790825743994	0.9720275977369630	0.2187572397593260	T	T	T
0.7183060959932931	0.9409018909098136	0.9975965574142386	T	T	T
0.8783259014377929	0.9337641114111107	0.9942166464852510	T	T	T
0.9313233929864201	0.9690874961425248	0.2059002554944594	T	T	T
0.8192369088167619	0.9402350099010444	0.3517751568219622	T	T	T
0.5807811970888153	0.1741247572496980	0.3336469417151842	T	T	T
0.6973451126650969	0.1293359343110304	0.1971794213248221	T	T	T
0.7319046780312720	0.1707903757379766	0.9764323895818279	T	T	T
0.8859795331502461	0.1726090073587565	0.9933352443096728	T	T	T
0.9343073471843362	0.1277599159827948	0.2053405684706174	T	T	T
0.8179027956649962	0.1669625643936755	0.3366494700359755	T	T	T
0.9232398885525561	0.0576539397539902	0.8605869645833550	T	T	T
0.8048752172109225	0.0290332450957226	0.7209351998663314	T	T	T
0.7808359651512321	0.0575147731003675	0.4955893039832404	T	T	T
0.6208349467255727	0.0677311170371454	0.4936757549243525	T	T	T
0.5666865838826298	0.0325370131411513	0.7015982322699978	T	T	T
0.6777481139035254	0.0561250345974018	0.8512986636905173	T	T	T
0.9173205947942662	0.8248605365533954	0.8379999215900676	T	T	T
0.8028059003214284	0.8736132581726420	0.7033603066942631	T	T	T
0.7669888828149964	0.8308784862830562	0.4867015008884543	T	T	T
0.6119876749695145	0.8259255599919343	0.4970864066530121	T	T	T
0.5621600787101259	0.8760090379350203	0.7033493286636479	T	T	T
0.6782498882663011	0.8369018232291906	0.8356019555325539	T	T	T
0.4222164570681411	0.4447739711066738	0.6398008261120827	T	T	T
0.3051608262076108	0.4727677892919284	0.7902500953548844	T	T	T
0.2850589081903922	0.4346057062250452	0.0099018054476763	T	T	T
0.1285374720172865	0.4326946645964471	0.0067102104231484	T	T	T
0.0759122068301978	0.4722442702232373	0.8003459361465539	T	T	T
0.1826156364936360	0.4489666144372862	0.6489639832590207	T	T	T

Structure files (CONTCAR) involved in this work:

0.4234290527572001	0.6724836954772063	0.6645702007376674	T	T	T
0.3022317768292726	0.6296377772608136	0.8004895228434178	T	T	T
0.2691235739720966	0.6718777641299860	0.0193513135976403	T	T	T
0.1149561946526540	0.6736489211722010	0.0078776659550375	T	T	T
0.0655113885740628	0.6292938964073886	0.7997372293061100	T	T	T
0.1797681075679491	0.6689345061835709	0.6644888380832442	T	T	T
0.0784550190556297	0.5540606022300177	0.1358811211180104	T	T	T
0.1990113787421386	0.5281981285199657	0.2813795322501950	T	T	T
0.2206890363765950	0.5672409155471922	0.5027037207323548	T	T	T
0.3820102448983765	0.5704934758069451	0.5044362452590508	T	T	T
0.4352111100291882	0.5280796932419441	0.2967736201291457	T	T	T
0.3273265242128763	0.5534316243309196	0.1464740781243043	T	T	T
0.0819420217321394	0.3270857338545006	0.1574261338773778	T	T	T
0.1955051817075981	0.3695021395779502	0.3047963528022759	T	T	T
0.2311924175029113	0.3301348819583668	0.5238160536509203	T	T	T
0.3852843275795894	0.3272099387653805	0.5077856107923647	T	T	T
0.4327547134763675	0.3711048816460149	0.2948327283402993	T	T	T
0.3162710245620334	0.3259870478950035	0.1677083689050859	T	T	T
0.8119581975424568	0.5644202722745142	0.3307342060989217	T	T	T
0.8236205259877392	0.3251983800107627	0.3293096663627022	T	T	T
0.7960123653997362	0.4718175285571727	0.7251994236374689	T	T	T
0.3563000229329619	0.0630065101810401	0.7189620708406025	T	T	T
0.3008544656497856	0.0653950072513101	0.8967881351152419	T	T	T
0.1992938507363962	0.0506774191447355	0.0254945062241416	T	T	T
0.0993728872070025	0.0661474137807370	0.8955036696108175	T	T	T
0.1017757304566228	0.0577256190916771	0.6976822148266482	T	T	T
0.2277690384508333	0.0332524113079692	0.7403573187276390	T	T	T
0.3575732202615626	0.8262358584212937	0.7490167713969094	T	T	T
0.3045247405985851	0.8443855560045657	0.9254107316827145	T	T	T
0.1891758043857086	0.8518799496596251	0.0203612178419121	T	T	T
0.0836037558788401	0.8325007773789462	0.9043127989804295	T	T	T
0.1020172904440298	0.8371826916698890	0.7084933656062010	T	T	T
0.2279294860301840	0.8545626226293793	0.7640950597038745	T	T	T
0.3199067231486346	0.9481190022148557	0.8031173088411201	T	T	T
0.0798889306873244	0.9493039566188122	0.8095907871139616	T	T	T
0.4297435081216573	0.1269579451852716	0.5852032451130914	T	T	T
0.4162309137458312	0.9949574403164653	0.5703576060845933	T	T	T
0.3971333005069481	0.8627259001570274	0.5673020482432082	T	T	T
0.1946883430115926	0.1306829421985159	0.6120196543958405	T	T	T
0.1796988403877567	0.0021586988967929	0.5609254255446771	T	T	T
0.1936926757031959	0.8682659405187407	0.5714828821400997	T	T	T
0.9876445237889868	0.0459283080450829	0.7890342531544877	T	T	T
0.9816287389351107	0.8608678373726488	0.7852140867230714	T	T	T
0.1417354668399100	0.9383861624589825	0.2201895439937550	T	T	T
0.1964438129245455	0.9305031651127059	0.3981367144126687	T	T	T
0.2971945943039676	0.9466520689566149	0.5277627041153806	T	T	T
0.3976745509575610	0.9296702764088819	0.3990087949848285	T	T	T
0.3956325769576349	0.9441605054559506	0.2015146984010451	T	T	T
0.2698252928131809	0.9690568385856149	0.2442227170134335	T	T	T
0.1419038315907242	0.1699579237929406	0.2400107077840636	T	T	T
0.1928307533033047	0.1618559698049286	0.4186053732480956	T	T	T
0.3081541605597896	0.1482774999873553	0.5135493366965604	T	T	T
0.4140502701311575	0.1705510837794020	0.3985747325447991	T	T	T

Structure files (CONTCAR) involved in this work:

0.3961591128031379	0.1549212169069720	0.2042201450050088	T	T	T
0.2704827344786986	0.1389613546168477	0.2610074774816007	T	T	T
0.1765919568026214	0.0506824551219490	0.3129526296373291	T	T	T
0.4183160088540585	0.0490120704676268	0.3209721160479147	T	T	T
0.0669275727571246	0.8713006594830632	0.0927584996779798	T	T	T
0.0804665691088888	0.0021381417831824	0.0680500031894433	T	T	T
0.0977591991054688	0.1342430832076878	0.0613342691680024	T	T	T
0.3022507453351305	0.8685435940559778	0.1209041736207486	T	T	T
0.3163914888699056	0.9949998326838517	0.0616742470904357	T	T	T
0.3029843410436688	0.1288514280679539	0.0677680852348399	T	T	T
0.5096326529075463	0.9527624153691904	0.2939046412398970	T	T	T
0.5166459731030835	0.1358778431549738	0.2837474428253126	T	T	T
0.6446378839664907	0.5598886893141082	0.2712717007061954	T	T	T
0.6823341142043382	0.5707643463131046	0.0850674315237941	T	T	T
0.7940468085329558	0.5462837484472607	0.9827709698324769	T	T	T
0.9026574965139192	0.5703488782937438	0.0959224702096120	T	T	T
0.9010272565475556	0.5639168894324542	0.2956413798442974	T	T	T
0.7718256126824193	0.5402399449452164	0.2234886018873227	T	T	T
0.6393045730827449	0.3367380167368731	0.2587813370724446	T	T	T
0.7170585197529279	0.3270670023286853	0.1050734187719498	T	T	T
0.8080399422744970	0.3544590557898726	0.9646707006120879	T	T	T
0.9037325038550856	0.3341586694101889	0.1001524077780581	T	T	T
0.9065266096931862	0.3403586305133079	0.2959495203332780	T	T	T
0.7661774652373660	0.3752929096832603	0.2711528675552022	T	T	T
0.6789103514481608	0.4495775708580901	0.1695800834750949	T	T	T
0.9152992024051603	0.4524681092601119	0.1878466591363548	T	T	T
0.5713205270275639	0.6268980595844134	0.4036638054403162	T	T	T
0.6013492593378157	0.4996217462774665	0.4355113104965799	T	T	T
0.5883177146307920	0.3666550019573904	0.4380414420068219	T	T	T
0.8015507201653551	0.6446265468218910	0.3758177514233477	T	T	T
0.8028896216102548	0.5067025260256469	0.4266836675164072	T	T	T
0.8323747928074383	0.3771456471967518	0.4453775502080841	T	T	T
0.0124717540674438	0.5451270657112351	0.2060388158001052	T	T	T
0.0171022872657172	0.3695726934012127	0.1931380938335956	T	T	T
0.8731819908992058	0.4344397972819505	0.7651947319412908	T	T	T
0.8106760809375084	0.4428563370554873	0.6017741148121438	T	T	T
0.7051142687812225	0.4201073669113299	0.4827125047794217	T	T	T
0.6016360515066560	0.4320882540707535	0.6059370521591614	T	T	T
0.5967542064249420	0.4323545038840908	0.8041128206688757	T	T	T
0.7275829942776619	0.4317702687482700	0.7701461513860369	T	T	T
0.8634917841094225	0.6740884111606154	0.7400080757870784	T	T	T
0.8071910525789749	0.6364710405369935	0.5734182293390675	T	T	T
0.6897780491070495	0.6468885276674951	0.4857388536446849	T	T	T
0.5805132620949840	0.6602268740305403	0.5954859850443045	T	T	T
0.6049384127394354	0.6623573538723805	0.7914110550682194	T	T	T
0.7299566894420367	0.6696124589518913	0.7254340948405227	T	T	T
0.8009416169740021	0.5571588823069474	0.7363315395567761	T	T	T
0.5853898774970154	0.5468062660522686	0.6997518432830401	T	T	T
0.9351807916887916	0.3705470351832161	0.9151244515431396	T	T	T
0.9128176492669522	0.5011969499533331	0.9302623407324292	T	T	T
0.8895968980051829	0.6323549617927151	0.9256715546104664	T	T	T
0.6772140347333082	0.3724432259650898	0.9304996496241846	T	T	T
0.6756204311027458	0.5064545427667891	0.9147921779877273	T	T	T

Structure files (CONTCAR) involved in this work:

0.7063261260058245	0.6361617481861822	0.9170046614449296	T	T	T
0.4879033101375402	0.4565094299468400	0.7068988288756161	T	T	T
0.4840846170561598	0.6336984835114544	0.7218606778004357	T	T	T
0.6405804058713249	0.9367021806053428	0.2930579131168030	T	T	T
0.6921872313524026	0.9341114895381526	0.1116127777500037	T	T	T
0.7989358477108015	0.9494834168459475	0.9920156554174234	T	T	T
0.9040735032074345	0.9284554355770959	0.1087180940210490	T	T	T
0.8945000672341359	0.9421504486276966	0.3063258052501754	T	T	T
0.7687993400489760	0.9647463559499180	0.2639826899758563	T	T	T
0.6424728808235517	0.1743484824273103	0.2556067977998623	T	T	T
0.6962461047489527	0.1537734738020406	0.0820047400144989	T	T	T
0.8094691808258030	0.1458524046518453	0.9834684200794852	T	T	T
0.9095314334533978	0.1710907829195854	0.1091624064703304	T	T	T
0.8960283628518249	0.1548501355437013	0.3042097239832236	T	T	T
0.7713315860143041	0.1380761291728109	0.2453334021732998	T	T	T
0.6750399705671974	0.0508361009874327	0.2054138668697022	T	T	T
0.9176793123481467	0.0486692888914376	0.1877262853764664	T	T	T
0.5659217338893558	0.8746701963667270	0.4283651169709529	T	T	T
0.5803808738839628	0.0067517082430575	0.4399874569380681	T	T	T
0.6035667804096372	0.1377384851360816	0.4370651566276403	T	T	T
0.8018369628048673	0.8641859962790358	0.3883825133312866	T	T	T
0.8142636717449250	0.9907421745972086	0.4467665596310878	T	T	T
0.8044168505848214	0.1249210251371281	0.4388063882186715	T	T	T
0.0107603293848102	0.9550142608064180	0.2213647540922217	T	T	T
0.0146498460692471	0.1377115214060717	0.2192317094851025	T	T	T
0.8572769408825905	0.0689319537245150	0.7919238408991901	T	T	T
0.8062785372754723	0.0619531131501309	0.6104627999624669	T	T	T
0.7000052988469363	0.0507871820002814	0.4891123602076322	T	T	T
0.5969028360745283	0.0759946924524532	0.6090353296563842	T	T	T
0.6026785321039226	0.0527112364719965	0.8059861364728359	T	T	T
0.7292311445039468	0.0339557777297081	0.7634919247057296	T	T	T
0.8550673779615459	0.8246803496544794	0.7604816909935028	T	T	T
0.8053154523176974	0.8588519648971954	0.5849948008742978	T	T	T
0.6886989153021520	0.8527974817301466	0.4915363211340658	T	T	T
0.5862210765060951	0.8276339308494501	0.6122798846851923	T	T	T
0.6016216085937663	0.8550921509923841	0.8048428204302738	T	T	T
0.7274574992235050	0.8618179211029188	0.7455160279935595	T	T	T
0.8271510603090840	0.9505021678811084	0.7217387016265309	T	T	T
0.5785949452563852	0.9535919545794449	0.6750664111172502	T	T	T
0.9348681843887654	0.1251530514875404	0.9269028272630513	T	T	T
0.9168302708291198	0.9938071215153796	0.9357015191274509	T	T	T
0.8960387086116776	0.8625914087028819	0.9408514160386167	T	T	T
0.6935627607606253	0.1321921633966668	0.8866212736195000	T	T	T
0.6836121401387573	0.0063908846249620	0.9471304013198992	T	T	T
0.6968888235286210	0.8730664722138574	0.9399311575877594	T	T	T
0.4876123676266310	0.0478869848390547	0.7171506974914842	T	T	T
0.4822501823564779	0.8670821694245847	0.7219229570788424	T	T	T
0.3579525175351845	0.4398939250776614	0.7131957377928789	T	T	T
0.3056510239828431	0.4293287009850782	0.8929213114225586	T	T	T
0.2061826613712131	0.4534085584728590	0.0224319937760147	T	T	T
0.1113362535105341	0.4289712485240855	0.8884247226571155	T	T	T
0.1065846323017420	0.4533499478675841	0.6915416372673463	T	T	T
0.2312559746282359	0.4701522705847455	0.7404669950552458	T	T	T

Structure files (CONTCAR) involved in this work:

0.3565886744077628	0.6677203378259091	0.7322948864957500	T	T	T
0.3012715031363784	0.6661527750446579	0.9085011431884752	T	T	T
0.1916020542152300	0.6467173538437928	0.0150257726675447	T	T	T
0.0909440545599077	0.6755876504318287	0.8920766786477512	T	T	T
0.1024842111304527	0.6545904312015914	0.6978122641217244	T	T	T
0.2288655784516824	0.6352990726867188	0.7478712875820677	T	T	T
0.3226579462839637	0.5510204007243040	0.8137939922131141	T	T	T
0.0852678820143440	0.5517042779771109	0.8240559501700557	T	T	T
0.4308045142830367	0.3751349245638543	0.5780285660622984	T	T	T
0.4139726745764318	0.5059218885404756	0.5605578931199967	T	T	T
0.4086070096633615	0.6391479931006490	0.5558648390906008	T	T	T
0.1961033811855137	0.3725468573895677	0.6130286936507403	T	T	T
0.1904712895101800	0.4998870001192640	0.5547934129286517	T	T	T
0.1912198461496416	0.6345971243561354	0.5554694847338020	T	T	T
0.9975307173758015	0.4531106025945681	0.7936488386829491	T	T	T
0.9853107373220258	0.6353523611016533	0.7850093416735119	T	T	T
0.1428511125156864	0.5614026013800277	0.2086089042170249	T	T	T
0.1962580568733079	0.5687330012288740	0.3868906604585025	T	T	T
0.3011622290047510	0.5660017011179304	0.5118028190841173	T	T	T
0.4053503483780678	0.5717063278448412	0.3890802845907838	T	T	T
0.4016103673308881	0.5570532180855550	0.1947152237624372	T	T	T
0.2727813298565425	0.5354458674664293	0.2331214454707522	T	T	T
0.1379763423449999	0.3294683483397322	0.2446742328991185	T	T	T
0.1921144946288245	0.3442677007984360	0.4196320621845840	T	T	T
0.3083917436876965	0.3542379914096953	0.5118528871008818	T	T	T
0.4108249990857173	0.3286031136451472	0.3931171383436362	T	T	T
0.3932294338774175	0.3418837303573835	0.1978752682338776	T	T	T
0.2686296064915477	0.3542769564821072	0.2573192919262810	T	T	T
0.1805983449059030	0.4497701425433186	0.2992510754598992	T	T	T
0.4139463782224418	0.4497388469913379	0.3122940877165722	T	T	T
0.0682695078179251	0.6226051501383850	0.0719173523631600	T	T	T
0.0831765197630002	0.4903306037947276	0.0604906753432183	T	T	T
0.1124527422841324	0.3598519974545248	0.0553731825076298	T	T	T
0.3101767193372739	0.6258638441515343	0.0976245081396311	T	T	T
0.3274053137498655	0.4946673571771613	0.0620076856615556	T	T	T
0.2990402437755308	0.3624308544302425	0.0620843049590772	T	T	T
0.5156433658839521	0.5345293727397130	0.2899702942734695	T	T	T
0.5119494209464999	0.3621765728771918	0.2749458547939629	T	T	T
0.4418176131801933	0.7507077541585730	0.6464387716847920	T	T	T
0.1939886154624893	0.7485888427323276	0.6534313935040217	T	T	T
0.2724813192583914	0.7491238783693979	0.0567036812981375	T	T	T
0.1077532738455202	0.7486557701961165	0.0536443366501246	T	T	T
0.0617534689690294	0.2497636817935525	0.1357748176071751	T	T	T
0.3044058194951421	0.2463284684062365	0.1532574384370967	T	T	T
0.2267996192969998	0.2517046945765585	0.5545477463336971	T	T	T
0.3899571965816506	0.2510465848148800	0.5502206118551832	T	T	T
0.5607064412935545	0.2511185678657021	0.3581805404862290	T	T	T
0.8026669440052790	0.2445923420590228	0.3573141205551698	T	T	T
0.7275286966429917	0.2496137066176497	0.9481625090594705	T	T	T
0.8911849791466865	0.2488758582896503	0.9511349372562438	T	T	T
0.9365135848812651	0.7476253853126998	0.8645880795043521	T	T	T
0.6859412431513856	0.7577180423223637	0.8565594219831427	T	T	T
0.7741008699793430	0.7506988850766281	0.4838452312657199	T	T	T

Structure files (CONTCAR) involved in this work:

0.6060009075161659	0.7497877832800993	0.4551663821058433	T	T	T
0.9838246231170946	0.6411977058458876	0.3751469869903006	T	T	T
0.9042481056000953	0.4005033675088933	0.6283514547234068	T	T	T
0.8981787994473640	0.3225592157244286	0.6356644827198540	T	T	T
0.9339571907751237	0.5975980316427764	0.3334999592575084	T	T	T
0.9886205493724906	0.6291703915894128	0.5319571351709774	T	T	T
0.9293512370423730	0.6886748914639752	0.4839865147845986	T	T	T
0.0166782507254650	0.7090058330052457	0.4841247501738851	T	T	T
0.0283585032754962	0.6233362998792348	0.3622173498896724	T	T	T
0.8772491725338446	0.3947783879595842	0.4300249016405303	T	T	T
0.9425633583788576	0.4822729358751182	0.4882504478629211	T	T	T
0.9574103375857151	0.5144452308528399	0.6100467037932948	T	T	T
1.0131178523341720	0.4530637660517953	0.5590912455470791	T	T	T
0.9799029859981041	0.6684324299764193	0.4756298762633120	T	T	T
0.9608685027927619	0.4691707031415402	0.5632690207652639	T	T	T

Figure S10 Mo-IS

Si Al O C Mo H

1.0000000000000000

20.0219999999999985 0.0000000000000000 0.0000000000000000

0.0000000000000000 19.8990000000000009 0.0000000000000000

0.0000000000000000 0.0000000000000000 13.3829999999999991

93 3 193 4 4 9

Selective dynamics

Direct

0.4246664902209824	0.0587209264422362	0.6534347706811185	T	T	T
0.3064949498886501	0.0288749535564183	0.7970402680786929	T	T	T
0.2819222713581835	0.0558257383721594	0.0206986735339816	T	T	T
0.1222220151399943	0.0636815993594990	0.0189785675542763	T	T	T
0.0670399910883241	0.0313808504435263	0.8078274455329444	T	T	T
0.1807794327755380	0.0646521661332542	0.6722446766182887	T	T	T
0.4172674170846367	0.8285096125070875	0.6710424003488904	T	T	T
0.3042473436316173	0.8699532803979432	0.8099515640007773	T	T	T
0.2692988644070388	0.8322181293280778	0.0296111498985106	T	T	T
0.1152816861885687	0.8266284493859927	0.0181680309669081	T	T	T
0.0702769724658523	0.8743669196775230	0.8042601578531841	T	T	T
0.1845864949575710	0.8280695330057476	0.6719782093062309	T	T	T
0.0788379303409230	0.9389742356557481	0.1555928922586296	T	T	T
0.1943084304168261	0.9686932688028178	0.2996623056524348	T	T	T
0.2181366254546342	0.9449649876537713	0.5229527739830354	T	T	T
0.3763014011351740	0.9370308155251420	0.5170687058937058	T	T	T
0.4340765820198905	0.9688228889559805	0.3077116564158341	T	T	T
0.3189164723110178	0.9371147514694000	0.1736584888902127	T	T	T
0.0800477411167840	0.1718163098773741	0.1751545336046381	T	T	T
0.1969624985597516	0.1269231232159061	0.3072204674462259	T	T	T
0.2330971695009784	0.1682144104165458	0.5249058606284274	T	T	T
0.3881160105223170	0.1738573573948573	0.5171913310430385	T	T	T
0.4359010135126813	0.1270661236005828	0.3046718175034934	T	T	T
0.3192524080261971	0.1695292640692629	0.1712427723788024	T	T	T
0.5749417613498665	0.5534927618321951	0.3598264195633850	T	T	T
0.6902519922721997	0.5237091427976505	0.2070064171021972	T	T	T
0.7072209201112407	0.5698963975990159	0.9951847381888033	T	T	T
0.8660477862813888	0.5735258584725235	0.9877365126611946	T	T	T
0.9299970707379708	0.5330173296640757	0.1924380416378488	T	T	T

Structure files (CONTCAR) involved in this work:

0.8151403094878947	0.5550077540691656	0.3338835206345092	T	T	T
0.5759513748107972	0.3268108179304135	0.3472171362362648	T	T	T
0.6983289376774706	0.3674621710523083	0.2113703924020932	T	T	T
0.7283034943736630	0.3234403774049931	0.9955216465076486	T	T	T
0.8824135297103877	0.3264794641029761	0.9930786665663177	T	T	T
0.9350343581261792	0.3747537576021940	0.1984073539534795	T	T	T
0.8249595885254617	0.3344482174690689	0.3408574854343559	T	T	T
0.7946611570359551	0.4668358322474175	0.7161358496058372	T	T	T
0.7737199229539644	0.4388997898051951	0.4827795937820307	T	T	T
0.6170585265633117	0.4334937068227898	0.4951470713945301	T	T	T
0.5726851312585874	0.4721034132430544	0.7081825047040706	T	T	T
0.6777824215411073	0.4373833620639992	0.8650953795828763	T	T	T
0.9231707998952366	0.6730936014994611	0.8312601231338235	T	T	T
0.7622907559466127	0.6664479272460234	0.4712369030062050	T	T	T
0.6088339160672107	0.6720728080883152	0.4861071692329581	T	T	T
0.5578412585349019	0.6304993950641291	0.7007467893093777	T	T	T
0.6680290782207960	0.6798083098546652	0.8382362906085816	T	T	T
0.5789629340423955	0.9436329129618733	0.3544282875969520	T	T	T
0.6949338751003655	0.9792662194422938	0.2090652586705381	T	T	T
0.7183995469012260	0.9438948305542156	0.9874939211901470	T	T	T
0.8767155560908423	0.9308707538440617	0.9882905085943182	T	T	T
0.9345915549383100	0.9652149018685420	0.1999258918128657	T	T	T
0.8178919627391489	0.9387547229305411	0.3329117529013944	T	T	T
0.5806192915252724	0.1739704864929789	0.3329028523272352	T	T	T
0.6958638833149643	0.1367726554940012	0.1939504251588590	T	T	T
0.7302819386847369	0.1670130030226638	0.9742521556371985	T	T	T
0.8843316101758200	0.1704029381149567	0.9883540236656011	T	T	T
0.9352290452479880	0.1242975910657410	0.2016833674737556	T	T	T
0.8180812223560701	0.1761507462590362	0.3236938024214652	T	T	T
0.9188113745381471	0.0572381741359204	0.8494933104692738	T	T	T
0.8071775559755990	0.0356664046264985	0.6945733646406533	T	T	T
0.7825783664324091	0.0610104532000292	0.4763419785127166	T	T	T
0.6243524119366959	0.0655241643862209	0.4889401114461029	T	T	T
0.5699917863388365	0.0305681790228497	0.6965510689751764	T	T	T
0.6868282494132931	0.0608471688979763	0.8289090879160680	T	T	T
0.9250819431194255	0.8276365806904838	0.8287325393881955	T	T	T
0.7655304393596951	0.8251902240726999	0.4715346778586970	T	T	T
0.6127356896086475	0.8258209500603032	0.4900789621661096	T	T	T
0.5621666226828864	0.8747813311221948	0.6965114471814281	T	T	T
0.6722773218134234	0.8334269914724327	0.8413517443194382	T	T	T
0.4258101597392652	0.4444649311829623	0.6454057214825297	T	T	T
0.3048961105765038	0.4699614141529111	0.7876737331145203	T	T	T
0.2826446341163345	0.4380618424958657	0.0128358355496152	T	T	T
0.1229098133353889	0.4326990026398489	0.0110015087383340	T	T	T
0.0723981881140318	0.4730027781217587	0.7993932326508797	T	T	T
0.1793771504692244	0.4389006461065837	0.6522525108088908	T	T	T
0.4165537151110919	0.6747047709652738	0.6592173317029103	T	T	T
0.2992108922984579	0.6295209911262933	0.7969461285819479	T	T	T
0.2717101439521378	0.6720385269222693	0.0186767137121045	T	T	T
0.1182948117868577	0.6727756602445566	0.0096567273317828	T	T	T
0.0698371870450460	0.6281655136817033	0.8011653850887592	T	T	T
0.1792987147547782	0.6708097560398981	0.6622768618835837	T	T	T
0.0753612353750781	0.5571462535684427	0.1414652975830314	T	T	T

Structure files (CONTCAR) involved in this work:

0.1963087871920005	0.5308557671897722	0.2817906570143994	T	T	T
0.2173439925244395	0.5589247517066815	0.5085262565128489	T	T	T
0.3782429424815399	0.5672185235872466	0.5086172167801811	T	T	T
0.4322462964244397	0.5262941668946584	0.2978056787666518	T	T	T
0.3241530634644335	0.5597204401359475	0.1509383152564279	T	T	T
0.0791972610830468	0.3260606358616489	0.1629560169713504	T	T	T
0.1983188859528910	0.3713861538189234	0.2974046487277098	T	T	T
0.2315675029588007	0.3292922025437747	0.5166257450424226	T	T	T
0.3868006812069530	0.3272574795551995	0.5107831404213300	T	T	T
0.4356195889344823	0.3687282839849609	0.2974339538660932	T	T	T
0.3210240586118147	0.3264937869313697	0.1653408079509196	T	T	T
0.9207694258018799	0.4455419053037601	0.8561382001053678	T	T	T
0.7931793294309362	0.6299801155092478	0.7014727152350957	T	T	T
0.7986686678261569	0.8721555904451197	0.6972674172561484	T	T	T
0.3610926640756314	0.0669000174446587	0.7278873047747978	T	T	T
0.3181620052194458	0.0496362443012651	0.9127066723099437	T	T	T
0.2016817604814236	0.0512387933218127	0.0076663366084278	T	T	T
0.0881607460728656	0.0695967495578892	0.9099950510835367	T	T	T
0.1046130930515905	0.0662169169488953	0.7135010841401798	T	T	T
0.2313225535646064	0.0509898409759926	0.7653468253723629	T	T	T
0.3632669713857657	0.8250851548459399	0.7616282050066155	T	T	T
0.3056351674725806	0.8608734987092399	0.9299793672788801	T	T	T
0.1912310027701821	0.8548870709208782	0.0273586091160779	T	T	T
0.0913903079647904	0.8325240479765506	0.9032068387517175	T	T	T
0.1082324456130573	0.8414130596303091	0.7081650074140937	T	T	T
0.2326412657528927	0.8435588055430794	0.7671581701586473	T	T	T
0.3152351022007781	0.9482324868886052	0.7800471115773648	T	T	T
0.0907298084787965	0.9529088417307575	0.8157036746824339	T	T	T
0.4339765851047047	0.1277801288713011	0.5897776233768177	T	T	T
0.4147712522989997	0.9963401988627419	0.5766298293173986	T	T	T
0.3841952899738281	0.8656036639715131	0.5746160822907452	T	T	T
0.1970344214674672	0.1373386373346602	0.6230195278628082	T	T	T
0.1877691466393547	0.0049249082493541	0.5905124473385424	T	T	T
0.2039688499866974	0.8725312763124488	0.5751639390803145	T	T	T
0.9872838712060458	0.0375542197481207	0.7907544945566719	T	T	T
0.9906811582558189	0.8677365302536600	0.7878527931914370	T	T	T
0.1425432134233627	0.9280409846990455	0.2286745099390210	T	T	T
0.1815452335294759	0.9468742210335553	0.4147351802717489	T	T	T
0.2977162193441711	0.9562924457176394	0.5087487103213770	T	T	T
0.4090846362660968	0.9290758992828982	0.4070416403063467	T	T	T
0.3957441687515523	0.9399376493031945	0.2101360088965966	T	T	T
0.2706445445511780	0.9496504350699480	0.2698558396123313	T	T	T
0.1380499796994810	0.1730039828523037	0.2601764053491595	T	T	T
0.1970130712597633	0.1368713321814448	0.4270106836111183	T	T	T
0.3114336406017273	0.1469053266158269	0.5235893550052843	T	T	T
0.4138580046486891	0.1695645432555704	0.4026867234753679	T	T	T
0.3957326390684486	0.1560395087656995	0.2078109776842588	T	T	T
0.2693723965362641	0.1486375295094119	0.2625412176070191	T	T	T
0.1816388080967966	0.0485722922919471	0.2811623753549214	T	T	T
0.4177077004833094	0.0483920484615488	0.3218926532754490	T	T	T
0.0674666091401903	0.8703054742585423	0.0914917243787226	T	T	T
0.0887202020997497	0.0013551065898695	0.0791806456794147	T	T	T
0.1081513229273886	0.1336859992540137	0.0766705449679728	T	T	T

Structure files (CONTCAR) involved in this work:

0.3053001212137453	0.8631083720983015	0.1273937374056699	T	T	T
0.3063437736119450	0.9939357579675751	0.0895769717917089	T	T	T
0.3030807004519511	0.1267411716564181	0.0710633428061071	T	T	T
0.5127714552015775	0.9559155654781624	0.2870654867265163	T	T	T
0.5158168986644390	0.1352403771320726	0.2867084122036861	T	T	T
0.6433991383267195	0.5515820253646567	0.2962738685323241	T	T	T
0.6744306263852258	0.5662332211237232	0.1067594075268851	T	T	T
0.7865763517461467	0.5811740224269415	0.0072707111856239	T	T	T
0.9032378864127200	0.5743756764523962	0.0965094842027828	T	T	T
0.8918071225696406	0.5561110508005365	0.2944794412410956	T	T	T
0.7678819307172077	0.5329267540157678	0.2407411372597877	T	T	T
0.6453932507798533	0.3326619916908674	0.2863155515890600	T	T	T
0.7013059412358654	0.3234393950175801	0.1102209937303375	T	T	T
0.8042183586818419	0.3523081027694779	0.9884844959259620	T	T	T
0.9053026728895889	0.3271835422789575	0.1109751116030387	T	T	T
0.9004561155224033	0.3527974581124375	0.3047076010375554	T	T	T
0.7721411271291349	0.3671298685383101	0.2628511345675492	T	T	T
0.6762441059795415	0.4442064122116057	0.1870155456235063	T	T	T
0.9187085989818770	0.4529047357496452	0.1743010060254747	T	T	T
0.5648559126589190	0.6275691993070869	0.4082557702734037	T	T	T
0.5777167090660115	0.4981842492457854	0.4497464128208371	T	T	T
0.5831592806741479	0.3644503868494800	0.4548091520124068	T	T	T
0.7947312995387823	0.6288439366464931	0.3749286781058670	T	T	T
0.8084500336054022	0.5014793782980146	0.4256894664702360	T	T	T
0.8126531316861246	0.3691764774780824	0.4509412880057642	T	T	T
0.0090336135854834	0.5491180952703226	0.2096816477544430	T	T	T
0.0153302967836384	0.3648246744297021	0.2113453157406734	T	T	T
0.8665039084401250	0.4288967903071900	0.7478708666504983	T	T	T
0.7850694637320430	0.4444328166892452	0.6008231348091796	T	T	T
0.6946161154381008	0.4354679644132332	0.4573546530162133	T	T	T
0.6115180301449518	0.4352356252290897	0.6157917360834192	T	T	T
0.6051364263110588	0.4459411078307328	0.8120683181403504	T	T	T
0.7357255044734500	0.4325779991358278	0.7805308457381392	T	T	T
0.8723003717832130	0.6677721480443777	0.7348647672631988	T	T	T
0.8044742532361525	0.6483276184978051	0.5719130013943866	T	T	T
0.6850621858870416	0.6426773939399116	0.4879133302343168	T	T	T
0.5767893027336275	0.6672984326595962	0.5964196685399221	T	T	T
0.5925914035334003	0.6693305868939770	0.7928813637962820	T	T	T
0.7236106085552553	0.6650431621226489	0.7542707303267211	T	T	T
0.7996396431024501	0.5458200812000764	0.7287925519826836	T	T	T
0.5824779453790505	0.5527114957007906	0.6965703047039286	T	T	T
0.9289013414152688	0.3727125346555953	0.9250783150217655	T	T	T
0.8831553587832783	0.5082423772449087	0.9239414643466105	T	T	T
0.8895397295140580	0.6424730328846355	0.9305739336182499	T	T	T
0.6776521731394280	0.3677402586403752	0.9277007075666927	T	T	T
0.6922208092026864	0.4992638704275705	0.9395016771276382	T	T	T
0.6732914296868928	0.6312248695046054	0.9357288804449038	T	T	T
0.4937411098284343	0.4534158853307277	0.7095960377275065	T	T	T
0.4767415710756979	0.6340800285709741	0.7142782492189895	T	T	T
0.6433816635355132	0.9389382411407997	0.2809781819099354	T	T	T
0.6817815866148652	0.9619824577587095	0.0927721381843727	T	T	T
0.7972372583499120	0.9312292474044832	0.0082975150721784	T	T	T
0.9154373903532815	0.9296738735285822	0.0949402191244021	T	T	T

Structure files (CONTCAR) involved in this work:

0.8943389613298882	0.9301609184698967	0.2923575082844974	T	T	T
0.7709285378236843	0.9576015901133004	0.2379915354812148	T	T	T
0.6371842486445403	0.1805943223160728	0.2463604820838150	T	T	T
0.6899244113642505	0.1433905848288888	0.0739616118508653	T	T	T
0.8077222706342068	0.1421013889031580	0.9841728403548278	T	T	T
0.9133788870916641	0.1629658674429642	0.1009024826685524	T	T	T
0.8946353252339897	0.1564822010116753	0.2954948377447283	T	T	T
0.7694417024419755	0.1640551573487875	0.2275779421442883	T	T	T
0.6856866490701358	0.0592732975432010	0.2298718029517313	T	T	T
0.9173809873919219	0.0447636173492354	0.1938680326866521	T	T	T
0.5702607715082959	0.8734941688266192	0.4151393465689355	T	T	T
0.5845567828141538	0.0047435002253469	0.4342664274542180	T	T	T
0.6108581078522427	0.1353061062266716	0.4295615043318388	T	T	T
0.7970140596453840	0.8659548285573082	0.3775692877135857	T	T	T
0.8152167649744536	0.9976432438001309	0.4164082182799239	T	T	T
0.7930488873316350	0.1312831142058779	0.4170667319224997	T	T	T
0.0131699756565005	0.9521889394189028	0.2240393589636424	T	T	T
0.0149296245500187	0.1334767557320545	0.2205982785943766	T	T	T
0.8604920793016708	0.0719788885843159	0.7690924347181035	T	T	T
0.8191608950489788	0.0674548893390330	0.5834847262382415	T	T	T
0.7031809177575048	0.0470888020786558	0.4892805840457146	T	T	T
0.5963430882521920	0.0747669915232958	0.6019413167502644	T	T	T
0.6090934856791685	0.0496167798195947	0.7987092207849115	T	T	T
0.7314908953709607	0.0564887966114031	0.7282185419859873	T	T	T
0.8713330752280923	0.8304673100772070	0.7388838470131897	T	T	T
0.8095971759187974	0.8401641118486333	0.5722226253561061	T	T	T
0.6900158235502419	0.8519322501489169	0.4920394773847085	T	T	T
0.5836280373738121	0.8274631869994575	0.6028169645070997	T	T	T
0.5972916146500918	0.8503731190759040	0.7988340418117464	T	T	T
0.7265167324663017	0.8489350542374414	0.7559765310962867	T	T	T
0.8162104995712890	0.9561755241735519	0.6959292924116822	T	T	T
0.5818830541862556	0.9518430545357104	0.6690715115846853	T	T	T
0.9307877266037626	0.1255629495233984	0.9140782992862899	T	T	T
0.8992257372886127	0.9962977435007873	0.9249224954855944	T	T	T
0.8970551235783968	0.8622446342287237	0.9301246360798797	T	T	T
0.6940548432328165	0.1348520367425751	0.8777129474604655	T	T	T
0.7112571083478016	0.0060498560231297	0.9104624747629106	T	T	T
0.6835214456878663	0.8775808462394254	0.9425920263631755	T	T	T
0.4916254646191657	0.0460874715238193	0.7185532224535590	T	T	T
0.4816589978597356	0.8696512950331283	0.7110030424682722	T	T	T
0.3627193773246595	0.4355231298880261	0.7204279401864805	T	T	T
0.3063443205988735	0.4360287937770170	0.8973276558638543	T	T	T
0.2024459490088031	0.4453996566567197	0.0253408964693047	T	T	T
0.1052474807785710	0.4329950393405025	0.8935090770996592	T	T	T
0.1041821717097266	0.4414580724495754	0.6968455131814022	T	T	T
0.2317230158867324	0.4573501748509980	0.7402597885188237	T	T	T
0.3503897282467276	0.6724372063187870	0.7293741586745267	T	T	T
0.3037212652597372	0.6558140094358996	0.9103954103355726	T	T	T
0.1946028971198266	0.6457359410278047	0.0221798964306215	T	T	T
0.0996484969801672	0.6735181318325613	0.8910543434904870	T	T	T
0.0979130021281754	0.6638188242742178	0.6938410918568801	T	T	T
0.2232867902801374	0.6424063391627491	0.7543616080726665	T	T	T
0.3178615767505596	0.5505764418062518	0.7923178704806344	T	T	T

Structure files (CONTCAR) involved in this work:

0.0975032118885600	0.5521497606385085	0.8056821068857315	T	T	T
0.4326443859328494	0.3770173485352550	0.5777698732905457	T	T	T
0.4155639259176642	0.5089755210303921	0.5724167695026474	T	T	T
0.3983498841151799	0.6405804655796657	0.55214427111105180	T	T	T
0.1936014078697268	0.3637038095581733	0.6106445535201183	T	T	T
0.1855552490957200	0.4933881195054049	0.5619618802451359	T	T	T
0.1898691851168345	0.6278009035836831	0.5612429222927214	T	T	T
0.9934342813492899	0.4682451685103960	0.7956744778525027	T	T	T
0.9895616006534133	0.6296656465306264	0.8001422998147597	T	T	T
0.1396770128736566	0.5668935864767621	0.2140492913566394	T	T	T
0.1915905126650672	0.5606785178331893	0.3942753778560693	T	T	T
0.2979477021858133	0.5558977001169613	0.5168492596202157	T	T	T
0.4018611270344035	0.5659957855556003	0.3933783170668627	T	T	T
0.3988722039812868	0.5558540228439044	0.1967085558731849	T	T	T
0.2704975788546737	0.5469182849203402	0.2399777732315130	T	T	T
0.1409463151907382	0.3286530643711590	0.2413231844838938	T	T	T
0.1950453189921530	0.3543828229249630	0.4153054424177933	T	T	T
0.3094585451721475	0.3529284398243565	0.5151963563709511	T	T	T
0.4123821255227763	0.3273002046507337	0.3959365636321241	T	T	T
0.3981167114073784	0.3377833896919787	0.2000683380016556	T	T	T
0.2719846168628948	0.3520542486892809	0.2550652428614461	T	T	T
0.1831689308544492	0.4505606261271688	0.2802073455709345	T	T	T
0.4148275388743175	0.4470422573731293	0.3110655877714115	T	T	T
0.0683476706627998	0.6237507926039109	0.0709339756503198	T	T	T
0.0827848309204893	0.4920618602517587	0.0690523035553060	T	T	T
0.1014041116958915	0.3604780963845167	0.0577595543247090	T	T	T
0.3141313882364710	0.6343868024501111	0.1048044713440114	T	T	T
0.3168584969202710	0.5033221456386606	0.0643152870520976	T	T	T
0.3069931986243419	0.3683727968135397	0.0637493571824081	T	T	T
0.5121353489675753	0.5372734034985521	0.2873838508947950	T	T	T
0.5159313718921985	0.3612289635813381	0.2822186416295980	T	T	T
0.4370345998130961	0.7523286763715317	0.6393833325906280	T	T	T
0.1919329956370166	0.7493671462613023	0.6382770172175288	T	T	T
0.2751622209205259	0.7517207935752590	0.0377414461234651	T	T	T
0.1110595209801204	0.7485457849920881	0.0527477349353969	T	T	T
0.0606284372486473	0.2479161292270824	0.1431191229611066	T	T	T
0.3081418419254626	0.2477663499468472	0.1422580950110822	T	T	T
0.2253848291328530	0.2488747490497403	0.5272163397281334	T	T	T
0.3925261037731135	0.2514073044490882	0.5545088751408139	T	T	T
0.5587716317550417	0.2486981857881522	0.3688321147982604	T	T	T
0.8150287959291911	0.2546355790576247	0.3560781978805664	T	T	T
0.7262232793806516	0.2469352458320703	0.9566302695220721	T	T	T
0.8865873652479741	0.2484838059682741	0.9556475031828958	T	T	T
0.9447228760163755	0.7501581470149083	0.8547181997856033	T	T	T
0.6740111815613057	0.7561218783926652	0.8793489875393425	T	T	T
0.7641531603591903	0.7460456783879191	0.4443871803533015	T	T	T
0.6077414502331298	0.7494350667909175	0.4482868363397325	T	T	T
0.9184995927719951	0.3744383708033158	0.5999456412124592	T	T	T
0.0182149730415772	0.8049001304787181	0.5231102213230164	T	T	T
0.9787495263062811	0.6838435981892674	0.4546151599277580	T	T	T
0.9609215455778637	0.4216072433779497	0.5461309753715979	T	T	T
0.1408043161371895	0.7202633419598081	0.3519559905003256	T	T	T
0.9567162457285455	0.7734281898914388	0.4185621263278921	T	T	T

Structure files (CONTCAR) involved in this work:

0.0290683556073645	0.7157505618458764	0.5736258428663120	T	T	T
0.9125123198707017	0.8015171796594923	0.5737833483152798	T	T	T
0.9154534620028237	0.6955227606030026	0.5898206530893543	T	T	T
0.8814996572748012	0.3616972791697720	0.5551808536255847	T	T	T
0.9394230523588691	0.4725583490647945	0.5484577885923083	T	T	T
0.9658969196714846	0.4052200611025593	0.4681739781604336	T	T	T
0.0096064823766787	0.4213575144807673	0.5833158383706273	T	T	T
0.8903846641271057	0.4035255418977884	0.6848975758681372	T	T	T
0.1050967535667662	0.7460426062261604	0.3028848181158650	T	T	T
0.1871147208515757	0.7102286311273692	0.3106985829676990	T	T	T
0.1518195019498433	0.7522610242468510	0.4166988883265971	T	T	T
0.1191043572043057	0.6724717483201729	0.3764837118601356	T	T	T

Figure S10 Mo-TS

Si Al O C Mo H

1.0000000000000000					
20.0219999999999985	0.0000000000000000	0.0000000000000000			
0.0000000000000000	19.8990000000000009	0.0000000000000000			
0.0000000000000000	0.0000000000000000	13.3829999999999991			
93	3	193	4	4	9

Selective dynamics

Direct

0.4244231827953097	0.0575374876032357	0.6553524317358952	T	T	T
0.3063875282926656	0.0284084201456036	0.7996717241587940	T	T	T
0.2810835927874104	0.0573503298194975	0.0227662149766350	T	T	T
0.1210498210238972	0.0630773217381503	0.0206384853841868	T	T	T
0.0663730442213009	0.0280171531720626	0.8080706121640362	T	T	T
0.1798112966676097	0.0623449050449701	0.6737157203815114	T	T	T
0.4149228257580991	0.8269316218302741	0.6681382617878608	T	T	T
0.3045944654574489	0.8690548599475951	0.8127107666634775	T	T	T
0.2695216345743511	0.8308967269301174	0.0312425736954734	T	T	T
0.1155578485238459	0.8258202552005062	0.0163800426418777	T	T	T
0.0693141642536722	0.8709434067485838	0.8012142064495261	T	T	T
0.1864158267423245	0.8266943909456751	0.6744360045235132	T	T	T
0.0789476719524093	0.9377983856346468	0.1568393802847097	T	T	T
0.1938434204247141	0.9684484705544244	0.3017420730277233	T	T	T
0.2176216610642558	0.9437973708586298	0.5243346787239148	T	T	T
0.3753852680523412	0.9368494282248867	0.5174548580220575	T	T	T
0.4333000155555161	0.9698851417273922	0.3075778080327929	T	T	T
0.3181809171103236	0.9381649580591364	0.1743041550094024	T	T	T
0.0795754521574302	0.1720353151983550	0.1749043233696085	T	T	T
0.1960814670172286	0.1270545918827611	0.3096689653468748	T	T	T
0.2330337217312378	0.1667918589309916	0.5278134448436340	T	T	T
0.3871508768612126	0.1721473817984047	0.5182623980405351	T	T	T
0.4355319103118962	0.1281853567503558	0.3051225978189563	T	T	T
0.3179298844196873	0.1705187288642012	0.1745958149107327	T	T	T
0.5759545491223073	0.5526297413469102	0.3575219554585758	T	T	T
0.6912729608393469	0.5234029132677676	0.2038625361123538	T	T	T
0.7100941408165961	0.5709842920258803	0.9932220021250063	T	T	T
0.8677714054988437	0.5722562051391766	0.9857085837357812	T	T	T
0.9313708110329548	0.5343750629364671	0.1918712740433300	T	T	T
0.8152042962720820	0.5566985395137451	0.3314344259255875	T	T	T
0.5768925893337613	0.3268820985574538	0.3486413468786535	T	T	T
0.6993655911701647	0.3672551087146800	0.2113722800738999	T	T	T

Structure files (CONTCAR) involved in this work:

0.7295130211103503	0.3223564465671518	0.9965171638121643	T	T	T
0.8839566462591824	0.3248729380134177	0.9933317555612479	T	T	T
0.9361665550499653	0.3756949361474077	0.1992239324578154	T	T	T
0.8259426342859011	0.3355212590230974	0.3425638707835055	T	T	T
0.7965608523122685	0.4688516295085278	0.7162743098869457	T	T	T
0.7753630823948744	0.4410972451892038	0.4824893202497334	T	T	T
0.6188446086022370	0.4342221648377173	0.4954349155835356	T	T	T
0.5748211150775200	0.4713517891303328	0.7097793076440460	T	T	T
0.6816920552822745	0.4373324054455975	0.8652464065556547	T	T	T
0.9257789540826419	0.6718147622283175	0.8250665029449327	T	T	T
0.7612555924652383	0.6667943216667063	0.4702908602358829	T	T	T
0.6079502815833957	0.6712428138517270	0.4839254878526167	T	T	T
0.5585077542275099	0.6301858569038895	0.6999765934580088	T	T	T
0.6705422883776019	0.6816735173594634	0.8367883614763107	T	T	T
0.5777389545308260	0.9438346603850734	0.3547173525259387	T	T	T
0.6968187275443788	0.9795513757350848	0.2125305918597792	T	T	T
0.7171007634155379	0.9424406581923047	0.9889605166961196	T	T	T
0.8754060871447433	0.9292926114527887	0.9902101352978869	T	T	T
0.9342552219640280	0.9641022688242242	0.2050488501488980	T	T	T
0.8187848006578961	0.9374730526389796	0.3381587979573120	T	T	T
0.5808106221226148	0.1736040954827696	0.3346158326737591	T	T	T
0.6978817073870935	0.1374126299878326	0.1961765730315822	T	T	T
0.7299090485813829	0.1661529724332988	0.9752545231640112	T	T	T
0.8843879041223583	0.1678128437756769	0.9904917540325913	T	T	T
0.9353344810608556	0.1235712503066982	0.2067266529220208	T	T	T
0.8183692520470238	0.1781791638175839	0.3255517627184539	T	T	T
0.9178059456703098	0.0553912394411203	0.8505260534704041	T	T	T
0.8073004568986309	0.0366651701707262	0.6943001469335409	T	T	T
0.7822536079088579	0.0617046584130775	0.4764426887072033	T	T	T
0.6241016601225262	0.0642829460837341	0.4904843525336369	T	T	T
0.5699679928301012	0.0288950164843263	0.6979784166709816	T	T	T
0.6872135687341538	0.0592394860348465	0.8303528547136346	T	T	T
0.9248194004320864	0.8266273291094927	0.8323527938612765	T	T	T
0.7623826815821293	0.8249409941385288	0.4776088622491284	T	T	T
0.6100843407868363	0.8254525220357193	0.4883221859857468	T	T	T
0.5596228259117200	0.8732663037463304	0.6958655102026524	T	T	T
0.6668357604941783	0.8352432518193519	0.8467036234230351	T	T	T
0.4289752704373512	0.4423658399475008	0.6487796559621765	T	T	T
0.3052922553509137	0.4706987180787683	0.7879001161207662	T	T	T
0.2842609113097884	0.4372397370075656	0.0133120855494395	T	T	T
0.1250252174326747	0.4329180327355658	0.0145164433725786	T	T	T
0.0749831895684595	0.4746022235126282	0.8024795644510322	T	T	T
0.1790900057151893	0.4391610342508257	0.6509479930030799	T	T	T
0.4162816421344094	0.6733619853882902	0.6619626253092609	T	T	T
0.3017183009643300	0.6302490031794399	0.8054603793624454	T	T	T
0.2728268772429734	0.6711387273402248	0.0237962054309836	T	T	T
0.1192146550500005	0.6722104267243127	0.0087430990183565	T	T	T
0.0727364040807534	0.6296330057861714	0.7967109384238286	T	T	T
0.1853251388682402	0.6703663959284605	0.6688776715434941	T	T	T
0.0777001055730124	0.5574316216228200	0.1459311985163955	T	T	T
0.1976383428227832	0.5296840418886027	0.2882618786940522	T	T	T
0.2234597686763718	0.5560801412475407	0.5127723792718650	T	T	T
0.3819338210110957	0.5624014723667919	0.5117833642140570	T	T	T

Structure files (CONTCAR) involved in this work:

0.4330367071877013	0.5247791671406343	0.2995533578740940	T	T	T
0.3243203447180180	0.5565868525425905	0.1521963364483567	T	T	T
0.0794320065185398	0.3265405513656346	0.1629941633079963	T	T	T
0.1978860897154979	0.3713945794890618	0.3006419052420050	T	T	T
0.2321027855445571	0.3271707911468685	0.5197377301543363	T	T	T
0.3864521950298448	0.3257546962407942	0.5148075637786523	T	T	T
0.4356147403761020	0.3674623907612656	0.3012951531041155	T	T	T
0.3208887350451750	0.3277097419602329	0.1674860624796470	T	T	T
0.9219882106613659	0.4443975572037170	0.8568855646992615	T	T	T
0.7954317411652400	0.6319669852695312	0.6997685183164446	T	T	T
0.7943982893347128	0.8744387928281598	0.7057644184206385	T	T	T
0.3608692409690508	0.0661716101784397	0.7298368563309487	T	T	T
0.3166178390537579	0.0527051121464512	0.9141609245469318	T	T	T
0.2007615433076815	0.0517780168040774	0.0114205869617156	T	T	T
0.0878118238457787	0.0649487862774343	0.9110042704791028	T	T	T
0.1037052475347217	0.0650470950555455	0.7153221648574353	T	T	T
0.2307317391255717	0.0473539260973767	0.7659193224094912	T	T	T
0.3608815387832554	0.8237065272409628	0.7585577523892714	T	T	T
0.3085558893436847	0.8562684232948324	0.9318763103530050	T	T	T
0.1917211343973503	0.8540817078765712	0.0226603775805278	T	T	T
0.0891696213269873	0.8312262381754673	0.9026189364467896	T	T	T
0.1083886853007878	0.8360219997588444	0.7070647492112527	T	T	T
0.2312183955418358	0.8462558499877392	0.7715734750153335	T	T	T
0.3174529384943903	0.9477457167688609	0.7875503141907119	T	T	T
0.0903619719462882	0.9495419997071647	0.8106027467339408	T	T	T
0.4333821723203908	0.1261184958459829	0.5904141843219910	T	T	T
0.4144217813587056	0.9944213996009936	0.5799415681373575	T	T	T
0.3822589364448390	0.8640482047901076	0.5714236741289969	T	T	T
0.1971781660692635	0.1347839095479776	0.6251056719966989	T	T	T
0.1852688602715561	0.0032690529067754	0.5907313501122351	T	T	T
0.2048844233757337	0.8715600009023590	0.5775819090250375	T	T	T
0.9863165217439678	0.0336457344846307	0.7935956933689391	T	T	T
0.9896010707020191	0.8647144475675029	0.7834856441635537	T	T	T
0.1428100193514803	0.9275373091322199	0.2297668086491967	T	T	T
0.1814630822961899	0.9441582036990809	0.4157871353705587	T	T	T
0.2969693075679091	0.9572801991254177	0.5104463168040833	T	T	T
0.4082770061589571	0.9306999001006016	0.4072976086339863	T	T	T
0.3951419129925747	0.9401498770055928	0.2104390219564128	T	T	T
0.2704529179870216	0.9516121329473000	0.2708091345976527	T	T	T
0.1387001223676754	0.1727875594020719	0.2580517160169331	T	T	T
0.1945990138137028	0.1398485156024095	0.4289073695893807	T	T	T
0.3108755589513773	0.1435244632327243	0.5225139618797310	T	T	T
0.4139666013041119	0.1697022232834124	0.4042144027136030	T	T	T
0.3950120561545043	0.1581333648025396	0.2092311319977653	T	T	T
0.2693327091162852	0.1472072205961904	0.2662459476613462	T	T	T
0.1798334868518159	0.0484176260077853	0.2867270534626132	T	T	T
0.4169397535090856	0.0494944936358848	0.3207245824218031	T	T	T
0.0687338321134562	0.8700705049675787	0.0905451082856977	T	T	T
0.0876310542087790	0.0020457147520227	0.0837849843559788	T	T	T
0.1053411045572557	0.1341247780007203	0.0746864710854365	T	T	T
0.3032462448514624	0.8642563611136620	0.1289843438509635	T	T	T
0.3065186214687092	0.9949479108654672	0.0898553072193098	T	T	T
0.3017680111632068	0.1281811269867049	0.0739235050831323	T	T	T

Structure files (CONTCAR) involved in this work:

0.5120896028227786	0.9575419655199331	0.2869552002712117	T	T	T
0.5154658134257941	0.1364766171922403	0.2871448147178725	T	T	T
0.6439780646845560	0.5505328766445653	0.2930911954754133	T	T	T
0.6757062056018778	0.5661426301515886	0.1037363722998154	T	T	T
0.7890107130174988	0.5843135402682168	0.0079468504807724	T	T	T
0.9067658951479757	0.5742854435291359	0.0932768759391372	T	T	T
0.8917922800384924	0.5592401818554714	0.2918969864678914	T	T	T
0.7686454285665795	0.5333708066385247	0.2383313463553089	T	T	T
0.6455364402376013	0.3335252094985130	0.2859490311137946	T	T	T
0.7030777431779668	0.3218412548496820	0.1115595143223620	T	T	T
0.8057137572269968	0.3500322714793443	0.9895025628467941	T	T	T
0.9076593917122370	0.3283868460050123	0.1106692169485817	T	T	T
0.9012606454464903	0.3526720965309150	0.3047208481409558	T	T	T
0.7726310821039276	0.3674121338050362	0.2646617204838324	T	T	T
0.6780978246131404	0.4437447813192065	0.1837915934119557	T	T	T
0.9197333108857692	0.4539929669966821	0.1764809694787046	T	T	T
0.5655517738936555	0.6273787273443430	0.4035028725577912	T	T	T
0.5798494909349359	0.4989239803137867	0.4494963299942995	T	T	T
0.5847213211872361	0.3651225043024569	0.4556602677345782	T	T	T
0.7930630687084509	0.6300615476959616	0.3727381163358823	T	T	T
0.8094327652935875	0.5032175362146724	0.4234739287279395	T	T	T
0.8149092218720362	0.3714489956040482	0.4520459824669149	T	T	T
0.0102133534095763	0.5502501251859482	0.2120926605521783	T	T	T
0.0163961336092251	0.3658180847404373	0.2129059926192262	T	T	T
0.8697067580946090	0.4324187914590686	0.7452451243074233	T	T	T
0.7870082683682521	0.4483845360786384	0.6001346579023827	T	T	T
0.6963498263710221	0.4360079063906402	0.4573911896423280	T	T	T
0.6137338137420822	0.4360624052180694	0.6160668158391254	T	T	T
0.6090091710324645	0.4463537145975309	0.8128079980063008	T	T	T
0.7395158599641956	0.4309583283598816	0.7804331148821950	T	T	T
0.8757687744153037	0.6678758725342504	0.7278735017205915	T	T	T
0.8048455671219388	0.6497616857002321	0.5697601114493034	T	T	T
0.6843935262913193	0.6424149809419132	0.4883304426679816	T	T	T
0.5745579819834788	0.6649592046552597	0.5930345159936901	T	T	T
0.5962155313811728	0.6701643696721402	0.7881594186959965	T	T	T
0.7282004748132982	0.6705146695164906	0.7547096647053357	T	T	T
0.7982907998499574	0.5479238068987478	0.7309481666792300	T	T	T
0.5820886683722685	0.5521402686206289	0.6979466057442784	T	T	T
0.9292366753307281	0.3696553890507121	0.9214654436906828	T	T	T
0.8809525752004267	0.5040768934353665	0.9265012839400142	T	T	T
0.8929643486275348	0.6379218116193985	0.9225508545491073	T	T	T
0.6799440615140037	0.3683869102741025	0.9295659484959252	T	T	T
0.6976955181249450	0.4999849729541436	0.9372944529283526	T	T	T
0.6755755044335252	0.6314828553918828	0.9325503281416138	T	T	T
0.4967449447086769	0.4493166050977684	0.7139110064026618	T	T	T
0.4778320880994725	0.6349136375780163	0.7171534453846745	T	T	T
0.6425496648217278	0.9407898002063848	0.2817636844668319	T	T	T
0.6848585283312448	0.9647784788838774	0.0954681868908176	T	T	T
0.7953640323113007	0.9226909194251360	0.0042304981501606	T	T	T
0.9111020226772257	0.9333320195280855	0.0989681926496419	T	T	T
0.8952538162397197	0.9260641924716381	0.2972041688192254	T	T	T
0.7711089303780797	0.9527962620914054	0.2429550657197360	T	T	T
0.6378038393403364	0.1791394998691881	0.2486215666884046	T	T	T

Structure files (CONTCAR) involved in this work:

0.6906216865536762	0.1429591298444904	0.0762303650712777	T	T	T
0.8073673097926348	0.1410337859041009	0.9837475238154592	T	T	T
0.9121865993242066	0.1577434541811422	0.1032183603762016	T	T	T
0.8952010693884234	0.1589868418840238	0.2983295898139608	T	T	T
0.7705085391342511	0.1681610027868315	0.2279266415093175	T	T	T
0.6921852890552930	0.0598192498461254	0.2343962321805369	T	T	T
0.9177144977029817	0.0437392941408641	0.2079839884853233	T	T	T
0.5674862101433018	0.8727848773901213	0.4129073203325748	T	T	T
0.5836902257771904	0.0033385981054681	0.4371822853709171	T	T	T
0.6097010330107929	0.1338515832489277	0.4311799643759762	T	T	T
0.8010271219008135	0.8652965997210487	0.3883544288995143	T	T	T
0.8166837092811388	0.9986373176895098	0.4175488349072881	T	T	T
0.7917910987262197	0.1315909621411488	0.4160591159723147	T	T	T
0.0127088335017278	0.9486295530464327	0.2252090589431361	T	T	T
0.0151284340957047	0.1337066887175763	0.2226704845343815	T	T	T
0.8612343060745805	0.0724922996891396	0.7683192733526635	T	T	T
0.8184326160615676	0.0695020743184704	0.5836340540819149	T	T	T
0.7030948046771273	0.0460100782937429	0.4885203962321427	T	T	T
0.5973484448984367	0.0733037392826582	0.6041700773814698	T	T	T
0.6097120188712358	0.0461361134676874	0.8003651532442352	T	T	T
0.7318043335029879	0.0569922072562315	0.7294301071013677	T	T	T
0.8659668517848981	0.8316468071788661	0.7500159664527966	T	T	T
0.8005185086898889	0.8374785245157714	0.5837052144299493	T	T	T
0.6868295458866626	0.8533347774201847	0.4877290431818614	T	T	T
0.5821876084068954	0.8265004564317004	0.6018562283219830	T	T	T
0.5922687442223920	0.8480084310308945	0.7997079276978682	T	T	T
0.7215138167485752	0.8570713476825111	0.7654155634145509	T	T	T
0.8165515235747418	0.9571244930489889	0.6934164898828380	T	T	T
0.5803943375667098	0.9501716856165032	0.6694124836424239	T	T	T
0.9309628984984371	0.1229893866280948	0.9162446951020629	T	T	T
0.8941940721756905	0.9950649625993100	0.9247393222404758	T	T	T
0.9038309593007410	0.8616159100558687	0.9373317166811903	T	T	T
0.6926235462129900	0.1330938386252458	0.8802825154011575	T	T	T
0.7137054042119723	0.0044053195604087	0.9107173423515874	T	T	T
0.6740549402754390	0.8792630228558388	0.9492755285593877	T	T	T
0.4918204835477816	0.0457113975628545	0.7199786419334185	T	T	T
0.4790101373996821	0.8686748438413467	0.7077522472711357	T	T	T
0.3650178304777776	0.4378885987473545	0.7227594519333219	T	T	T
0.3028845810507015	0.4342295713264129	0.8958435761898028	T	T	T
0.2045266366724178	0.4432167328003667	0.0338238980137860	T	T	T
0.1100690659661030	0.4361446919779894	0.8963685193305179	T	T	T
0.1050470650038699	0.4416211268623825	0.6995918088184279	T	T	T
0.2338319078479395	0.4594695159229270	0.7345526210958695	T	T	T
0.3519263184936227	0.6725164353417179	0.7354462859011752	T	T	T
0.3104748711301912	0.6550903705848312	0.9193640540810302	T	T	T
0.1957513697306368	0.6450704683493196	0.0180316422918740	T	T	T
0.0978740149177621	0.6736990069319158	0.8915075916077463	T	T	T
0.1036761133962264	0.6641588557058961	0.6919357028145434	T	T	T
0.2252688521319970	0.6464806496476758	0.7683749289835570	T	T	T
0.3183475269491320	0.5509381747881199	0.7978049731843109	T	T	T
0.1001339996380765	0.5534641615170379	0.8050856155954985	T	T	T
0.4329322458344695	0.3735145238591502	0.5838232591510737	T	T	T
0.4242055274345509	0.5061661126524287	0.5728486804822084	T	T	T

Structure files (CONTCAR) involved in this work:

0.3962018522271397	0.6364484687802612	0.5577481800532450	T	T	T
0.1922441933901723	0.3635853384017758	0.6101979519046425	T	T	T
0.1830183578494212	0.4924287979725703	0.5583574373708814	T	T	T
0.2057210733796279	0.6243503999371381	0.5743782904020269	T	T	T
0.9960041020836955	0.4693746144247170	0.8027221147520431	T	T	T
0.9925872947003331	0.6311039371069904	0.7901860898298245	T	T	T
0.1409236468716928	0.5668969726424775	0.2213608819291106	T	T	T
0.2001355835045826	0.5653271816654607	0.3976026539669029	T	T	T
0.3032051462928117	0.5426644573894840	0.5206046760820996	T	T	T
0.4047783165605490	0.5653284552681705	0.3959980768901267	T	T	T
0.3988466240587416	0.5540543899477118	0.1989095417630190	T	T	T
0.2708915151445213	0.5367978379326943	0.2384807466803786	T	T	T
0.1421323881022461	0.3297509223833945	0.2394111163332025	T	T	T
0.1963139775476453	0.3456464248880110	0.4149637259329141	T	T	T
0.3094800486697194	0.3527745281520007	0.5183452996200957	T	T	T
0.4129942610077865	0.3264120410517030	0.4004320616598939	T	T	T
0.3978187864801473	0.3359711162160668	0.2046845308656087	T	T	T
0.2716297928739891	0.3585244157771972	0.2532584009751011	T	T	T
0.1788621866422073	0.4506841618037230	0.2979088289078442	T	T	T
0.4149301831879177	0.4458123039383597	0.3144928569767592	T	T	T
0.0714255981199171	0.6232626223280266	0.0739851412695547	T	T	T
0.0856129911478589	0.4916841921938224	0.0749662846701153	T	T	T
0.1004309161148887	0.3603139735251604	0.0567072891171406	T	T	T
0.3109095654325182	0.6326645281201767	0.1137081645171832	T	T	T
0.3198317595237020	0.5036453561356539	0.0600632164588757	T	T	T
0.3114189393074324	0.3681368584064127	0.0632702627499930	T	T	T
0.5129302982999360	0.5347919840230948	0.2864164744366413	T	T	T
0.5158098979064357	0.3601880384270590	0.2848414386672803	T	T	T
0.4351867455676895	0.7508189072106475	0.6368613478330545	T	T	T
0.1986765953874599	0.7486568548716231	0.6412314531300912	T	T	T
0.2751032733060331	0.7506864001465782	0.0450656295868610	T	T	T
0.1124162496972064	0.7480198605874134	0.0524304403587433	T	T	T
0.0602169562607389	0.2483823336286989	0.1443168018387669	T	T	T
0.3048070227752769	0.2489657928336700	0.1483739240175274	T	T	T
0.2279561258334349	0.2472911855141106	0.5374616792705772	T	T	T
0.3901808778992946	0.2493958025101202	0.5571076134383918	T	T	T
0.5608341832739925	0.2486545180187938	0.3713189783241964	T	T	T
0.8154393430365098	0.2560247160031321	0.3609922505321364	T	T	T
0.7258083567928293	0.2460272211045700	0.9565441352376775	T	T	T
0.8883483461143131	0.2460971275141061	0.9599126427505693	T	T	T
0.9443497022744890	0.7487781345786471	0.8545901559618374	T	T	T
0.6731913480673818	0.7575009379840870	0.8812874952963533	T	T	T
0.7620066085324896	0.7467116379601068	0.4449377786425256	T	T	T
0.6065124494631881	0.7488879384458118	0.4472333852735066	T	T	T
0.9201997337058052	0.3754419525524996	0.5985243963688410	T	T	T
0.0108879030254821	0.8182846993362360	0.5164491976666882	T	T	T
0.9643802795524493	0.6996860060384723	0.4395564433320063	T	T	T
0.9650688894207227	0.4198578378800584	0.5442348694410540	T	T	T
0.1068274377301549	0.6956300439245202	0.4262888964950091	T	T	T
0.9410213808147044	0.7927193343614842	0.4192712491378475	T	T	T
0.0315990210686810	0.7286732079416331	0.5496708721321788	T	T	T
0.9074556645257966	0.8070739703743314	0.5814500273357948	T	T	T
0.9143490837314223	0.7017183560976975	0.5805795739970073	T	T	T

Structure files (CONTCAR) involved in this work:

0.8831123646370117	0.3635350335398803	0.5533086526742227	T	T	T
0.9424325057760886	0.4699262199665819	0.5345905131227563	T	T	T
0.9761451578246099	0.3980089010677181	0.4707489160193259	T	T	T
0.0107602277198875	0.4238596029983304	0.5887336561492932	T	T	T
0.8927551610262556	0.4064139204926596	0.6822911340357327	T	T	T
0.1067229519948205	0.7334829131234889	0.3664417328626160	T	T	T
0.1100427185196942	0.6455178423447376	0.3923670838722663	T	T	T
0.1521358868578093	0.7032003686314583	0.4709831987308957	T	T	T
0.0297034052874995	0.6873832036537436	0.4265144143130500	T	T	T

Figure S10 Mo-FS

Si Al O C Mo H

1.0000000000000000

20.0219999999999985 0.0000000000000000 0.0000000000000000

0.0000000000000000 19.8990000000000009 0.0000000000000000

0.0000000000000000 0.0000000000000000 13.3829999999999991

93 3 193 4 4 9

Selective dynamics

Direct

0.4245751308555158	0.0579859873876220	0.6549682177981823	T	T	T
0.3068757556041276	0.0289884147303938	0.7994399374509317	T	T	T
0.2812210378179626	0.0570839125245635	0.0225790151895217	T	T	T
0.1213263770688871	0.0631541025551981	0.0203865521480242	T	T	T
0.0666484382533847	0.0284936352274413	0.8078627759666923	T	T	T
0.1803316803802856	0.0629918559756957	0.6738544869430517	T	T	T
0.4151450023749582	0.8272481028591914	0.6688496997085874	T	T	T
0.3049009618296071	0.8699591533565449	0.8128115283761190	T	T	T
0.2696061505977268	0.8313977811193610	0.0310566090003006	T	T	T
0.1156364743930478	0.8260893279951523	0.0166931909202638	T	T	T
0.0697099798309914	0.8713598018614821	0.8013983037607521	T	T	T
0.1869422065855460	0.8270784600207474	0.6748828279970218	T	T	T
0.0791260577519651	0.9379393245991280	0.1568883960977743	T	T	T
0.1939183956715614	0.9683247607093876	0.3018730426775888	T	T	T
0.2178062917051179	0.9440793886841505	0.5245012123902895	T	T	T
0.3755442883283631	0.9369367185835927	0.5175687501129194	T	T	T
0.4333793307958262	0.9697906847664016	0.3077004023510839	T	T	T
0.3181309421717146	0.9379116119589079	0.1746375987767178	T	T	T
0.0796563990339498	0.1719322120696074	0.1749001641028790	T	T	T
0.1961878594267606	0.1268520427397392	0.3093355779736588	T	T	T
0.2331989681127323	0.1668871066694802	0.5271892534095595	T	T	T
0.3873717168792635	0.1724637341924899	0.5177975615795136	T	T	T
0.4355021289507728	0.1280469752987332	0.3048707287492454	T	T	T
0.3180151284227040	0.1704841331524661	0.1740893619515698	T	T	T
0.5759168303844655	0.5525825432991548	0.3575477321132813	T	T	T
0.6912305853117998	0.5232480184334306	0.2043771388416659	T	T	T
0.7096198857155657	0.5710125741401743	0.9935645541527961	T	T	T
0.8674005124311089	0.5726976325418496	0.9852087309723537	T	T	T
0.9309441797344878	0.5343008534405791	0.1912720701138017	T	T	T
0.8151437122738815	0.5561446715062618	0.3317129560147450	T	T	T
0.5765828238092078	0.3267497335823875	0.3483511369415160	T	T	T
0.6990361088594664	0.3671522690953165	0.2113519233440943	T	T	T
0.7292227337911876	0.3225780156578995	0.9962699309109987	T	T	T
0.8836473725646995	0.3252640111773064	0.9931486765272833	T	T	T
0.9358079174422983	0.3755954014965739	0.1990424050648222	T	T	T

Structure files (CONTCAR) involved in this work:

0.8256240034169862	0.3352146539854821	0.3423370703695614	T	T	T
0.7963293118344286	0.4686966265322930	0.7163063430695013	T	T	T
0.7749931814387416	0.4405743695418957	0.4826280712591261	T	T	T
0.6183480895337997	0.4339592271978078	0.4953519206621013	T	T	T
0.5742973488349770	0.4713784020233605	0.7095745665970881	T	T	T
0.6810477762898804	0.4375436129958792	0.8652523160084222	T	T	T
0.9259849887811328	0.6721609765265141	0.8247911162232507	T	T	T
0.7614309190875495	0.6663380163841022	0.4705151379432896	T	T	T
0.6079670780484917	0.6711788786673940	0.4840330803795605	T	T	T
0.5583425657771097	0.6301859571947431	0.6999272615915847	T	T	T
0.6704783024387925	0.6813983203162265	0.8371009317152005	T	T	T
0.5777902149094983	0.9437095043079868	0.3544868466410216	T	T	T
0.6963327650244868	0.9794904507969652	0.2117682459961893	T	T	T
0.7174856673927208	0.9427873310951045	0.9886162101796291	T	T	T
0.8759301140969672	0.9295120354905823	0.9897416907923580	T	T	T
0.9344508660808776	0.9639694157082421	0.2041539309630462	T	T	T
0.8185215016329521	0.9374965192896272	0.3369354183314157	T	T	T
0.5806957743589402	0.1735819844816725	0.3340368374467965	T	T	T
0.6973506463107015	0.1372738454817476	0.1954692072500701	T	T	T
0.7298735586736856	0.1663397922827262	0.9746993730774300	T	T	T
0.8843170614753679	0.1682949769330765	0.9896370303516846	T	T	T
0.9352088846435328	0.1233870408571235	0.2054261898363764	T	T	T
0.8182813124952185	0.1776341744899487	0.3249494599511265	T	T	T
0.9181903963921604	0.0556958731023708	0.8501849804166443	T	T	T
0.8073054195019301	0.0362235221208582	0.6941780773596601	T	T	T
0.7823452112148962	0.0613222201143923	0.4762568339369119	T	T	T
0.6241655302119544	0.0643765723994411	0.4899718028238790	T	T	T
0.5700201039765680	0.0291682190069194	0.6974979018501501	T	T	T
0.6872261819750809	0.0594648606833148	0.8298809299666940	T	T	T
0.9250633755214905	0.8267726604195463	0.8308307521122085	T	T	T
0.7624125548731978	0.8247591638203525	0.4759296285213613	T	T	T
0.6100890301927515	0.8253686268312053	0.4882795591175181	T	T	T
0.5599211759838137	0.8735601162822347	0.6957874865333256	T	T	T
0.6675815107124888	0.8348982935904916	0.8458031985202886	T	T	T
0.4284882458630148	0.4426458866148236	0.6483739474879804	T	T	T
0.3052774340615023	0.4705242493104109	0.7880891364454530	T	T	T
0.2838822939437468	0.4378313909344166	0.0135347302391998	T	T	T
0.1243676315198989	0.4331798541435817	0.0139079798888506	T	T	T
0.0743654464455783	0.4748156033341529	0.8014161928127193	T	T	T
0.1792926262196011	0.4388238871122465	0.6516259055099159	T	T	T
0.4161415737642462	0.6736079796743963	0.6619396993520986	T	T	T
0.3012110412237282	0.6300990628252835	0.8046255178200715	T	T	T
0.2729207692257214	0.6713589855617826	0.0231324033462388	T	T	T
0.1192729495392869	0.6724469016976545	0.0090055225523305	T	T	T
0.0728664537736885	0.6299548403391914	0.7968096755728472	T	T	T
0.1851219970364227	0.6708687971606161	0.6686294753692605	T	T	T
0.0773853576901831	0.5576723810549100	0.1455585465851006	T	T	T
0.1972582017217732	0.5305788242808135	0.2882555751746214	T	T	T
0.2231149254431992	0.5563903556905931	0.5128094347883817	T	T	T
0.3818936052672827	0.5631241282455890	0.5112225482670931	T	T	T
0.4332921530851988	0.5251710922784938	0.2991400352919397	T	T	T
0.3241279249118001	0.5576475919498771	0.1528842645715425	T	T	T
0.0794045376470705	0.3265797072123106	0.1631265275309124	T	T	T

Structure files (CONTCAR) involved in this work:

0.1977810689744876	0.3717834734319672	0.3006491056139700	T	T	T
0.2319811309427147	0.3275597107850035	0.5194548845944461	T	T	T
0.3864815011083285	0.3260411930316211	0.5141985769548392	T	T	T
0.4355349327877309	0.3678200005067789	0.3006688223541556	T	T	T
0.3206566217763791	0.3276739224225609	0.1675160584768249	T	T	T
0.9218449600642515	0.4447229289481717	0.8565846271869423	T	T	T
0.7957236325602692	0.6318137498774592	0.6997487666892657	T	T	T
0.7950219053691903	0.8737489458482092	0.7044868086472160	T	T	T
0.3611870762523622	0.0670667252126980	0.7296829237407605	T	T	T
0.3173421139771802	0.0522282039618390	0.9143812974863936	T	T	T
0.2009515128517730	0.0517487965361364	0.0101016152547563	T	T	T
0.0875640906651241	0.0653682224610101	0.9110851401369937	T	T	T
0.1041978877614961	0.0655507511761425	0.7153770888707920	T	T	T
0.2312185813225071	0.0484078471360591	0.7662565060649916	T	T	T
0.3612066510746683	0.8241482024601495	0.7594544006162427	T	T	T
0.3084285011403362	0.8580575861107640	0.9322125689152337	T	T	T
0.1917199455593287	0.8544737478496074	0.0235277951818016	T	T	T
0.0895689926985177	0.8316074326445569	0.9027774425469313	T	T	T
0.1088197275400889	0.8361184518141164	0.7075015557505427	T	T	T
0.2314832998055042	0.8472337474408949	0.7719735111466179	T	T	T
0.3179940808135164	0.9484016335272161	0.7861023976762662	T	T	T
0.0906845761873711	0.9500059438989229	0.8105636417757165	T	T	T
0.4337574324663700	0.1263963356067836	0.5896908200792690	T	T	T
0.4143831113549936	0.9947688852891953	0.5798264348567310	T	T	T
0.3824709280281551	0.8643490394152142	0.5721254398026612	T	T	T
0.1974216326272761	0.1354481582298263	0.6249895178208420	T	T	T
0.1860617363151627	0.0037253073601192	0.5912452272918839	T	T	T
0.2050431373640481	0.8719005628288992	0.5778218208655682	T	T	T
0.9866075781386029	0.0342382724198775	0.7927666704390445	T	T	T
0.9900013605145787	0.8653494148948611	0.7838318023402353	T	T	T
0.1427914414045159	0.9274244846782036	0.2300361730174794	T	T	T
0.1812839082685713	0.9448033188907108	0.4161992193344392	T	T	T
0.2971518462532539	0.9572409682044154	0.5099441983244648	T	T	T
0.4086604858339891	0.9305337134181345	0.4075395478396441	T	T	T
0.3951259814502170	0.9402099271353892	0.2105669847415725	T	T	T
0.2704889993047223	0.9509906955294845	0.2713368085506852	T	T	T
0.1383723249920125	0.1725728657559695	0.2586955976939300	T	T	T
0.1949943109574000	0.1388572691130508	0.4287538918654425	T	T	T
0.3111144111817667	0.1438720038081487	0.5225190401223065	T	T	T
0.4139179331844683	0.1699175094581976	0.4036212464724796	T	T	T
0.3950281456162697	0.1577785805850879	0.2088266005020518	T	T	T
0.2692111204796431	0.1476543023216501	0.2657602766859875	T	T	T
0.1802704378478130	0.0482720533629722	0.2855782555206365	T	T	T
0.4169877406524719	0.0493910473852505	0.3210427991340795	T	T	T
0.0685512694445126	0.8702248778133431	0.0906898498666009	T	T	T
0.0881198832704117	0.0020132194214854	0.0835633807982772	T	T	T
0.1059801759521530	0.1341315015272708	0.0749097900380089	T	T	T
0.3035318002495151	0.8639424296324770	0.1292627724134843	T	T	T
0.3060278781345812	0.9947788903404656	0.0903989908832157	T	T	T
0.3017839383594069	0.1279859649777209	0.0736224742574832	T	T	T
0.5121595630183986	0.9574336006723193	0.2867207761553346	T	T	T
0.5154481318204438	0.1361933934680570	0.2868286012497693	T	T	T
0.6443076981631690	0.5506501433328760	0.2938450641104335	T	T	T

Structure files (CONTCAR) involved in this work:

0.6757947240468878	0.5661865831734947	0.1044350374912140	T	T	T
0.7886068080757817	0.5843781366112762	0.0073680780091121	T	T	T
0.9060087653779365	0.5746398206928371	0.0932423190261412	T	T	T
0.8918685420659741	0.5592446252130814	0.2920461282166318	T	T	T
0.7687785945078902	0.5327864424313346	0.2385009534753459	T	T	T
0.6453756600725963	0.3332359640669929	0.2859533628511222	T	T	T
0.7027753306334696	0.3220054004356915	0.1113014647923224	T	T	T
0.8053830894078562	0.3504278869329988	0.9890975561067760	T	T	T
0.9069952081796473	0.3282914083001758	0.1107186991371348	T	T	T
0.9009090775881226	0.3529002580272642	0.3047267376059771	T	T	T
0.7723486216997512	0.3672552615067732	0.2645248952834440	T	T	T
0.6776393484399387	0.4436925855798053	0.1842666804429781	T	T	T
0.9194432068941988	0.4539649687397169	0.1760180073437133	T	T	T
0.5654567277327671	0.6272056051998632	0.4039073000202779	T	T	T
0.5793441771258576	0.4985536708735741	0.4491613236241586	T	T	T
0.5844068460477576	0.3647967452823710	0.4555234770940201	T	T	T
0.7933594337219758	0.6296617399441684	0.3728361644515148	T	T	T
0.8095164513540766	0.5025328366355071	0.4235414542822540	T	T	T
0.8142643258232924	0.3707680241150806	0.4520814872546136	T	T	T
0.0096708975814778	0.5507709317827955	0.2116226466190740	T	T	T
0.0160196249652701	0.3656660500791563	0.2125348485271226	T	T	T
0.8690806948757858	0.4316956762052731	0.7457468819750400	T	T	T
0.7866426272781002	0.4479267335437321	0.6002787754089893	T	T	T
0.6959558961152740	0.4359461251168631	0.4575151024654077	T	T	T
0.6130849659771761	0.4357888436562163	0.6159756812706805	T	T	T
0.6083872424758608	0.4464308810135761	0.8127530609005407	T	T	T
0.7388918678252966	0.4314988511397407	0.7804715248073114	T	T	T
0.8764696601112936	0.6681245703351129	0.7266539151728747	T	T	T
0.8048217600772719	0.6484717500199313	0.5696557820246915	T	T	T
0.6844180795419166	0.6423030830700780	0.4881336293826914	T	T	T
0.5746953421688454	0.6651477192121878	0.5932255624501305	T	T	T
0.5962825665375374	0.6699382183623448	0.7881211517325567	T	T	T
0.7286019597376038	0.6699166058103492	0.7557610761348830	T	T	T
0.7991403009888449	0.5477499244995173	0.7307358200729017	T	T	T
0.5819048995548961	0.5521208947579818	0.6975218650935634	T	T	T
0.9292519096735063	0.3703475512876090	0.9221284207358452	T	T	T
0.8810480163292714	0.5045737889334846	0.9261893989953590	T	T	T
0.8923347369151384	0.6384843197480156	0.9219649098809437	T	T	T
0.6795229993986125	0.3685117854915571	0.9293928732036262	T	T	T
0.6968747116106226	0.5000753208890661	0.9376390426059720	T	T	T
0.6748888096252115	0.6315750308941657	0.9333508151807483	T	T	T
0.4961615949183354	0.4497066161261524	0.7137706259364667	T	T	T
0.4776837150358351	0.6350322684664473	0.7171280746768232	T	T	T
0.6426768275009285	0.9402967832328273	0.2815719616144496	T	T	T
0.6842434848619023	0.9643130251636334	0.0948346027849216	T	T	T
0.7959030614852568	0.9242656076830648	0.0050053771227631	T	T	T
0.9121218847269057	0.9321099850483334	0.0983379061952656	T	T	T
0.8952498080959889	0.9261129211318331	0.2965885782340536	T	T	T
0.7711456191941808	0.9537640380224965	0.2417694505857080	T	T	T
0.6375109659506762	0.1794197768235292	0.2477724764031006	T	T	T
0.6904854519344694	0.1429179440491321	0.0754848842268243	T	T	T
0.8073499348740194	0.1413222477009109	0.9832505033481793	T	T	T
0.9122528387242799	0.1581958877705587	0.1023123727527919	T	T	T

Structure files (CONTCAR) involved in this work:

0.8950185527705743	0.1583557352171812	0.2973582517224505	T	T	T
0.7701471998582824	0.1673850094526207	0.2277240876697498	T	T	T
0.6908205436684555	0.0597053945611020	0.2334656560719954	T	T	T
0.9173940549936676	0.0435286699746240	0.2055531631203478	T	T	T
0.5675124240018609	0.8727737386564405	0.4129695933560736	T	T	T
0.5838401065945391	0.0034021306244475	0.4366372394715866	T	T	T
0.6100188022493670	0.1339047443194591	0.4304186772627931	T	T	T
0.8001828449146912	0.8650290010105759	0.3857810182789986	T	T	T
0.8165027645158531	0.9980461508092999	0.4173829771604916	T	T	T
0.7921235360450634	0.1311880994660319	0.4159139004252728	T	T	T
0.0128950358325228	0.9491557684297827	0.2253054063327903	T	T	T
0.0149834567259604	0.1333989639890103	0.2217351111279049	T	T	T
0.8611140216648144	0.0719528961816783	0.7683934396553154	T	T	T
0.8186148656748041	0.0688805184224968	0.5834314642606834	T	T	T
0.7031467773803048	0.0459771378023735	0.4883804852850083	T	T	T
0.5972924082932423	0.0735747625937384	0.6035784919210759	T	T	T
0.6097233090951086	0.0464385679007491	0.7999335921195657	T	T	T
0.7317939740322440	0.0566923718210798	0.7289494938929684	T	T	T
0.8668931137115855	0.8309380176219060	0.7472920603238264	T	T	T
0.8014999631062989	0.8383599041713649	0.5812094733571559	T	T	T
0.6869567208469003	0.8530142083961492	0.4874612017760497	T	T	T
0.5823745679760410	0.8266488073612025	0.6018762210755177	T	T	T
0.5930240938529073	0.8485888128706979	0.7994644153370143	T	T	T
0.7222459581623039	0.8552596816168105	0.7636042179531700	T	T	T
0.8164987375417803	0.9566711656977466	0.6935939062858830	T	T	T
0.5805500369095659	0.9504509324192066	0.6689094902675370	T	T	T
0.9309061923291860	0.1237276436929660	0.9150862756117255	T	T	T
0.8955190558044690	0.9955442696769782	0.9254259582541761	T	T	T
0.9027641373046728	0.8617847634442328	0.9352763156698995	T	T	T
0.6928174547771807	0.1334398229521470	0.8793824583459258	T	T	T
0.7136073105861197	0.0048251724351718	0.9106157300042728	T	T	T
0.6757692129315293	0.8790714961825394	0.9479575023806482	T	T	T
0.4919207541456020	0.0459896413381336	0.7196484977607461	T	T	T
0.4793761451767928	0.8688961256371526	0.7082243093797160	T	T	T
0.3644697497381075	0.4374173839518098	0.7221342285046956	T	T	T
0.3043478296193491	0.4349186573004344	0.8967160020847486	T	T	T
0.2039281345859332	0.4440529702223831	0.0313644618447273	T	T	T
0.1082613295675901	0.4361388736663861	0.8960938121720016	T	T	T
0.1048523250413989	0.4415115682843429	0.6990594318949492	T	T	T
0.2332885027128008	0.4585346549732551	0.7366705240701262	T	T	T
0.3514669357476210	0.6725535637630752	0.7347931470737539	T	T	T
0.3102079898141302	0.6543592210496739	0.9187883408997637	T	T	T
0.1957692138988229	0.6453256795260696	0.0187068907558485	T	T	T
0.0980801339384629	0.6737286246090899	0.8917672966203984	T	T	T
0.1033533899727242	0.6656900210104743	0.6925558375426515	T	T	T
0.2246584983115300	0.6463769479020497	0.7684069809447033	T	T	T
0.3181287667071334	0.5508713657917695	0.7961296010744517	T	T	T
0.0999632246855741	0.5535984907776448	0.8037928196669305	T	T	T
0.4329329123696070	0.3739910300105169	0.5829819730037620	T	T	T
0.4234517103584367	0.5066696284762692	0.5730208981312638	T	T	T
0.3965356270955220	0.6370884257083853	0.5572306691709770	T	T	T
0.1926352606617409	0.3631455025713147	0.6111570183218195	T	T	T
0.1842131404621256	0.4920080644642690	0.5592299454884332	T	T	T

Structure files (CONTCAR) involved in this work:

0.2054632129356286	0.6241042536532853	0.5752805484723862	T	T	T
0.9953141529156819	0.4698308517075382	0.8008056070528888	T	T	T
0.9926440887167706	0.6309671825886928	0.7910545191925432	T	T	T
0.1405410962090538	0.5671815186713941	0.2207265827201808	T	T	T
0.1984048977362114	0.5650446612042672	0.3982394119384232	T	T	T
0.3030829990273521	0.5439800368910934	0.5185966709436969	T	T	T
0.4056334825853654	0.5657141398160058	0.3958537173646192	T	T	T
0.3988592324828656	0.5546661689451670	0.1988511079510228	T	T	T
0.2708477343469800	0.5393030474776954	0.2400127171417040	T	T	T
0.1417645323205468	0.3299004185990420	0.2401481523142429	T	T	T
0.1956607079559406	0.3476952074937588	0.4157536590523510	T	T	T
0.3094557673533153	0.3528241678464120	0.5178530884420752	T	T	T
0.4128957131707111	0.3267281590864825	0.3997622653760257	T	T	T
0.3977035062090511	0.3364269829053428	0.2040000149031465	T	T	T
0.2715609124520985	0.3573493659865109	0.2543442893707846	T	T	T
0.1796237610416371	0.4511359909963883	0.2952417523869107	T	T	T
0.4150144284483080	0.4462000835107000	0.3138569309361239	T	T	T
0.0710668401694322	0.6235663215455775	0.0737413102956380	T	T	T
0.0849291578740983	0.4918118785873912	0.0747195725121553	T	T	T
0.1006648147577327	0.3604986281485930	0.0570491465126124	T	T	T
0.3114299670245177	0.6336016842782803	0.1132936009010188	T	T	T
0.3187978586121606	0.5040586170452519	0.0616903042713539	T	T	T
0.3100932636054747	0.3685389525253495	0.0639857531294562	T	T	T
0.5132336678634143	0.5349659077679528	0.2856405527610006	T	T	T
0.5157529119102293	0.3603243899164296	0.2843281434715420	T	T	T
0.4353091883249344	0.7511165306173986	0.6376401614225402	T	T	T
0.1997937048949259	0.7491084827803326	0.6426609247381740	T	T	T
0.2753042985105942	0.7510799802941449	0.0427521327752163	T	T	T
0.1123664211945510	0.7482638977174608	0.0525450519968366	T	T	T
0.0603881673030901	0.2483429013965572	0.1443789214224988	T	T	T
0.3052769322443711	0.2488991056486081	0.1474191932396881	T	T	T
0.2276825956222653	0.2474419087659367	0.5347971890291766	T	T	T
0.3904839677093102	0.2497067737449387	0.5565906121176594	T	T	T
0.5603957921595450	0.2485251361192188	0.3708316822456603	T	T	T
0.8154312482845213	0.2555985371469438	0.3599787880331623	T	T	T
0.7256771559318446	0.2462372911374132	0.9563509128406257	T	T	T
0.8880631226696477	0.2466070575347043	0.9590984372266596	T	T	T
0.9446747990578551	0.7490699635715747	0.8541995484594638	T	T	T
0.6730521295633687	0.7572928470051640	0.8812387684854623	T	T	T
0.7621553177744620	0.7462765211825106	0.4449065468753601	T	T	T
0.6064713889438905	0.7488115231778494	0.4472264823402433	T	T	T
0.9197477843222295	0.3749587847677121	0.5989750283210907	T	T	T
0.0112992036702948	0.8207773445627801	0.5213866484581310	T	T	T
0.9677560490071609	0.6995985704251065	0.4425586279850984	T	T	T
0.9639888457926188	0.4201678041604158	0.5449731794677372	T	T	T
0.1047748624171734	0.6966351290109792	0.4446159419002713	T	T	T
0.9430115624774965	0.7951651235507394	0.4204212772450551	T	T	T
0.0336770928822466	0.7316251069800340	0.5554455436327671	T	T	T
0.9072275313179992	0.8080429527093205	0.5759648148092559	T	T	T
0.9163017253867415	0.6994389144478839	0.5800761070424926	T	T	T
0.8826637189637595	0.3628993338797648	0.5538621387645482	T	T	T
0.9414601707876737	0.4705175621362211	0.5384568993066765	T	T	T
0.9736638378867817	0.3997580777787166	0.4701498567935550	T	T	T

Structure files (CONTCAR) involved in this work:

0.0104292899090883	0.4231038977658170	0.5878890893342998	T	T	T
0.8921694600825765	0.4056285194055957	0.6829418404152507	T	T	T
0.0941532336080566	0.7202204604374202	0.3719245997507580	T	T	T
0.1055888970650161	0.6419613564522995	0.4331132030900851	T	T	T
0.1551386158606496	0.7133100555731662	0.4672196688201289	T	T	T
-0.0204154141375875	0.6651307415371117	0.3806154894003054	T	T	T

Figure S11(a)

Si Al O Zn H C

1.0000000000000000

20.0219999999999985 0.0000000000000000 0.0000000000000000

0.0000000000000000 19.8990000000000009 0.0000000000000000

0.0000000000000000 0.0000000000000000 13.3829999999999991

92 4 194 4 5 1

Selective dynamics

Direct

0.4231838210650298	0.0606477214309719	0.6495118426761683	T	T	T
0.3039853269931352	0.0331884009319595	0.7913382621185588	T	T	T
0.2835159238902571	0.0559364263231130	0.0175070470144385	T	T	T
0.1237200985552016	0.0646653651397147	0.0122609252932074	T	T	T
0.0689353696631324	0.0329623263050749	0.7984795042885564	T	T	T
0.1811472406321772	0.0695314179034853	0.6630769824197725	T	T	T
0.4147471513845578	0.8293953631125836	0.6692304469032192	T	T	T
0.2978430676733867	0.8742753111068803	0.8037161190331218	T	T	T
0.2682574286899668	0.8321972966274943	0.0189510416806378	T	T	T
0.1119468314354306	0.8286950138447960	0.0099508090593289	T	T	T
0.0623427192833771	0.8758879867786652	0.7970413894162763	T	T	T
0.0770705440913959	0.9428150313685165	0.1481041716337163	T	T	T
0.1962600913020758	0.9745321148636725	0.2865957317372937	T	T	T
0.2189969791176910	0.9496883839635922	0.5120398473096617	T	T	T
0.3780613777012410	0.9378846130083379	0.5121060861855949	T	T	T
0.4352444868880143	0.9688184438450760	0.3002877229277980	T	T	T
0.3212812017321446	0.9353252386291461	0.1646987803313020	T	T	T
0.0831295282550949	0.1765180475794114	0.1641585096567700	T	T	T
0.1997900739574304	0.1312040596912620	0.2962850016242231	T	T	T
0.2313332039412911	0.1697395360494861	0.5134213109986654	T	T	T
0.3871472746080930	0.1734520504425217	0.5079795932706201	T	T	T
0.4357752373291251	0.1265774563962709	0.2944897275962041	T	T	T
0.3212244828719958	0.1734889230380006	0.1645346060566746	T	T	T
0.5752727033750529	0.5560556479341043	0.3582404784526453	T	T	T
0.6875831304061930	0.5257787466299856	0.2041404858983864	T	T	T
0.7112909060748862	0.5682653465583379	0.9896412511009743	T	T	T
0.8708357692968847	0.5702036418175752	0.9811302653757066	T	T	T
0.8119598929304997	0.5504125713865118	0.3354498286286189	T	T	T
0.5727352124163948	0.3276889082948215	0.3308130215625833	T	T	T
0.6921102961201053	0.3726628160581363	0.1927080203012920	T	T	T
0.7314179767043396	0.3285230974073575	0.9776180215543022	T	T	T
0.8860226016886903	0.3263184006678193	0.9898238165689386	T	T	T
0.9397102285207449	0.3771643254585843	0.1896012721414196	T	T	T
0.9198161354521458	0.4432245466098897	0.8549475178116828	T	T	T
0.8013220916032222	0.4713963665262277	0.7184098021431116	T	T	T
0.7778697082409984	0.4357879216137152	0.4902855185042005	T	T	T
0.6191688535195896	0.4290063390039954	0.4879749466168406	T	T	T
0.5692956935553773	0.4692927048235346	0.6989211124854058	T	T	T

Structure files (CONTCAR) involved in this work:

0.6756790792272404	0.4486871058705152	0.8548458589952762	T	T	T
0.9178951654304678	0.6781019032183567	0.8258082546082013	T	T	T
0.7685376213288158	0.6674126339996586	0.4626404747913962	T	T	T
0.6125160856883185	0.6753397432460095	0.4876805444309852	T	T	T
0.5607281882836918	0.6280279558871324	0.6978188543154089	T	T	T
0.6733433506650199	0.6732230571374900	0.8283911264499031	T	T	T
0.5795404030872137	0.9470855632895094	0.3576844114593105	T	T	T
0.7003041382337680	0.9753613977957005	0.2134454561551301	T	T	T
0.7195577745483170	0.9348889616860088	0.9937376434686102	T	T	T
0.8797020537706794	0.9330604702132969	0.9992154761254423	T	T	T
0.9330870800715704	0.9752589690179223	0.2052594188275587	T	T	T
0.8237311920108233	0.9515754984722802	0.3543841753871365	T	T	T
0.5774511336880290	0.1727243820197991	0.3324653479112743	T	T	T
0.6985738831017646	0.1317226729451999	0.1953968077726005	T	T	T
0.7322351313420628	0.1730984717394139	0.9756476031692565	T	T	T
0.8869818143605297	0.1744658582019972	0.9866403862783090	T	T	T
0.9378463257126567	0.1319570441730276	0.1975619467066017	T	T	T
0.8211454471475241	0.1727075011726024	0.3309011268534407	T	T	T
0.9235917444283195	0.0544665183526348	0.8590973850892628	T	T	T
0.8025406121410891	0.0289929687749656	0.7121703247831144	T	T	T
0.7812215209665009	0.0698991707111191	0.4939604190766688	T	T	T
0.6204883190822358	0.0712553703630938	0.4933398069015267	T	T	T
0.5677206809326495	0.0322975726847302	0.7024668518695930	T	T	T
0.6787719090658747	0.0536562689123823	0.8530465566676221	T	T	T
0.9220774532326369	0.8314347384205412	0.8464919099493418	T	T	T
0.8018020541788413	0.8719997350000729	0.7043383092304123	T	T	T
0.6127228140476993	0.8287219830877532	0.4912841323307854	T	T	T
0.5589920196167945	0.8750088919957837	0.6979080703764611	T	T	T
0.6754475061904803	0.8330462924617562	0.8314457609106259	T	T	T
0.4230226980272157	0.4421361761118913	0.6431385511746295	T	T	T
0.3039168598142225	0.4683145928900605	0.7868782819170064	T	T	T
0.2807696613915613	0.4464266801434529	0.0123779204410254	T	T	T
0.1232085174048096	0.4390799346101607	0.0115747545765094	T	T	T
0.0644207207714426	0.4669463945734763	0.7992956699629270	T	T	T
0.1781740987364503	0.4305216373880956	0.6625366999959359	T	T	T
0.4149260430745514	0.6749368988863411	0.6655920672781951	T	T	T
0.2973637409394690	0.6275508810597371	0.7968399629800481	T	T	T
0.2667417893226438	0.6706490201510360	0.0161811824541911	T	T	T
0.1113428641193158	0.6738222577255565	0.0096165097303308	T	T	T
0.0613297613024371	0.6258236322852651	0.7970391735606692	T	T	T
0.1760332725731639	0.6696844473052203	0.6599447649432435	T	T	T
0.0728711835595573	0.5601634677495250	0.1477056694686986	T	T	T
0.1928232649839036	0.5302489431142909	0.2865044125808170	T	T	T
0.2140837623724175	0.5512984258029738	0.5149280998258210	T	T	T
0.3737374962785072	0.5664886384897675	0.5132226583799812	T	T	T
0.4291248299656541	0.5322006002793430	0.3025454661076071	T	T	T
0.3190983550481409	0.5658961542313509	0.1610160017698748	T	T	T
0.0848922623138532	0.3289981325534767	0.1618646821997457	T	T	T
0.1980924599661272	0.3727079271990731	0.2975396277421559	T	T	T
0.2301816886851468	0.3308908351597440	0.5143104361142793	T	T	T
0.3849057986483755	0.3276824962235431	0.5053412957438136	T	T	T
0.4303445568462733	0.3746300368008449	0.2926779541822007	T	T	T
0.3172344004050597	0.3298154863789799	0.1597857537802018	T	T	T

Structure files (CONTCAR) involved in this work:

0.9269814857468651	0.5314359011908115	0.1875148660991479	T	T	T
0.8214221227415256	0.3356121968277442	0.3238000155259274	T	T	T
0.7988271083908491	0.6301846672501210	0.6946408719302077	T	T	T
0.1809452621924061	0.8311797403776380	0.6614863975799109	T	T	T
0.7710733788861425	0.8298247339222410	0.4782449059708280	T	T	T
0.0040896524827087	0.5515192692086078	0.2109599694735698	T	T	T
0.3589610926068847	0.0706749115927053	0.7218732197076581	T	T	T
0.3161542116075952	0.0545320832583324	0.9067932519155336	T	T	T
0.2029038096358613	0.0484701780722329	0.0112052042916240	T	T	T
0.0958012018362363	0.0690981604136056	0.8990310888742731	T	T	T
0.1039490695733132	0.0669436678765679	0.7015352773856930	T	T	T
0.2294151935381431	0.0578999055240623	0.7595131293708557	T	T	T
0.3558345305079127	0.8288408045316734	0.7518399213106416	T	T	T
0.3055387067398254	0.8657763105847647	0.9241609938309050	T	T	T
0.1893029138524439	0.8523141656202888	0.0174557307578988	T	T	T
0.0853443448617566	0.8349989857039730	0.8957324105762967	T	T	T
0.0930459569338845	0.8382087045153293	0.6974290353688902	T	T	T
0.2254023612111246	0.8492679101620765	0.7681352427469966	T	T	T
0.3116315283252752	0.9527346605719904	0.7746711159741644	T	T	T
0.0876494341649234	0.9528965516584927	0.8014919597538415	T	T	T
0.4326155761456749	0.1279638308370107	0.5818829311051011	T	T	T
0.4151479610901285	0.9964124982869336	0.5759672317702129	T	T	T
0.3893800965795252	0.8661650269175860	0.5677166349481703	T	T	T
0.1948036779591202	0.1433306316637781	0.6143077547859346	T	T	T
0.1938135933343511	0.0123707298253038	0.5801485960177041	T	T	T
0.1974888222685224	0.8793079067789523	0.5588155632236548	T	T	T
0.9885959898430998	0.0417852784457844	0.7891166039229461	T	T	T
0.9809980410207675	0.8715838514016125	0.7870422503756194	T	T	T
0.1420654963879605	0.9339374946423216	0.2191864360300825	T	T	T
0.1836215224872020	0.9591834951001456	0.4031221116442298	T	T	T
0.2998038683464719	0.9557837116967925	0.5000407032318985	T	T	T
0.4123703829780336	0.9322640595250786	0.4029289631209297	T	T	T
0.3976608975203447	0.9340795673126829	0.2056089021317228	T	T	T
0.2715462990641526	0.9510808857698366	0.2579839943676489	T	T	T
0.1424465461955498	0.1780740433720814	0.2468257905699947	T	T	T
0.1954599346559617	0.1359359163258419	0.4169059284079205	T	T	T
0.3097664416349108	0.1484713562915820	0.5145888283064897	T	T	T
0.4137432641479057	0.1675489346336561	0.3941471462250657	T	T	T
0.3982003332898148	0.1600682755968209	0.1985004924749933	T	T	T
0.2730771365525789	0.1571234290154993	0.2600479770256860	T	T	T
0.1872201657415829	0.0542214166997748	0.2604720076446324	T	T	T
0.4146174659070612	0.0481135591499768	0.3050550478981153	T	T	T
0.0665538870083364	0.8741052739105497	0.0838497671589584	T	T	T
0.0848478236227445	0.0048475704577485	0.0703059763659506	T	T	T
0.1077030562547712	0.1361571507818899	0.0653543297061610	T	T	T
0.3031539697600872	0.8616951375065389	0.1191295730474975	T	T	T
0.3137367835244935	0.9934799818364320	0.0804551542702618	T	T	T
0.3022511490737415	0.1271419810122998	0.0693470057182717	T	T	T
0.5152898016406844	0.9600041780189961	0.2854963599867997	T	T	T
0.5161823634695325	0.1323490986340360	0.2789946662619118	T	T	T
0.6385662105133612	0.5618226877991102	0.2835925264904194	T	T	T
0.6920233425635323	0.5741403601346019	0.1069356123095399	T	T	T
0.7913534926499630	0.5558203694494682	0.9758516846096091	T	T	T

Structure files (CONTCAR) involved in this work:

0.8957399576284474	0.5766260952858010	0.0967514524033296	T	T	T
0.8873308406141936	0.5440416122212114	0.2927313411050064	T	T	T
0.7617928032193407	0.5208803368299934	0.2536795204285192	T	T	T
0.6374671822945817	0.3325705854176012	0.2597121929315667	T	T	T
0.6932420986944509	0.3369754206676133	0.0832405689189590	T	T	T
0.8090927628139136	0.3526731466756513	0.9874863571200911	T	T	T
0.9124793028238902	0.3258284576929445	0.1044542309762729	T	T	T
0.9044016066797476	0.3610389137482782	0.2955648715230820	T	T	T
0.7641063015584318	0.3721203692848389	0.2447203747950743	T	T	T
0.6644740246045796	0.4499909256917251	0.1774298272553184	T	T	T
0.9218114529661191	0.4534860589262329	0.1533610059338903	T	T	T
0.5670678456103249	0.6265155788467411	0.4179220620369898	T	T	T
0.5865834261327241	0.4958027141199128	0.4386294471808416	T	T	T
0.5871057075169032	0.3619358139001045	0.4397302655304010	T	T	T
0.7970563447977587	0.6280369956121794	0.3646012571225786	T	T	T
0.8044670323334688	0.5095662248566946	0.4442195919616658	T	T	T
0.8250145788453561	0.3780012986041049	0.4431880284948029	T	T	T
0.0200890686741750	0.3701894295880043	0.2014371140060579	T	T	T
0.8551967003431145	0.4294631998934346	0.7834731771454384	T	T	T
0.7921010259468084	0.4371029563230048	0.6092576229064339	T	T	T
0.6996161614127914	0.4281312081250232	0.4654044629100081	T	T	T
0.6056689866920293	0.4295357480887972	0.6071689973169057	T	T	T
0.6030337821775621	0.4444605446115730	0.8026031426169191	T	T	T
0.7298800612850203	0.4761829885595493	0.7729071131978916	T	T	T
0.8619322967320457	0.6854179030547728	0.7366188015967552	T	T	T
0.8120413308781642	0.6376792096846629	0.5610669778387203	T	T	T
0.6905008614579790	0.6497686032419318	0.4814280890766582	T	T	T
0.5877258115476017	0.6702944709313662	0.6024318067207814	T	T	T
0.5956114221267741	0.6579686159136168	0.7983703214369182	T	T	T
0.7216170381410533	0.6442930009975104	0.7415310134603283	T	T	T
0.8312727881983782	0.5472396761560071	0.6981073293632309	T	T	T
0.5803237944424487	0.5493715419171092	0.6824892232056294	T	T	T
0.9319115499423815	0.3773013506154688	0.9236507730494365	T	T	T
0.9098892282816637	0.5094719548911472	0.9246756940120517	T	T	T
0.8867355396000342	0.6405517173200964	0.9230099763560590	T	T	T
0.6959389899925479	0.3744784633644553	0.8926834810211118	T	T	T
0.6726894920873029	0.5028070361583385	0.9453160797698176	T	T	T
0.6891320418689350	0.6372338628494193	0.9353414801238455	T	T	T
0.4906662814827154	0.4512924456970469	0.7078827793575335	T	T	T
0.4801542206519589	0.6352242195436926	0.7079096849294468	T	T	T
0.6460954352024689	0.9429453932603433	0.2890612091620502	T	T	T
0.7011017226793602	0.9307557477664834	0.1113228051343335	T	T	T
0.8002343929009907	0.9387010749298915	0.9773549182890976	T	T	T
0.8963315074494324	0.9323163638761085	0.1171854898886780	T	T	T
0.8998422957255613	0.9598251445888980	0.3124818940433574	T	T	T
0.7737382004940212	0.9745708549664929	0.2638419172061296	T	T	T
0.6423344237864973	0.1706589334969111	0.2604846873281527	T	T	T
0.6977862220872545	0.1645445566756563	0.0843433145196113	T	T	T
0.8098930972704061	0.1483895439886835	0.9818174608924812	T	T	T
0.9132201925752463	0.1749396373219396	0.1009891477572572	T	T	T
0.8980384918790789	0.1556970607059368	0.2967647775639242	T	T	T
0.7716905535840846	0.1397671333043351	0.2462080114156328	T	T	T
0.6796712121813506	0.0524610668261654	0.1871588225743068	T	T	T

Structure files (CONTCAR) involved in this work:

0.9245991821601321	0.0533885339904285	0.1733508943652691	T	T	T
0.5695186533622850	0.8764383052647116	0.4163839240112567	T	T	T
0.5844734408735743	0.0077325522470246	0.4392355054010262	T	T	T
0.5951134865198654	0.1404492658303494	0.4408942659327297	T	T	T
0.8120657742798666	0.8760375123014511	0.3899917758559546	T	T	T
0.8152464359569102	1.0028542213344707	0.4484803263504255	T	T	T
0.8077539407402010	0.1372411246232105	0.4390047093375662	T	T	T
0.0113599580631402	0.9549451058445992	0.2160224418344910	T	T	T
0.0174899346920584	0.1431098957644649	0.2151126047777963	T	T	T
0.8583448023058703	0.0582349132923752	0.7880276867744777	T	T	T
0.8019417327691534	0.0741687533029642	0.6116377217870176	T	T	T
0.7006490817759576	0.0640345221499735	0.4816479517627247	T	T	T
0.6000238801556464	0.0749931586048311	0.6106236213858878	T	T	T
0.6038271449636976	0.0510468746317293	0.8075802991491631	T	T	T
0.7297252502302872	0.0317389993015322	0.7644343535914934	T	T	T
0.8543505798636691	0.8367132643685149	0.7807738189907134	T	T	T
0.8133280283324125	0.8303766711148625	0.5994072322087933	T	T	T
0.6892710370765959	0.8518190707496618	0.4974165154717947	T	T	T
0.5790627939548727	0.8295566625182307	0.6022272403977701	T	T	T
0.5994698366134312	0.8496316765976333	0.7968414003836060	T	T	T
0.7265383738220816	0.8622445030510332	0.7460620358689517	T	T	T
0.8190481230247696	0.9504215798236429	0.6861494467925174	T	T	T
0.5771742531288565	0.9531135074379655	0.6763413551032028	T	T	T
0.9326651515605279	0.1256075990385432	0.9175117339912968	T	T	T
0.9172111923734355	0.9942065782954048	0.9410469682451771	T	T	T
0.9088614192854568	0.8618245299893968	0.9565264743736526	T	T	T
0.6936317686666810	0.1294569140898009	0.8914244620427415	T	T	T
0.6858388288638280	0.0020622998632610	0.9465213265056804	T	T	T
0.6911704547628107	0.8679690701623110	0.9385645274840443	T	T	T
0.4893850080613756	0.0507499256754684	0.7176699937657318	T	T	T
0.4793405302788887	0.8668274253278335	0.7181291827204337	T	T	T
0.3601430227958923	0.4318487904905157	0.7185119928820817	T	T	T
0.3156774255388403	0.4481225729836377	0.9028737348166844	T	T	T
0.2010313902064521	0.4603633771258702	0.0010781339267224	T	T	T
0.0892768758146669	0.4326489384109223	0.9020911791934706	T	T	T
0.1019257586354539	0.4329491600297846	0.7045820949389144	T	T	T
0.2294055829010104	0.4437993015496933	0.7547657665274545	T	T	T
0.3564354786363698	0.6727001559764881	0.7496631899760765	T	T	T
0.2985205449121381	0.6375507804613706	0.9163132758545526	T	T	T
0.1882369766148962	0.6490300348376664	0.0203385904466140	T	T	T
0.0869330251834507	0.6662508471006643	0.8942230819082498	T	T	T
0.0968506439946418	0.6595968631705531	0.6978317852387231	T	T	T
0.2246888607389518	0.6510102543922568	0.7531310072821289	T	T	T
0.3097831900265881	0.5490486283492594	0.7691841033323806	T	T	T
0.0812361517813301	0.5472186698210684	0.8024313279725575	T	T	T
0.4321610450107533	0.3763988314839180	0.5723716280563926	T	T	T
0.4133774446897136	0.5080606643380656	0.5732181898786771	T	T	T
0.3867771984971620	0.6389775262749059	0.5647533696041820	T	T	T
0.1915872013811581	0.3571240133088694	0.6138653349089397	T	T	T
0.1857736006923647	0.4881748439025593	0.5779451325961987	T	T	T
0.1885254067643265	0.6207218993539618	0.5654334726554445	T	T	T
0.9846575769140380	0.4553969794117793	0.7836701549166787	T	T	T
0.9811576595055833	0.6350009110083262	0.7824028412020905	T	T	T

Structure files (CONTCAR) involved in this work:

0.1352751601162279	0.5693669789255034	0.2238288614557644	T	T	T
0.1826524928426619	0.5476689423925684	0.4036089393763380	T	T	T
0.2947174613987927	0.5485084778795433	0.5121308608477493	T	T	T
0.4017373121571054	0.5713299797672362	0.4003639065380933	T	T	T
0.3947248420536444	0.5651067533190709	0.2042830326443568	T	T	T
0.2668239959963863	0.5544031981287113	0.2528473653092415	T	T	T
0.1389154307317546	0.3266934936876024	0.2521084179824051	T	T	T
0.1965243939262620	0.3672895443569882	0.4179781311637673	T	T	T
0.3082128567504706	0.3534104987981479	0.5192335127714466	T	T	T
0.4058819499758278	0.3308202642653955	0.3883440546289871	T	T	T
0.3937478561667700	0.3475645324840017	0.1917554630574289	T	T	T
0.2700093774949332	0.3474070897671058	0.2558651158268702	T	T	T
0.1846002534608917	0.4502906991117791	0.2643868567402949	T	T	T
0.4103535402563996	0.4529024975149835	0.3117236010227224	T	T	T
0.0644522097837485	0.6275494723540862	0.0803124253349316	T	T	T
0.0830755536255099	0.4959558752630084	0.0744792620041308	T	T	T
0.1170344184254949	0.3664395957204482	0.0650999453566976	T	T	T
0.3053048097112489	0.6389659456642437	0.1115959833117038	T	T	T
0.3122934976438744	0.5060406966902304	0.0796037410349772	T	T	T
0.2945624084408798	0.3736563587618781	0.0630752550980571	T	T	T
0.5091891121824764	0.5416072488778310	0.2921451479869424	T	T	T
0.5104364856126864	0.3666621999984177	0.2777845136312620	T	T	T
0.4336269449368328	0.7521003402187394	0.6406265792860906	T	T	T
0.1781662771353333	0.7464799308208424	0.6238995346544559	T	T	T
0.2756485731056140	0.7510420428558457	0.0171228812810801	T	T	T
0.1035291030854666	0.7509966130628807	0.0444122538286460	T	T	T
0.0658112975234315	0.2530085214830505	0.1298951879841035	T	T	T
0.3112445984560336	0.2512176724327170	0.1301658416234203	T	T	T
0.2233832756928067	0.2505485858452342	0.5064609977899801	T	T	T
0.3928524516084411	0.2511556516000212	0.5443192129051811	T	T	T
0.5540675571799489	0.2498455252738154	0.3506914928694206	T	T	T
0.8102430496415930	0.2516249111869728	0.3408698131531541	T	T	T
0.7279491351847266	0.2511226741962326	0.9406651897022927	T	T	T
0.8921869182456509	0.2510617900810013	0.9439829226516743	T	T	T
0.9436421393235314	0.7526987652858217	0.8563877598605881	T	T	T
0.6857156706138123	0.7529581172924736	0.8441606000800712	T	T	T
0.7870969750639507	0.7448726349514360	0.4548507479610320	T	T	T
0.6059019680314498	0.7516968008824102	0.4485317059005314	T	T	T
0.9369600798946239	0.4925298684590089	0.5080493109820784	T	T	T
0.9670671505546743	0.7340677911585787	0.5685526595435093	T	T	T
0.9312327824119984	0.3898996610698079	0.4539643900906705	T	T	T
0.8750595614737431	0.5562393972024867	0.5531899804024007	T	T	T
0.8734202750598132	0.7500081475009107	0.5999197059773677	T	T	T
0.0533284425218044	0.7600662595522453	0.6238190041716897	T	T	T
0.9803019976541348	0.4937651671554154	0.5411710943214051	T	T	T
0.9722303588333099	0.7029906539502816	0.5117420390434975	T	T	T
0.0570664858791693	0.3824591883639774	0.4648707098014087	T	T	T
1.0213526247604028	0.3499302944988369	0.5771750173569750	T	T	T
1.0221697730429045	0.3000223352730980	0.4655769295354522	T	T	T
1.0166254754890385	0.3511145417964245	0.4954468506487578	T	T	T

Figure S11(b)

Si Al O Zn H C

1.00000000000000

Structure files (CONTCAR) involved in this work:

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20.0219999999999985 0.0000000000000000 0.0000000000000000
0.0000000000000000 19.8990000000000009 0.0000000000000000
0.0000000000000000 0.0000000000000000 13.3829999999999991
92 4 194 4 5 1
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Selective dynamics

Direct

0.4230478913395930	0.0606995066226580	0.6495574144719807	T	T	T
0.3028471376809496	0.0335325728038454	0.7903798477111619	T	T	T
0.2836674619047568	0.0555391849494489	0.0176304461180819	T	T	T
0.1236182428434898	0.0635260134847896	0.0118413659922997	T	T	T
0.0692813709786083	0.0310176327664656	0.7957845015612012	T	T	T
0.1808880744682046	0.0716575826354718	0.6623241264205242	T	T	T
0.4145466088094605	0.8295917867821724	0.6710494456684493	T	T	T
0.2948157056700850	0.8745711899886431	0.8011210995559104	T	T	T
0.2681793550812962	0.8323797813282560	0.0177152638751251	T	T	T
0.1117044647052147	0.8288126878064099	0.0109017003924977	T	T	T
0.0622902528170683	0.8741194231480210	0.7955625102442826	T	T	T
0.0770952726788001	0.9423574704918777	0.1493643271110928	T	T	T
0.1969483071153135	0.9738853190315999	0.2862762508388957	T	T	T
0.2176905425369641	0.9503725504183075	0.5131497814095439	T	T	T
0.3777221910223407	0.9374024060613108	0.5129875862481784	T	T	T
0.4353162002299107	0.9687290563736289	0.3008071196461664	T	T	T
0.3218806254367325	0.9345751779770126	0.1646289896920936	T	T	T
0.0830970193895040	0.1759604794487486	0.1621143539719823	T	T	T
0.2005762796700185	0.1304622977692454	0.2938599097401709	T	T	T
0.2308649320833629	0.1697907915268809	0.5108905366940414	T	T	T
0.3867320410584675	0.1734561233851205	0.5077374049174345	T	T	T
0.4359849447207698	0.1266681541656878	0.2943464740323611	T	T	T
0.3220223726211782	0.1735278332938777	0.1631172637827762	T	T	T
0.5750381574829799	0.5584683152713774	0.3583868981480244	T	T	T
0.6896530003281632	0.5269017575314807	0.2095447702385720	T	T	T
0.7129454146115762	0.5670661290334950	0.9917416253635051	T	T	T
0.8719877474008609	0.5706349036463524	0.9849013858518110	T	T	T
0.8139500077992160	0.5515807624907585	0.3452697724568982	T	T	T
0.5744585263331448	0.3280704165288169	0.3300035809523067	T	T	T
0.6916387443709142	0.3736721283065941	0.1895455953410376	T	T	T
0.7306370893236823	0.3291270489410078	0.9744335382504541	T	T	T
0.8858558440448534	0.3265386222443613	0.9880456599426518	T	T	T
0.9398198299167714	0.3767534846786824	0.1895284586443244	T	T	T
0.9205684586303740	0.4460028271729279	0.8551759461169046	T	T	T
0.8012143531386571	0.4740726185177070	0.7130686871843498	T	T	T
0.7793694375733048	0.4375274904970591	0.4918843214000554	T	T	T
0.6209783770336732	0.4314316951217878	0.4859733612692693	T	T	T
0.5705262483818856	0.4701693461318159	0.6969474747377766	T	T	T
0.6777408346404379	0.4500412684720603	0.8527732534026973	T	T	T
0.9177143633841952	0.6774218487440137	0.8301703709000224	T	T	T
0.7645796438944439	0.6743329560943597	0.4609922848067622	T	T	T
0.6127402291486024	0.6757840027126766	0.4894688970127141	T	T	T
0.5602441370124340	0.6285255898984934	0.6986309510102333	T	T	T
0.6732756174066811	0.6709349128110974	0.8308374335983225	T	T	T
0.5799530838866166	0.9463885827743304	0.3585413940539398	T	T	T
0.7007467125568180	0.9740372868654302	0.2139160526411734	T	T	T
0.7197605174278354	0.9337793520352879	0.9942568395780845	T	T	T

Structure files (CONTCAR) involved in this work:

0.8797702503345493	0.9327768595280862	1.0001321193917669	T	T	T
0.9332909751527554	0.9752075036042208	0.2055564300788024	T	T	T
0.8246254543956624	0.9533457787084885	0.3561101717566099	T	T	T
0.5777410014964836	0.1727606798087018	0.3336503892815966	T	T	T
0.6988726240587800	0.1303371430401295	0.1966758443332741	T	T	T
0.7318160056192202	0.1728453222347233	0.9765441228078462	T	T	T
0.8871997345130089	0.1742103694074758	0.9847909136316340	T	T	T
0.9379327178953735	0.1318088244486575	0.1966700092022125	T	T	T
0.8211868126641959	0.1726051242250023	0.3315705438153003	T	T	T
0.9235068133581789	0.0522212001194135	0.8582574465058316	T	T	T
0.8014737424837253	0.0248633143782322	0.7106395428550067	T	T	T
0.7814441446485647	0.0720606582459158	0.4949519203039183	T	T	T
0.6207788722112644	0.0712958852632357	0.4937700698056393	T	T	T
0.5678683234987911	0.0319397587309673	0.7032226863033282	T	T	T
0.6788312365567736	0.0521074006445236	0.8542740125122352	T	T	T
0.9213911852406607	0.8310604827122792	0.8460103285257760	T	T	T
0.8009583249210769	0.8676392427056943	0.6998500257186920	T	T	T
0.6133242629709716	0.8300898974703337	0.4944173195279771	T	T	T
0.5583820429539064	0.8744478831502798	0.7003275152739110	T	T	T
0.6757421324469505	0.8309175649002525	0.8318085788764991	T	T	T
0.4234293754934574	0.4425901549431365	0.6425590010479227	T	T	T
0.3037502368719455	0.4677342447770479	0.7862868952177480	T	T	T
0.2810858129362175	0.4467142218655947	0.0124903894036977	T	T	T
0.1231604701585499	0.4401113615215655	0.0111300513300771	T	T	T
0.0656869270049768	0.4688395626519403	0.7966015499206923	T	T	T
0.1787723534598272	0.4285763581087300	0.6614390199472964	T	T	T
0.4147184059142333	0.6748928437520217	0.6665366414526109	T	T	T
0.2949826874643076	0.6269030076691999	0.7949472710817086	T	T	T
0.2667461113371302	0.6708628071991399	0.0151844179953114	T	T	T
0.1112673263384369	0.6735635427926383	0.0109544031224939	T	T	T
0.0616622547061624	0.6271944896270780	0.7962656641679384	T	T	T
0.1747712969937391	0.6707990432838690	0.6579823341592581	T	T	T
0.0725337050756568	0.5603124476264757	0.1487442476445619	T	T	T
0.1933532514924628	0.5307149209963330	0.2859472428710128	T	T	T
0.2131117464339969	0.5509693563142987	0.5154289418516639	T	T	T
0.3734459026120248	0.5676149355484086	0.5131442929280485	T	T	T
0.4292915920946320	0.5328740070291753	0.3021503693313445	T	T	T
0.3194206557599304	0.5667178824592102	0.1603815609984605	T	T	T
0.0849591698758118	0.3289625482582403	0.1603271074161120	T	T	T
0.1989121026673491	0.3731096952818094	0.2957808130703185	T	T	T
0.2299302582482014	0.3305422921264685	0.5120448038217884	T	T	T
0.3846289333132843	0.3278861279124867	0.5047410340859839	T	T	T
0.4311523158195186	0.3749471256444700	0.2924660834745047	T	T	T
0.3182829494137006	0.3298550159103741	0.1589818356523385	T	T	T
0.9265426559254774	0.5315552110104499	0.1920141833162674	T	T	T
0.8192581224742980	0.3353255573490472	0.3211775939516790	T	T	T
0.7973583748117513	0.6325613372280237	0.6899301448687950	T	T	T
0.1792053016000125	0.8285379567308992	0.6581699916989635	T	T	T
0.7680883293353193	0.8306980312899114	0.4764055350013646	T	T	T
0.0041902456667896	0.5509651765956680	0.2125922138784504	T	T	T
0.3591736935874396	0.0703431187350651	0.7226497673639904	T	T	T
0.3156330087114945	0.0525796865640039	0.9065834551000295	T	T	T
0.2029924933322054	0.0488582515753617	0.0120351400045436	T	T	T

Structure files (CONTCAR) involved in this work:

0.0963737969065403	0.0645107028420638	0.8981192045238917	T	T	T
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0.2293510356266825	0.0616999283479070	0.7590230857805809	T	T	T
0.3538011769312922	0.8297255895798066	0.7507566521235338	T	T	T
0.3026642019425218	0.8673574610604302	0.9218094752296869	T	T	T
0.1890456364214556	0.8518567875296359	0.0203230988684059	T	T	T
0.0861668182081237	0.8366742557615522	0.8962836843898884	T	T	T
0.0902762151854666	0.8299345050196671	0.6983587803438793	T	T	T
0.2226479506167570	0.8484160256218883	0.7656107981114755	T	T	T
0.3073661953925132	0.9531446326091070	0.7709505376311674	T	T	T
0.0885225601234028	0.9507456713608424	0.7909557897432266	T	T	T
0.4319650198854297	0.1282079991930902	0.5821082655292052	T	T	T
0.4144161292402643	0.9967346764927489	0.5757416121177207	T	T	T
0.3912735053645933	0.8660269517958127	0.5681681391984104	T	T	T
0.1931621445095475	0.1453216832038668	0.6119522263974694	T	T	T
0.1947404917688836	0.0145139198771010	0.5800368644208136	T	T	T
0.1913407724358885	0.8815690884142435	0.5596927142867673	T	T	T
0.9888721716704205	0.0393966973875786	0.7889221458607660	T	T	T
0.9809261018305880	0.8710437607973280	0.7871242884503945	T	T	T
0.1420613747710169	0.9331841677231760	0.2203383829010582	T	T	T
0.1841861044532703	0.9610321990327995	0.4032599040642690	T	T	T
0.2987901883141682	0.9529713958206306	0.5033788724080930	T	T	T
0.4109686646463129	0.9326582748029022	0.4030006450402308	T	T	T
0.3981566780823486	0.9339219750973247	0.2057061577746625	T	T	T
0.2716732037302134	0.9485324021812384	0.2580475905853330	T	T	T
0.1430561653893424	0.1768879112894615	0.2437252327967699	T	T	T
0.1956760402531464	0.1350599519338690	0.4144625903484833	T	T	T
0.3092598788724613	0.1485508623265457	0.5143752452222423	T	T	T
0.4132988725056495	0.1674070713896341	0.3939195810091060	T	T	T
0.3987623655211511	0.1600183065654843	0.1979070908389494	T	T	T
0.2736079752597940	0.1574181917999806	0.2584340124792797	T	T	T
0.1891567414611721	0.0533900614235267	0.2577419436635411	T	T	T
0.4150893884968796	0.0481774929317188	0.3047017526247492	T	T	T
0.0659990556628501	0.8739692951720249	0.0845860276313882	T	T	T
0.0852790762233030	0.0044720101645849	0.0719124766472603	T	T	T
0.1060214310772987	0.1357155300563996	0.0621490731485412	T	T	T
0.3048642185393758	0.8613014348885453	0.1168497412833350	T	T	T
0.3136095458157574	0.9936352300290771	0.0819139089616534	T	T	T
0.3031259764298102	0.1271668259118418	0.0678517300304080	T	T	T
0.5153598008238953	0.9597234325565062	0.2871192152936266	T	T	T
0.5162802490911731	0.1333077342918039	0.2791931880820152	T	T	T
0.6381267819353023	0.5647738881313005	0.2834208393097037	T	T	T
0.6973621885307819	0.5728267227567585	0.1101781809621481	T	T	T
0.7929561459172704	0.5558344035414956	0.9740173734578089	T	T	T
0.8942645882863062	0.5760185237754845	0.1016895382351283	T	T	T
0.8883965912572718	0.5438431119302429	0.2980773416472302	T	T	T
0.7617212101312131	0.5213330896414156	0.2658708853874224	T	T	T
0.6379938585379964	0.3317530733720495	0.2560153666549219	T	T	T
0.6905317566314538	0.3414407276647078	0.0776726458793939	T	T	T
0.8086793680717127	0.3516109490700923	0.9869361408577275	T	T	T
0.9126778868408945	0.3268206625850886	0.1028636935017422	T	T	T
0.9044934393537911	0.3586649869401113	0.2960399369907288	T	T	T
0.7649427252563444	0.3709420078482927	0.2376714209375458	T	T	T

Structure files (CONTCAR) involved in this work:

0.6650416969502847	0.4515939037734791	0.1822897510805049	T	T	T
0.9212578393908719	0.4534367660898614	0.1577414809703897	T	T	T
0.5657629371864450	0.6284938623606694	0.4189590111121893	T	T	T
0.5859718730433160	0.4972842823526105	0.4376036820882988	T	T	T
0.5909966261692330	0.3633321685210129	0.4374207478976984	T	T	T
0.7999583354568277	0.6287347624958736	0.3743323825181351	T	T	T
0.8110881914940336	0.5102840072080718	0.4533076758032103	T	T	T
0.8234444784258778	0.3782178618971541	0.4400171872771089	T	T	T
0.0200183550053124	0.3691356626509242	0.2026012121328328	T	T	T
0.8565548742299302	0.4367699593462980	0.7818117442011102	T	T	T
0.7906685955156294	0.4311314093298477	0.6112379070505254	T	T	T
0.7013054344740272	0.4336035982999082	0.4625386125208742	T	T	T
0.6075209800952630	0.4307580820670929	0.6053313628007885	T	T	T
0.6047444796157252	0.4465695021625653	0.8010628823002905	T	T	T
0.7313019564486674	0.4806033019031302	0.7720440265125761	T	T	T
0.8605864305482196	0.6827813975302010	0.7442948344385736	T	T	T
0.8070497887942505	0.6656002875264414	0.5673498728334130	T	T	T
0.6892370321521283	0.6462177890120170	0.4829623792682519	T	T	T
0.5864186123843536	0.6718604188375542	0.6038426185113153	T	T	T
0.5953930188558471	0.6565800877528239	0.8001177485820404	T	T	T
0.7216551652260460	0.6404266643936097	0.7458315443160095	T	T	T
0.8288233139799855	0.5489156779547717	0.6790652948606855	T	T	T
0.5800152033386133	0.5502534285151236	0.6798419641588214	T	T	T
0.9304784195379046	0.3780725932385217	0.9206378694096889	T	T	T
0.9128516213924178	0.5107488492311949	0.9285866406409965	T	T	T
0.8895740516146597	0.6417726863229161	0.9306824789193665	T	T	T
0.6986651799435053	0.3746497776214930	0.8857079967350998	T	T	T
0.6749977251922613	0.5008968676726950	0.9477052509258002	T	T	T
0.6880819638513805	0.6356334686520982	0.9388690697478437	T	T	T
0.4919578616563085	0.4512871676608015	0.7053886800782170	T	T	T
0.4795684317358540	0.6353700326576037	0.7106695477085677	T	T	T
0.6461255633303623	0.9419311827628037	0.2891322363442461	T	T	T
0.7017170881066177	0.9291618224504536	0.1119760516577188	T	T	T
0.8004487971384191	0.9394083802884259	0.9780340325938683	T	T	T
0.8966920438952591	0.9315803838250213	0.1180265511189180	T	T	T
0.9004382824818495	0.9610163540115378	0.3130747251949940	T	T	T
0.7740251603480283	0.9734760075064626	0.2647020169794085	T	T	T
0.6429167159368898	0.1691799224712069	0.2623894835902851	T	T	T
0.6984503875642277	0.1641023248678994	0.0860791410454158	T	T	T
0.8098319551316426	0.1493241322002025	0.9819209593724458	T	T	T
0.9143348742704438	0.1741588432245544	0.0988205680157208	T	T	T
0.8979824859325904	0.1561932427170921	0.2956490913832706	T	T	T
0.7717690194805797	0.1377520337170169	0.2487266871315012	T	T	T
0.6801370266497389	0.0511617275477282	0.1868617405063442	T	T	T
0.9248603175512644	0.0532588215883597	0.1727223006115418	T	T	T
0.5694317704989618	0.8759647793051117	0.4174298939391137	T	T	T
0.5858547331806981	0.0072943237187608	0.4395876766654829	T	T	T
0.5935945062576417	0.1402418040500966	0.4425119909575103	T	T	T
0.8139549542615959	0.8794414704361748	0.3972665174812500	T	T	T
0.8168208165264725	0.0070559962271078	0.4468341909514000	T	T	T
0.8089659009527691	0.1400711943081966	0.4421661473085586	T	T	T
0.0115000136268966	0.9550145527494487	0.2169386576493837	T	T	T
0.0175468237791308	0.1434929631921241	0.2147944405856673	T	T	T

Structure files (CONTCAR) involved in this work:

0.8586839244137188	0.0514315300650546	0.7864363201039190	T	T	T
0.8006838160906590	0.0734073158833610	0.6133969186565280	T	T	T
0.7010420258341086	0.0665876733755423	0.4804745397249403	T	T	T
0.6010677743896186	0.0739351566670522	0.6113795775386872	T	T	T
0.6039348967612538	0.0509501499074798	0.8082764050674718	T	T	T
0.7298112089630818	0.0284111320075840	0.7664798664973944	T	T	T
0.8548277269134288	0.8360563951077520	0.7781372664447093	T	T	T
0.8120266611169775	0.8224200244897036	0.5974515960547185	T	T	T
0.6883310588617836	0.8580046397927618	0.5042410075192356	T	T	T
0.5770449208347661	0.8294694894432031	0.6036299278705315	T	T	T
0.5997180711258402	0.8486377805728980	0.7982483426045853	T	T	T
0.7265567522220281	0.8582681784236416	0.7448986354041979	T	T	T
0.8158662019458387	0.9465935175417733	0.6784902490965998	T	T	T
0.5766069988653824	0.9525612970780778	0.6786927872119288	T	T	T
0.9308953206700609	0.1249290659854225	0.9132433393480134	T	T	T
0.9184687241454633	0.9938567015674878	0.9433577951750598	T	T	T
0.9078602638170095	0.8614884989441163	0.9558464163036874	T	T	T
0.6942632790993031	0.1279174747628194	0.8926902351181750	T	T	T
0.6846313939692228	0.0006157221537998	0.9480949958279150	T	T	T
0.6927804295977280	0.8667125315674888	0.9380078580826838	T	T	T
0.4895874598652071	0.0511083036543978	0.7170388103025733	T	T	T
0.4787094610164090	0.8666262949296778	0.7220903056094184	T	T	T
0.3612883123822993	0.4322254978664757	0.7193651540717310	T	T	T
0.3154703263016774	0.4489017002115527	0.9027243266701437	T	T	T
0.2012178853088089	0.4601684164923658	0.0022139839423292	T	T	T
0.0905763858499965	0.4363315312675149	0.9004701955377575	T	T	T
0.1021040700832676	0.4322667095022912	0.7027121416087064	T	T	T
0.2299275125925525	0.4406316231540131	0.7540353064617639	T	T	T
0.3541808360987523	0.6717337803219441	0.7475216252179256	T	T	T
0.2962631698404163	0.6367423831837613	0.9145656684810408	T	T	T
0.1882265241258244	0.6496973710888531	0.0238299550221036	T	T	T
0.0885091935269817	0.6643900352650457	0.8951558798711455	T	T	T
0.0945708975872491	0.6677264980686332	0.6992050672868014	T	T	T
0.2218118766355583	0.6497834609913763	0.7522444803845072	T	T	T
0.3072149676136932	0.5483760968430171	0.7671911332319237	T	T	T
0.0836132945997690	0.5490455483956268	0.7926297553978054	T	T	T
0.4316879788640530	0.3766777172435893	0.5717792647537457	T	T	T
0.4121517426446821	0.5083445447563020	0.5728767738880808	T	T	T
0.3889002683267470	0.6398482937784776	0.5636927621161180	T	T	T
0.1903301092594754	0.3549511708393677	0.6120050363716183	T	T	T
0.1882028061917575	0.4853587899153749	0.5762338529023191	T	T	T
0.1819470345396032	0.6174315477061257	0.5676084242501127	T	T	T
0.9856559518909180	0.4578486540523642	0.7838551857667555	T	T	T
0.9812054279782855	0.6344157804612162	0.7863873055327230	T	T	T
0.1351795376448692	0.5695202283895278	0.2242130432269033	T	T	T
0.1829820331220720	0.5465482402205308	0.4033721091381473	T	T	T
0.2937190518576677	0.5528104903370571	0.5141439387450736	T	T	T
0.4003409051984619	0.5711469579532598	0.3996751876497812	T	T	T
0.3948758170066147	0.5654890404237850	0.2036793658497643	T	T	T
0.2667690709488230	0.5563128240285572	0.2521071416236244	T	T	T
0.1394679873195163	0.3274851957541171	0.2498841968009380	T	T	T
0.1961967828282113	0.3678733831040021	0.4163668993681232	T	T	T
0.3077277288838872	0.3534166951693092	0.5188160742226723	T	T	T

Structure files (CONTCAR) involved in this work:

0.4056515236868249	0.3312810451925155	0.3878038835570792	T	T	T
0.3945975074709890	0.3479091348188263	0.1913591716176818	T	T	T
0.2706500422315043	0.3469092129336339	0.2550303711419287	T	T	T
0.1861712076062891	0.4507201007886931	0.2623066918826190	T	T	T
0.4114645795713440	0.4532905351977624	0.3108315768600815	T	T	T
0.0638078395326843	0.6275844814688344	0.0811962282343569	T	T	T
0.0829389349026040	0.4962834903734009	0.0750848541430463	T	T	T
0.1150495402398119	0.3668719926680947	0.0625345150764538	T	T	T
0.3066697486879659	0.6395677888937411	0.1095711803166766	T	T	T
0.3122326166215134	0.5063119603467077	0.0799017544570556	T	T	T
0.2953816056798733	0.3738261708723573	0.0625084263716914	T	T	T
0.5090622123665552	0.5437286156475950	0.2920107616242338	T	T	T
0.5112310117593070	0.3665138022672350	0.2784988743570462	T	T	T
0.4333617871037121	0.7522553597344487	0.6436255885121357	T	T	T
0.1840993867996240	0.7454787462797448	0.6182926306213148	T	T	T
0.2761095627025776	0.7512555327047238	0.0139131315721495	T	T	T
0.1021758433379413	0.7509705206762985	0.0434846659767522	T	T	T
0.0664505916217108	0.2528330407717418	0.1287009822893557	T	T	T
0.3123892783352141	0.2513118438566905	0.1287982965977918	T	T	T
0.2230009879967444	0.2504456943075835	0.5008457353243894	T	T	T
0.3924489753773174	0.2512962818864042	0.5435633535976860	T	T	T
0.5560015333846253	0.2503690365016022	0.3517770048985662	T	T	T
0.8090982346644949	0.2515375039762069	0.3389285143268707	T	T	T
0.7260663919840413	0.2508722989183138	0.9414265632717482	T	T	T
0.8932475688791296	0.2511148137792081	0.9430630772474530	T	T	T
0.9445307781516331	0.7527254965164695	0.8561729160208961	T	T	T
0.6854366097131985	0.7508898284460419	0.8458608645666499	T	T	T
0.7698386354523771	0.7503588001479831	0.4279376265211803	T	T	T
0.6098194818310225	0.7528223059465557	0.4519178152279769	T	T	T
0.9420711842824515	0.4739706795801577	0.5190879090164109	T	T	T
0.9639347549769633	0.7290397516115614	0.5762513500427134	T	T	T
0.9274156567444950	0.3862734121681886	0.4462554014388959	T	T	T
0.9027649672876055	0.5574194527453854	0.5643141789416818	T	T	T
0.8738560138851039	0.7431152223276484	0.6043332662854738	T	T	T
0.0364619926362224	0.7574674030046999	0.6451874190673524	T	T	T
0.9877124035181132	0.4707249287912466	0.5442123059317739	T	T	T
0.9425518571051178	0.6271730872958826	0.5610660132020553	T	T	T
0.0536035278061373	0.3737287886826403	0.4562405016359924	T	T	T
0.0160660713559711	0.3432755167796484	0.5711502633154011	T	T	T
0.0136272855058397	0.2919430396092320	0.4582889387602254	T	T	T
0.0137554065399465	0.3429644701507766	0.4892844795110726	T	T	T

Figure S11(c)

Si Al O Zn H C

1.0000000000000000

20.0219999999999985 0.0000000000000000 0.0000000000000000

0.0000000000000000 19.8990000000000009 0.0000000000000000

0.0000000000000000 0.0000000000000000 13.3829999999999991

92 4 194 4 5 1

Selective dynamics

Direct

0.4222757230660297 0.0608810927790594 0.6490161140636577 T T T

0.3036494706797880 0.0337119849426710 0.7919173470167010 T T T

0.2831238908022459 0.0561307424073906 0.0178281981953883 T T T

Structure files (CONTCAR) involved in this work:

0.1233808373826584	0.0632284689254410	0.0120145713813207	T	T	T
0.0687480105072962	0.0318110097764809	0.7964532736595711	T	T	T
0.1812112996422737	0.0698641912888415	0.6628757911900737	T	T	T
0.4146678559492542	0.8292516114503795	0.6697090393382796	T	T	T
0.2968157586001396	0.8746558253118059	0.8034563076883414	T	T	T
0.2682476730294914	0.8315944963120762	0.0193439850848068	T	T	T
0.1120681776513772	0.8280631780767304	0.0109169566768144	T	T	T
0.0625322723940161	0.8745036270801092	0.7967183468060267	T	T	T
0.0771218615998308	0.9418468338404440	0.1489964394173545	T	T	T
0.1963773474334412	0.9742665044240072	0.2866355384998247	T	T	T
0.2173751226253944	0.9491594413685491	0.5126970147418514	T	T	T
0.3773525214753879	0.9374869602677457	0.5119878677066310	T	T	T
0.4349616911256587	0.9686220783088297	0.3001000508028163	T	T	T
0.3213427602477943	0.9354647689160261	0.1642417488159598	T	T	T
0.0834664004398352	0.1756562394314551	0.1627514906081649	T	T	T
0.1996236735553600	0.1308676753477133	0.2966221742839287	T	T	T
0.2314926820987295	0.1695893516405741	0.5132244206713082	T	T	T
0.3869902641541699	0.1734507452655125	0.5074114454730820	T	T	T
0.4361043511496822	0.1264586373837731	0.2942449630817325	T	T	T
0.3208364744245957	0.1732783185919796	0.1656872507261217	T	T	T
0.5768952746781554	0.5542771030255473	0.3585870979111920	T	T	T
0.6888624970773897	0.5258849226922941	0.2002740934202462	T	T	T
0.7117103545054286	0.5696026352975891	0.9882223876697971	T	T	T
0.8715920845791693	0.5708802241423101	0.9839775528834656	T	T	T
0.8113880057232608	0.5506514626347114	0.3351243484087123	T	T	T
0.5728866514752831	0.3279381274499524	0.3309587077867457	T	T	T
0.6939689534777687	0.3718851746857052	0.1925068632130827	T	T	T
0.7308968093198304	0.3275875216956589	0.9790503769964010	T	T	T
0.8853902267546970	0.3265328252866800	0.9943735029599018	T	T	T
0.9409063269629159	0.3779706127516058	0.1917433628675878	T	T	T
0.9198632971115146	0.4429435341015218	0.8585739445198516	T	T	T
0.8025254985160799	0.4701674914820035	0.7203185515953864	T	T	T
0.7751917867503618	0.4359702608987077	0.4911320414953764	T	T	T
0.6162304006408681	0.4269593439765491	0.4911606787399302	T	T	T
0.5668493278260697	0.4688167699993545	0.7020520275574943	T	T	T
0.6756976925320783	0.4484920385063322	0.8551162818183508	T	T	T
0.9180326877335384	0.6774755279315268	0.8273030664468164	T	T	T
0.7756797463278468	0.6661941819678489	0.4673077667982191	T	T	T
0.6157463308891051	0.6756230062177278	0.4879222165957411	T	T	T
0.5613294170621608	0.6278299330592557	0.6974862100636003	T	T	T
0.6751581420542528	0.6729152261900271	0.8244792579633118	T	T	T
0.5795796290805290	0.9469343421778778	0.3568665479694280	T	T	T
0.7000554543707338	0.9750879634343567	0.2117704470157594	T	T	T
0.7197667268173107	0.9347412821324145	0.9920196495281116	T	T	T
0.8800204711305438	0.9332471821493618	0.9986459095746826	T	T	T
0.9334082458845218	0.9737509035915667	0.2052865831927810	T	T	T
0.8229100241177986	0.9498981664357413	0.3524479581498975	T	T	T
0.5779456401955312	0.1726555242763284	0.3304705055864778	T	T	T
0.6991830495212054	0.1320397449019476	0.1938656724980104	T	T	T
0.7326949819227446	0.1727059397166243	0.9738627910112684	T	T	T
0.8874171491476144	0.1742671048379026	0.9874230397696275	T	T	T
0.9385079009728704	0.1301442579791028	0.1975474970591606	T	T	T
0.8224016158669842	0.1717267064889808	0.3303892775242590	T	T	T

Structure files (CONTCAR) involved in this work:

0.9238622967057999	0.0551947388573582	0.8591993252768136	T	T	T
0.8034412066537914	0.0300528573527582	0.7127984303645762	T	T	T
0.7809922312279084	0.0681748663770020	0.4932646892742910	T	T	T
0.6201821396896975	0.0712296512284265	0.4923219536008887	T	T	T
0.5669626232031194	0.0320690082825245	0.7012041945960384	T	T	T
0.6786202525482598	0.0534885301594043	0.8512362117761143	T	T	T
0.9220322514954643	0.8302385391618509	0.8461226739259787	T	T	T
0.8037593019231087	0.8731093611062313	0.7040272924184882	T	T	T
0.6120737775836284	0.8270236350135268	0.4906616815053371	T	T	T
0.5590823907649838	0.8746882933727126	0.6978031942456193	T	T	T
0.6772359938579207	0.8329535936669912	0.8282265073835330	T	T	T
0.4216475666069114	0.4416297444560007	0.6457044997557647	T	T	T
0.3026651226246574	0.4676151761832640	0.7881220618585710	T	T	T
0.2807663307638979	0.4462026204627902	0.0141949081951526	T	T	T
0.1228894259920541	0.4401837284086942	0.0128077761939888	T	T	T
0.0645222919472222	0.4677794894464020	0.7978823768420187	T	T	T
0.1774331394514730	0.4296729621905829	0.6630061680744535	T	T	T
0.4146161502083915	0.6746939647090301	0.6660717250499997	T	T	T
0.2969378144538901	0.6267737727870776	0.7979291933813421	T	T	T
0.2669044745632296	0.6700630220111312	0.0173618958846972	T	T	T
0.1114224226364986	0.6726695567281453	0.0098318106274934	T	T	T
0.0617333221984794	0.6266791008586740	0.7945254600388283	T	T	T
0.1766303228938589	0.6704393490711035	0.6608472659348423	T	T	T
0.0728983189894396	0.5604387435279765	0.1499468930045188	T	T	T
0.1931203245515322	0.5298706189372361	0.2874441986992572	T	T	T
0.2132116621494932	0.5507093917400953	0.5165762938246266	T	T	T
0.3730891201961489	0.5657863318930156	0.5149091346620037	T	T	T
0.4296583691296467	0.5325428540457169	0.3037491544054849	T	T	T
0.3199002215751045	0.5652661184299416	0.1614794203258909	T	T	T
0.0854848510516421	0.3281713897013911	0.1610141790486023	T	T	T
0.1979780658369391	0.3723491368546245	0.2987775334340253	T	T	T
0.2304659414153548	0.3307288016226781	0.5147764898355471	T	T	T
0.3851496689576797	0.3280477475034015	0.5055074234093690	T	T	T
0.4314746726692156	0.3747968594744574	0.2925920437381185	T	T	T
0.3171448945649834	0.3298219918771610	0.1621213527748263	T	T	T
0.9275414548941193	0.5317160222114330	0.1902164247861135	T	T	T
0.8221694987635335	0.3355150384419464	0.3262378014910130	T	T	T
0.8015751646872513	0.6292142845155066	0.6954755780848685	T	T	T
0.1812665613798378	0.8287399778612979	0.6605113124730962	T	T	T
0.7724922200163686	0.8284217874947561	0.4777246034108804	T	T	T
0.0044196121039592	0.5522367655325912	0.2140525578878084	T	T	T
0.3583445224463633	0.0711677403564310	0.7218596135959884	T	T	T
0.3157047696083937	0.0560114528706913	0.9070395017871318	T	T	T
0.2026035864125260	0.0474649055228731	0.0113737790117573	T	T	T
0.0955345330166238	0.0658390375764869	0.8986196623510279	T	T	T
0.1038138647547249	0.0675184483842378	0.7010341259307989	T	T	T
0.2289363262143944	0.0578115627841444	0.7598274435354111	T	T	T
0.3545831694164771	0.8295209963047316	0.7503884275618091	T	T	T
0.3048557818915955	0.8645603201659899	0.9236276254547525	T	T	T
0.1892807445443839	0.8518221864364892	0.0186775616446790	T	T	T
0.0857136704919737	0.8361544674514935	0.8967880232904892	T	T	T
0.0922204327122280	0.8318517096059700	0.6992496117074426	T	T	T
0.2238338597226610	0.8516673019664150	0.7673272784357390	T	T	T

Structure files (CONTCAR) involved in this work:

0.3118531509773496	0.9533077591936662	0.7766724495262388	T	T	T
0.0875266661592245	0.9515025717002191	0.7943569616901450	T	T	T
0.4322870023715801	0.1285267258012443	0.5822572304608528	T	T	T
0.4133201774354183	0.9974249818977585	0.5743436029466004	T	T	T
0.3913517498057739	0.8664333608295178	0.5675872827660360	T	T	T
0.1952523629492081	0.1437399000281310	0.6146605370568629	T	T	T
0.1940557261170492	0.0133609788431500	0.5793168005368955	T	T	T
0.1919964309786863	0.8802695989781762	0.5597380775549005	T	T	T
0.9883463918690574	0.0412062902099039	0.7883965845416934	T	T	T
0.9812610400071577	0.8700561874201296	0.7856452369745527	T	T	T
0.1425340091330068	0.9333461664556055	0.2191623598921205	T	T	T
0.1834311517419870	0.9591073280201977	0.4029512629087302	T	T	T
0.2984000382053273	0.9525147287542659	0.5020587604888128	T	T	T
0.4109979930305446	0.9323147031871294	0.4022947444463594	T	T	T
0.3977347278649895	0.9342925428933774	0.2048517185942752	T	T	T
0.2717839522297408	0.9514741691453539	0.2577372208327056	T	T	T
0.1428927791767936	0.1775858438438375	0.2451331304294674	T	T	T
0.1943055612364953	0.1365217834558952	0.4170226240692123	T	T	T
0.3097937648762376	0.1476628664572025	0.5126642542115322	T	T	T
0.4145312101911200	0.1675602624965280	0.3940520307608600	T	T	T
0.3980230672918892	0.1597257925648656	0.1984458138174659	T	T	T
0.2733756639689796	0.1562781869087562	0.2617537053180503	T	T	T
0.1867576625429287	0.0539322925324763	0.2609987472790626	T	T	T
0.4150630683949698	0.0480607516276982	0.3051856183365631	T	T	T
0.0664222883556014	0.8732154889747277	0.0848199882810690	T	T	T
0.0843482894245705	0.0041778864516989	0.0714523374290222	T	T	T
0.1073388174592283	0.1353417639448773	0.0634978282278040	T	T	T
0.3033858847606293	0.8618250989137837	0.1188968290768653	T	T	T
0.3139499504168677	0.9936168171424780	0.0798750884198356	T	T	T
0.3009636969699910	0.1273470185991927	0.0704558002829563	T	T	T
0.5149334746433938	0.9589175579407136	0.2854250648281482	T	T	T
0.5164671656393991	0.1320959512084069	0.2778852035101813	T	T	T
0.6395981432721614	0.5575151929485181	0.2830785404053767	T	T	T
0.6893134599662375	0.5755684086470056	0.1043037370030040	T	T	T
0.7919404507943957	0.5570950245822718	0.9778031715142342	T	T	T
0.8954305660703957	0.5764695687253735	0.1002635202865041	T	T	T
0.8874302751392674	0.5408051725600149	0.2955650830595999	T	T	T
0.7639818866704939	0.5252485635968056	0.2465286645168454	T	T	T
0.6394574495106662	0.3353510965098465	0.2641510744168590	T	T	T
0.6927089653689750	0.3328901624239368	0.0853422259652985	T	T	T
0.8083762466657693	0.3522730780146023	0.9907803880950540	T	T	T
0.9104902684514079	0.3256967447208363	0.1104944135288577	T	T	T
0.9061515075496234	0.3654280559475750	0.3011066960346044	T	T	T
0.7667093446113057	0.3703257445859070	0.2427299118502714	T	T	T
0.6690339423644289	0.4493589368536784	0.1719763095763646	T	T	T
0.9244031541904114	0.4537737140257740	0.1539420493138207	T	T	T
0.5731817097676731	0.6248364098364310	0.4180600568652170	T	T	T
0.5859780217592262	0.4939943398972366	0.4393708262827010	T	T	T
0.5839170489750254	0.3603569890412853	0.4418099925327264	T	T	T
0.7997727695022369	0.6290680345294548	0.3649328707697662	T	T	T
0.7966556642548585	0.5089536849840754	0.4400226574782052	T	T	T
0.8224520669835054	0.3786704342125887	0.4432153881064890	T	T	T
0.0207229519391277	0.3679920717223711	0.2045655747831941	T	T	T

Structure files (CONTCAR) involved in this work:

0.8554624700421590	0.4275214396666463	0.7866835863164464	T	T	T
0.7943877804075550	0.4384829027106797	0.6090141642919679	T	T	T
0.6968146053239067	0.4240440741887052	0.4728871624346003	T	T	T
0.6003705377277890	0.4277353638496688	0.6094314078894686	T	T	T
0.6025802922094524	0.4440055080596810	0.8042594213223726	T	T	T
0.7300876379608733	0.4738970332828139	0.7720003990672464	T	T	T
0.8608758903317318	0.6840415575658825	0.7428017983801537	T	T	T
0.8158148408250927	0.6303641286122624	0.5621759730800223	T	T	T
0.6958384386220343	0.6579250374906066	0.4828122352545101	T	T	T
0.5904371798312125	0.6686488909804725	0.6020626004608012	T	T	T
0.5968351746069189	0.6579832389904712	0.7973307466452846	T	T	T
0.7223865917985669	0.6423864956825459	0.7375356777860160	T	T	T
0.8342339570276187	0.5456317583470174	0.7031915587630595	T	T	T
0.5788937627379029	0.5485168196248276	0.6839117988666226	T	T	T
0.9318186935727346	0.3777390852953567	0.9295137488497879	T	T	T
0.9095104781329227	0.5092565690222177	0.9276649567972078	T	T	T
0.8902176930010341	0.6409283410812883	0.9281583759721860	T	T	T
0.6952684130618008	0.3747329206971936	0.8959304212244698	T	T	T
0.6736209839403315	0.5040969541620265	0.9433035736641250	T	T	T
0.6911362215698238	0.6384388658303312	0.9324920614441821	T	T	T
0.4880895185255942	0.4515876887893803	0.7133172449857433	T	T	T
0.4809454088418700	0.6364390697780276	0.7074903007214797	T	T	T
0.6459940946626511	0.9428968244097167	0.2878564035706564	T	T	T
0.7000971784688068	0.9308017383297787	0.1093361999376622	T	T	T
0.8005393489176192	0.9399725037208271	0.9778644415089358	T	T	T
0.8971080567425925	0.9311798947254626	0.1165553372144197	T	T	T
0.8993325900987872	0.9585420853938382	0.3121488618291514	T	T	T
0.7737190121501796	0.9735995269490129	0.2615670157826313	T	T	T
0.6426823653178247	0.1710009740769176	0.2582811947667177	T	T	T
0.6980167773768753	0.1637502228157544	0.0822576418013544	T	T	T
0.8104365464486692	0.1481298233927363	0.9804822841592430	T	T	T
0.9128873849234185	0.1736275727828221	0.1022025774570905	T	T	T
0.8989966385076040	0.1525728240738315	0.2976218973675741	T	T	T
0.7722778034620661	0.1418166848054808	0.2442396301824939	T	T	T
0.6805606834063429	0.0526539274899850	0.1871069154394940	T	T	T
0.9254295872983664	0.0517678773027810	0.1726236928360572	T	T	T
0.5706676466341926	0.8767037387156805	0.4167024126939270	T	T	T
0.5841760220088991	0.0080109117501806	0.4376217991091400	T	T	T
0.5962545763008223	0.1405892121460223	0.4389134901783677	T	T	T
0.8107102795438770	0.8737014493253034	0.3856649505925299	T	T	T
0.8136309102122441	1.0001966173369417	0.4478290005756509	T	T	T
0.8071206926332292	0.1352364069026598	0.4370872520112843	T	T	T
0.0115663807625872	0.9535930109853041	0.2175070517968689	T	T	T
0.0181047898221937	0.1421112973140509	0.2144020217876062	T	T	T
0.8582769890809113	0.0610492946330174	0.7888326311903565	T	T	T
0.8030986578903623	0.0732667804877323	0.6102799604881348	T	T	T
0.7003680878636414	0.0628377557765015	0.4827621135965260	T	T	T
0.5986682493561368	0.0750668692788961	0.6091367594648528	T	T	T
0.6036478469128573	0.0511313024756523	0.8058081127717839	T	T	T
0.7298670745407183	0.0320705683071326	0.7626372228525103	T	T	T
0.8546287207031285	0.8357432969358894	0.7801262928454004	T	T	T
0.8168414760312033	0.8359382326779666	0.5959790475820071	T	T	T
0.6900366177984378	0.8452981954141974	0.4959213865950719	T	T	T

Structure files (CONTCAR) involved in this work:

0.5792572429506385	0.8293711927340315	0.6019820455890528	T	T	T
0.6009505279780797	0.8501564593716642	0.7958287606272759	T	T	T
0.7277145175790636	0.8627971147652024	0.7421211077532524	T	T	T
0.8220968756941825	0.9516307852099702	0.6906488682920341	T	T	T
0.5766830244601951	0.9528860311843181	0.6751639129583777	T	T	T
0.9338768881084207	0.1262143697717645	0.9179811556521124	T	T	T
0.9172766037843954	0.9947736108110180	0.9408496556464385	T	T	T
0.9088879120920494	0.8622390151393666	0.9551364012398823	T	T	T
0.6940615052454882	0.1291302101655053	0.8896877622185178	T	T	T
0.6854286621740625	0.0014509693702817	0.9442224138208215	T	T	T
0.6936459687662803	0.8673124877230245	0.9357204928627890	T	T	T
0.4885601554564626	0.0499104557730593	0.7167748658658013	T	T	T
0.4797131133693539	0.8655882108630839	0.7196464415340382	T	T	T
0.3578387430225349	0.4302974718073383	0.7188358941042110	T	T	T
0.3140413699202609	0.4461094639139269	0.9036406717164043	T	T	T
0.2010064854271549	0.4611630277174233	0.0061861340886602	T	T	T
0.0908378644572235	0.4362905418797584	0.9021062846184796	T	T	T
0.1010667175776874	0.4303607900212208	0.7049406459776060	T	T	T
0.2277650053403175	0.4444535925749654	0.7558662278284605	T	T	T
0.3560545834300608	0.6717803952572362	0.7500318273786372	T	T	T
0.2989538266643050	0.6375023546774670	0.9174001561931604	T	T	T
0.1884263186604408	0.6484434696983715	0.0216569526075754	T	T	T
0.0875714401608983	0.6636162347021134	0.8948471562509097	T	T	T
0.0968053002192406	0.6661385863744067	0.6993311478834061	T	T	T
0.2236250296558416	0.6485459222007419	0.7553133522279635	T	T	T
0.3105268793541126	0.5481776449750969	0.7717158106896473	T	T	T
0.0819696528333321	0.5479015608843099	0.7937857332864338	T	T	T
0.4317412870861573	0.3759296493951579	0.5749235834682788	T	T	T
0.4127609322492502	0.5074443716739029	0.5753329990991303	T	T	T
0.3869686034946374	0.6384641364290432	0.5652991441294151	T	T	T
0.1924201667229090	0.3560631129241981	0.6153069910381421	T	T	T
0.1852864484758514	0.4860817493919743	0.5768071786150160	T	T	T
0.1864261084593443	0.6187542506911723	0.5687196006234854	T	T	T
0.9845969132479276	0.4548612569330168	0.7872279263120392	T	T	T
0.9814681838557333	0.6348398865644902	0.7830647832598587	T	T	T
0.1360897203900454	0.5694204943654192	0.2244283442152947	T	T	T
0.1835893341810946	0.5477683470767423	0.4041695677136119	T	T	T
0.2940476629904112	0.5482791076830518	0.5150427931830596	T	T	T
0.4011499001076234	0.5702290898665793	0.4020051510954977	T	T	T
0.3953223678883130	0.5655267826909403	0.2054744380410589	T	T	T
0.2674193849096445	0.5521988483217637	0.2524885159399689	T	T	T
0.1401689835341161	0.3257911580163369	0.2502015173198318	T	T	T
0.1942777828598387	0.3657746376176865	0.4191432516990992	T	T	T
0.3082578091620793	0.3541948598083781	0.5166367455384071	T	T	T
0.4082716020334236	0.3313788036461663	0.3894299574286333	T	T	T
0.3938907572797319	0.3471244117075277	0.1928509906104970	T	T	T
0.2707150632591502	0.3479524113520519	0.2590483504706630	T	T	T
0.1835699797689805	0.4497624792018550	0.2663166557878748	T	T	T
0.4117210749166669	0.4529597536232712	0.3113231405235098	T	T	T
0.0644515153752678	0.6272754059758111	0.0815605010109061	T	T	T
0.0820174860949085	0.4955419646732819	0.0775125948844614	T	T	T
0.1152772640548096	0.3665388591699004	0.0636246774487631	T	T	T
0.3053961483207572	0.6384035887354845	0.1128320913193588	T	T	T

Structure files (CONTCAR) involved in this work:

0.3146035422101414	0.5058136919524775	0.0788942185880709	T	T	T
0.2939227041085067	0.3735064078294791	0.0656669633607019	T	T	T
0.5096054717907579	0.5430863025895362	0.2938772713184379	T	T	T
0.5114164004035450	0.3667063574867870	0.2754864927738201	T	T	T
0.4326020417102423	0.7519717944420123	0.6408720691239147	T	T	T
0.1874366752606286	0.7455677744869065	0.6237777673719702	T	T	T
0.2756598953164224	0.7505453906171577	0.0189217017636135	T	T	T
0.1033364936384700	0.7502142795375801	0.0432148751380123	T	T	T
0.0660972707104503	0.2522558865029781	0.1288950558786986	T	T	T
0.3103954266360314	0.2511699523636111	0.1327487605398535	T	T	T
0.2243763194276372	0.2503748915648337	0.5070384628821735	T	T	T
0.3917243613102072	0.2511702306541185	0.5437787334455824	T	T	T
0.5545251608101647	0.2497164772036389	0.3476442985532779	T	T	T
0.8151179652675283	0.2510422254610662	0.3422575581890072	T	T	T
0.7284750113485697	0.2507648776216268	0.9390655926610789	T	T	T
0.8927503218748312	0.2515587341842366	0.9478675680409707	T	T	T
0.9448433439484187	0.7522962068807184	0.8574755081638387	T	T	T
0.6878041895070145	0.7528795523344215	0.8384221071537177	T	T	T
0.8010337121443201	0.7435599456262434	0.4680712935084331	T	T	T
0.6023841420581416	0.7507993408077701	0.4474222086197299	T	T	T
0.9400840472664070	0.4982606691822339	0.4937634009328292	T	T	T
0.9666597246286481	0.7312052633077497	0.5729471030249865	T	T	T
0.9265403566366750	0.4137454362194609	0.4373024115709548	T	T	T
0.8796695034303531	0.5495299992957463	0.5617213490426803	T	T	T
0.8828446098276792	0.7642380106887341	0.5756320443014979	T	T	T
0.0353215025045205	0.7658069157281350	0.6405250943785060	T	T	T
0.0248418354041899	0.5905989267402525	0.4697797355614989	T	T	T
0.0263221877032915	0.6282794960439501	0.4764778691568116	T	T	T
0.0490287727245238	0.3907246738086373	0.4612898430559312	T	T	T
1.0040249762248510	0.3632327417705440	0.5733480246976527	T	T	T
1.0005951127837605	0.3116835783345944	0.4579681095675276	T	T	T
1.0076045050551665	0.3612662541667891	0.4919473775367549	T	T	T

Figure S11(d) TS1

Si Al O Zn H C

1.0000000000000000

20.0219999999999985 0.0000000000000000 0.0000000000000000

0.0000000000000000 19.8990000000000009 0.0000000000000000

0.0000000000000000 0.0000000000000000 13.3829999999999991

92 4 194 4 5 1

Selective dynamics

Direct

0.4232584593288608 0.0605073829887106 0.6497099664301753 T T T

0.3038792322014952 0.0323829469258136 0.7913411194849924 T T T

0.2835572167459676 0.0559200199622134 0.0174852190063241 T T T

0.1238348901929515 0.0649529985543235 0.0128686213922932 T T T

0.0687825522064813 0.0332737970643994 0.7993044762133134 T T T

0.1809979505043519 0.0685508820040364 0.6632610776266576 T T T

0.4148996795718936 0.8293150191442195 0.6682238455576952 T T T

0.2977981842124934 0.8730863105498730 0.8028002122853805 T T T

0.2681773589422623 0.8320540599656917 0.0189766652335264 T T T

0.1120703629210484 0.8286834840096381 0.0092536473723230 T T T

0.0613201352186862 0.8760168787806510 0.7973933908638596 T T T

0.0768656385021641 0.9428300476149687 0.1476635378096931 T T T

Structure files (CONTCAR) involved in this work:

0.1960084980092915	0.9746256719693573	0.2864926391465996	T	T	T
0.2192267275500799	0.9492908353029108	0.5116239494247579	T	T	T
0.3779923983656830	0.9382405554409546	0.5120980511384738	T	T	T
0.4353118864687673	0.9687117555854985	0.3004104856875243	T	T	T
0.3213321570866479	0.9355231689676839	0.1646206111780655	T	T	T
0.0831493510625831	0.1767473242924601	0.1649282185961443	T	T	T
0.1995775763717887	0.1314775255775730	0.2970576753248263	T	T	T
0.2314142019384058	0.1698592815582549	0.5145293228229331	T	T	T
0.3873099076770291	0.1735182541527315	0.5083214885952831	T	T	T
0.4357525521218129	0.1264871491710900	0.2947247249944300	T	T	T
0.3210337207222187	0.1734554191124897	0.1646889014667119	T	T	T
0.5756551277808589	0.5550336092264785	0.3577814215348676	T	T	T
0.6876035936759426	0.5265684702405848	0.2018275322759217	T	T	T
0.7099215903233996	0.5688052797393601	0.9886563756574969	T	T	T
0.8694472263181552	0.5700179788226329	0.9781974493583001	T	T	T
0.8120987918177007	0.5517014718963057	0.3318103828665585	T	T	T
0.5727920158095237	0.3280630485863573	0.3312466604889447	T	T	T
0.6929468429411475	0.3728365199581453	0.1942710119667773	T	T	T
0.7315614492499629	0.3287854482114435	0.9790624873308892	T	T	T
0.8858752781452598	0.3266930423927070	0.9917361016886509	T	T	T
0.9391842284666000	0.3782165885903397	0.1907809629900135	T	T	T
0.9189859481228757	0.4420881508131045	0.8545532515928161	T	T	T
0.8037097562705344	0.4736920752876563	0.7198364695008304	T	T	T
0.7792014486321895	0.4390454203628536	0.4902035731256104	T	T	T
0.6203751253573715	0.4287426109390766	0.4882826207721270	T	T	T
0.5697060497458006	0.4690590428152475	0.6988395363741333	T	T	T
0.6762235764091636	0.4486762147810286	0.8541548648105913	T	T	T
0.9159050003717648	0.6779312551324488	0.8218155482694651	T	T	T
0.7703707955589294	0.6648956637773468	0.4647013562465910	T	T	T
0.6117835089636378	0.6756852439677962	0.4848904843202310	T	T	T
0.5615375640098421	0.6280495092317206	0.6963470820752404	T	T	T
0.6741314125739836	0.6739094012658517	0.8266772898775329	T	T	T
0.5798961806753044	0.9477969828432335	0.3577268930807601	T	T	T
0.7009599402946275	0.9754421445252613	0.2135714660771035	T	T	T
0.7197850490218656	0.9352968499883271	0.9933330130729612	T	T	T
0.8797483426983213	0.9329520244460505	0.9997514309568233	T	T	T
0.9328095101141873	0.9748034258773485	0.2062275885141051	T	T	T
0.8238224202687944	0.9497112898773756	0.3556222414560533	T	T	T
0.5774573924776840	0.1731085821379929	0.3324816669704343	T	T	T
0.6989619805237641	0.1324761361927946	0.1954219288792922	T	T	T
0.7321667432899103	0.1735589257130390	0.9757101637693789	T	T	T
0.8867452008844623	0.1746274578214722	0.9880585286157333	T	T	T
0.9379404835121516	0.1316802074571427	0.1986683693016050	T	T	T
0.8216878670957845	0.1730920162510253	0.3316430525823697	T	T	T
0.9234562086347821	0.0549586831508453	0.8600625410876340	T	T	T
0.8028350681113468	0.0299010792952493	0.7128268832481356	T	T	T
0.7812582616550764	0.0689555111399836	0.4939023846953921	T	T	T
0.6205201372332221	0.0718529432210533	0.4933944009807071	T	T	T
0.5677935081480586	0.0326156402036747	0.7024101962890029	T	T	T
0.6788655893900326	0.0543407214358995	0.8530610577872707	T	T	T
0.9216661090904636	0.8309277427211390	0.8488201519543538	T	T	T
0.8025798580726113	0.8727707012882548	0.7060430245419148	T	T	T
0.6133601185392660	0.8274146812975411	0.4906070270322905	T	T	T

Structure files (CONTCAR) involved in this work:

0.5595086382556798	0.8753490341131932	0.6969577739373843	T	T	T
0.6755453755383064	0.8335873937918711	0.8305249635826039	T	T	T
0.4233039705225289	0.4426341767859346	0.6431505608223024	T	T	T
0.3037072505901044	0.4695351139538360	0.7865063223455402	T	T	T
0.2809361228465586	0.4463969020364451	0.0118163806255537	T	T	T
0.1234576597885319	0.4384608474451107	0.0113591063418040	T	T	T
0.0638355815693664	0.4658624621812285	0.8002924196137582	T	T	T
0.1779984359803739	0.4316010311579084	0.6629343018480874	T	T	T
0.4154098142859425	0.6750177809902732	0.6644699274760634	T	T	T
0.2969750514253542	0.6291599968152808	0.7951524867989298	T	T	T
0.2664845033357883	0.6705730507371108	0.0156950606399881	T	T	T
0.1111899664484605	0.6738736805200098	0.0082813051746454	T	T	T
0.0599035582242384	0.6245304627195343	0.7980644303770851	T	T	T
0.1741086074775898	0.6698280345339944	0.6585076701209774	T	T	T
0.0730135322084661	0.5601581267301191	0.1462865493430938	T	T	T
0.1925021081832765	0.5304460330671952	0.2862650672668932	T	T	T
0.2141809301491019	0.5519051527130788	0.5143088381326829	T	T	T
0.3737983520602937	0.5664242302603807	0.5125499019855475	T	T	T
0.4292657848809271	0.5318927805817494	0.3022814023855808	T	T	T
0.3190008781082878	0.5656560494921594	0.1610995321662005	T	T	T
0.0844631369835642	0.3292615752661905	0.1627750190221827	T	T	T
0.1977822530933709	0.3726936935544908	0.2979341692087027	T	T	T
0.2302820675431334	0.3309828154451585	0.5151932887072340	T	T	T
0.3851066747522687	0.3277126942848279	0.5056816300938005	T	T	T
0.4301755199083983	0.3746427022957959	0.2928373475895193	T	T	T
0.3170648800277076	0.3298955319982569	0.1594324749551859	T	T	T
0.9269506772774312	0.5326921984411530	0.1847102772062874	T	T	T
0.8217173410851667	0.3363209268766037	0.3273774186289953	T	T	T
0.7996208876608349	0.6278978772449607	0.6935050616698296	T	T	T
0.1789483268745126	0.8313966616281298	0.6603841392441993	T	T	T
0.7743426588374159	0.8262042074293412	0.4806153289288504	T	T	T
0.0043602425282374	0.5514184564126895	0.2090243364699790	T	T	T
0.3587438063750337	0.0698993705081274	0.7217345880928669	T	T	T
0.3160094476459394	0.0542780840604601	0.9065869532957299	T	T	T
0.2029199338228491	0.0481349337648687	0.0115859469858053	T	T	T
0.0960253852873620	0.0696163710811536	0.8994742461481406	T	T	T
0.1038305371600030	0.0665446270282667	0.7019655197185568	T	T	T
0.2292204075805136	0.0567593817461124	0.7596788987307914	T	T	T
0.3565452347814687	0.8283155587734693	0.7518132207265489	T	T	T
0.3051741708648105	0.8646693326385086	0.9232840801090757	T	T	T
0.1893043402187220	0.8525236452076758	0.0167273373232771	T	T	T
0.0857117851681724	0.8343791396586493	0.8945915737371746	T	T	T
0.0903902411820608	0.8379737500728797	0.6962066336751955	T	T	T
0.2256756540582707	0.8470666686106116	0.7657643544985970	T	T	T
0.3111253614619220	0.9518404185615041	0.7747496551121844	T	T	T
0.0870130736389601	0.9528172584442380	0.8023966343870735	T	T	T
0.4325052161299503	0.1279107322508477	0.5823052891313953	T	T	T
0.4156348505766589	0.9963124499599532	0.5759854341170394	T	T	T
0.3880903199792417	0.8663934573330144	0.5677107955467859	T	T	T
0.1950783017042625	0.1422177346433023	0.6147377699474909	T	T	T
0.1926658158541796	0.0108489360235056	0.5807985876947780	T	T	T
0.1987554191297810	0.8781829420235455	0.5578843085154199	T	T	T
0.9885261467055211	0.0423243123126396	0.7899991114170754	T	T	T

Structure files (CONTCAR) involved in this work:

0.9801104348623760	0.8712598353506789	0.7883312300952411	T	T	T
0.1419657518403180	0.9341437861306950	0.2186673271466467	T	T	T
0.1836116489678764	0.9584394157195242	0.4029198831531039	T	T	T
0.2998440826009149	0.9571180337608078	0.4998763153753525	T	T	T
0.4123069332608437	0.9321868493045536	0.4030266493229067	T	T	T
0.3975787469515679	0.9339209978757758	0.2058432105842696	T	T	T
0.2713761959192370	0.9517296983437908	0.2574849413221905	T	T	T
0.1422253402892121	0.1784799556121810	0.2479941117071143	T	T	T
0.1955350889125058	0.1366385304862412	0.4175804240906893	T	T	T
0.3098521934405012	0.1488228180180245	0.5150463949740294	T	T	T
0.4135833392361120	0.1673246729896783	0.3943999876112317	T	T	T
0.3979437576703948	0.1598936983420567	0.1988133485229721	T	T	T
0.2728505673949304	0.1568792884318256	0.2601138812399629	T	T	T
0.1864626625860908	0.0544163198213493	0.2619276185340056	T	T	T
0.4146678116051551	0.0479836603211036	0.3050747256400402	T	T	T
0.0666081359022371	0.8743768462092355	0.0825851295734674	T	T	T
0.0844497729938714	0.0051966221045371	0.0703317192301825	T	T	T
0.1083990857801061	0.1364366430927508	0.0663343776247895	T	T	T
0.3029787606076630	0.8619769712546141	0.1189304874635485	T	T	T
0.3142013234049601	0.9935275773421700	0.0800974351791903	T	T	T
0.3020527632516010	0.1271871616611843	0.0693144379454888	T	T	T
0.5152975059233480	0.9595777257762015	0.2857950437064613	T	T	T
0.5161484021884233	0.1323327324848808	0.2795393052150555	T	T	T
0.6391154211412838	0.5608223132565606	0.2837890610357558	T	T	T
0.6875593180508746	0.5751007201106343	0.1045744959014807	T	T	T
0.7900880902232068	0.5552389485015424	0.9791096878974942	T	T	T
0.8976349703299835	0.5776152261699761	0.0921330006794833	T	T	T
0.8879135919604687	0.5468562955634682	0.2894010385177641	T	T	T
0.7633354060421479	0.5248493475484216	0.2454884041918293	T	T	T
0.6374946457296491	0.3330776395628745	0.2603081358314335	T	T	T
0.6948360992537943	0.3354744437713637	0.0860750226091717	T	T	T
0.8091505512716273	0.3532221589190251	0.9882629708545434	T	T	T
0.9114971330153664	0.3260455828686783	0.1069943011697014	T	T	T
0.9047075683435841	0.3626489950680208	0.2978865481412837	T	T	T
0.7643577231252431	0.3725241262492036	0.2482063702908171	T	T	T
0.6658245373816137	0.4500047900990630	0.1766396093224334	T	T	T
0.9211922514375702	0.4541279518798383	0.1531117068541412	T	T	T
0.5666337638900371	0.6256856785980541	0.4166221119028657	T	T	T
0.5872621674449943	0.4953645970566602	0.4387814185140286	T	T	T
0.5875125381014693	0.3618151685457942	0.4401599495708355	T	T	T
0.7971041851371318	0.6292938116616905	0.3625798042627622	T	T	T
0.8045768555972794	0.5085120677905566	0.4354549940144330	T	T	T
0.8255408895463154	0.3781846084425609	0.4471415771029373	T	T	T
0.0197258111708068	0.3707997699509870	0.2015535521975837	T	T	T
0.8553866062704450	0.4264447091242722	0.7824702056264411	T	T	T
0.7936797615087262	0.4436777417549230	0.6083890715098162	T	T	T
0.7006657565192778	0.4277153230759471	0.4670826932132904	T	T	T
0.6055000709309986	0.4291973424901888	0.6070577361309771	T	T	T
0.6035178928160608	0.4435564306670303	0.8018476837740246	T	T	T
0.7310934852871471	0.4748560580139856	0.7731332810807949	T	T	T
0.8623673781679411	0.6877805988779083	0.7292591060715147	T	T	T
0.8071579522490522	0.6271140559842703	0.5606119170660102	T	T	T
0.6904467404274234	0.6544426803794847	0.4754201928073435	T	T	T

Structure files (CONTCAR) involved in this work:

0.5886343192368825	0.6695042054915860	0.6003545733354481	T	T	T
0.5963147634554129	0.6588201478686116	0.7963507895766719	T	T	T
0.7228524973257787	0.6459715921261175	0.7402282961616942	T	T	T
0.8354669854705327	0.5488820263048236	0.7133435755834716	T	T	T
0.5806282779386658	0.5492120114110354	0.6827751047308480	T	T	T
0.9321915351170394	0.3774056404775639	0.9258872443654750	T	T	T
0.9084984434451747	0.5090378975993496	0.9226820317715908	T	T	T
0.8822539004631756	0.6399392437674916	0.9165407364654375	T	T	T
0.6950668424182616	0.3749589528643216	0.8958526093963708	T	T	T
0.6714731335742163	0.5038487321017074	0.9430761710279478	T	T	T
0.6896566141095469	0.6380990059702824	0.9337046559625028	T	T	T
0.4907946495025149	0.4516797101285947	0.7079833466243611	T	T	T
0.4808163501422262	0.6355725275617357	0.7061353878528600	T	T	T
0.6460754733830776	0.9436094032334853	0.2885244196336316	T	T	T
0.7015916669830840	0.9312506196483989	0.1110087851013723	T	T	T
0.8004924257108172	0.9381464624337793	0.9765056574123219	T	T	T
0.8955248257575876	0.9326652016249440	0.1178821069062394	T	T	T
0.8999106699435707	0.9585690242037816	0.3135152065872271	T	T	T
0.7740575137756900	0.9728559570936463	0.2649402275675242	T	T	T
0.6421966164378009	0.1707290835313448	0.2603003778268111	T	T	T
0.6973329970374633	0.1646629778232343	0.0840813807109375	T	T	T
0.8097369900154066	0.1483720726646749	0.9823781770826402	T	T	T
0.9128277857153515	0.1746080039372197	0.1024961380176309	T	T	T
0.8985682015437205	0.1554228001401718	0.2981314424493339	T	T	T
0.7720764959738008	0.1419975704028912	0.2456571729880189	T	T	T
0.6814319317385255	0.0528518140371621	0.1879765843487241	T	T	T
0.9246626008053326	0.0530492415408687	0.1750751428322577	T	T	T
0.5715836839493094	0.8777228969727655	0.4179059306128644	T	T	T
0.5840877788518483	0.0089245485298020	0.4384659559005739	T	T	T
0.5957416651566417	0.1412636965212178	0.4410536853221133	T	T	T
0.8127997405343141	0.8739167658208734	0.3912229098955982	T	T	T
0.8147748488744284	0.0011603750629002	0.4495669409159750	T	T	T
0.8076459939785007	0.1360170014374814	0.4383226147822325	T	T	T
0.0111167421058583	0.9542390774009597	0.2156415610043697	T	T	T
0.0176685241975979	0.1428034987845840	0.2154107860070503	T	T	T
0.8584324527799011	0.0596398641834236	0.7885976273061152	T	T	T
0.8025053465858953	0.0740112644188684	0.6113323553228611	T	T	T
0.7006193139068755	0.0634248468713517	0.4821938116471152	T	T	T
0.5999046216132863	0.0755263192426013	0.6106499288718805	T	T	T
0.6038936598855492	0.0510361701593016	0.8076583107043029	T	T	T
0.7298074006781956	0.0328099045480894	0.7641990407953081	T	T	T
0.8535628060890994	0.8373226705694669	0.7844742049533139	T	T	T
0.8180502336411226	0.8314928202124178	0.6014921830729489	T	T	T
0.6914605986935104	0.8449204947803247	0.4963360398111035	T	T	T
0.5808734987472499	0.8297884410755850	0.6022549464921866	T	T	T
0.5995246416132901	0.8505497733618509	0.7965313991717221	T	T	T
0.7266549165029815	0.8625047006194847	0.7443758576952686	T	T	T
0.8198131395488509	0.9511411567429653	0.6884596434530654	T	T	T
0.5773256637556951	0.9535746781164379	0.6754520523069742	T	T	T
0.9327738123599727	0.1256958009667920	0.9193096235768156	T	T	T
0.9170807949684480	0.9939417878633873	0.9408687904985734	T	T	T
0.9098221482290852	0.8614288146182596	0.9589647867311087	T	T	T
0.6934384210305015	0.1301837906506726	0.8912119033122736	T	T	T

Structure files (CONTCAR) involved in this work:

0.6865917518224506	0.0028818059078840	0.9466057344446345	T	T	T
0.6911637165036408	0.8688272464361240	0.9374759417662969	T	T	T
0.4894300762887414	0.0508715977573055	0.7179867511055132	T	T	T
0.4797250046001259	0.8668828607664029	0.7159422555396230	T	T	T
0.3600725810472474	0.4333392798513463	0.7182266302134258	T	T	T
0.3161051386823332	0.4497088319014449	0.9024870545829521	T	T	T
0.2011958854250590	0.4597949225737720	0.9998538638719462	T	T	T
0.0894758055240502	0.4308827199444271	0.9021116442863329	T	T	T
0.1017601055202938	0.4334712399606785	0.7047215995121543	T	T	T
0.2292910008788220	0.4442007822799770	0.7551593194210376	T	T	T
0.3572399085764247	0.6731595088077132	0.7492830977987522	T	T	T
0.2977783053140338	0.6385638696046171	0.9147039150349729	T	T	T
0.1879886349942244	0.6488999400551764	0.0187815677162363	T	T	T
0.0867770252258595	0.6670709715704433	0.8924985804062818	T	T	T
0.0951539362726380	0.6574900769965291	0.6971938989841140	T	T	T
0.2250294025866971	0.6554312038819525	0.7503185881653898	T	T	T
0.3076012556737506	0.5504297735419580	0.7674226975960344	T	T	T
0.0803948745991742	0.5464120539947146	0.8055161926641173	T	T	T
0.4319836368738090	0.3765392851327434	0.5729272616343289	T	T	T
0.4136451860653789	0.5082347147923978	0.5725295371692702	T	T	T
0.3860333395724732	0.6389366968937011	0.5644998130576140	T	T	T
0.1915585654483092	0.3584990928349380	0.6137291285239339	T	T	T
0.1850010505929303	0.4901919309144572	0.5794166333423034	T	T	T
0.1895912581144530	0.6223101541936202	0.5638773871729960	T	T	T
0.9845039458878134	0.4539314566275908	0.7842644566045449	T	T	T
0.9801544977905758	0.6343763923845327	0.7826602440802936	T	T	T
0.1353406209782025	0.5694954478862362	0.2226798282871215	T	T	T
0.1821761422633408	0.5480412622073454	0.4034224913424109	T	T	T
0.2946968977497255	0.5481180856613558	0.5111573263088082	T	T	T
0.4019230629423528	0.5714792299811321	0.3998560215573850	T	T	T
0.3946357373917802	0.5650394089304868	0.2041896694885042	T	T	T
0.2666004230357256	0.5545055937349731	0.2529406547393364	T	T	T
0.1380858608649357	0.3268524144998460	0.2536204458197675	T	T	T
0.1967036859196861	0.3667306596595184	0.4183531180717458	T	T	T
0.3083127948364364	0.3531165748247062	0.5198376724762047	T	T	T
0.4057131876607092	0.3307736595633299	0.3885725826564441	T	T	T
0.3934658501038241	0.3475299412362519	0.1919521179500550	T	T	T
0.2694095333804691	0.3475929503745407	0.2550199413361660	T	T	T
0.1842084077138198	0.4503616084994807	0.2653635348296403	T	T	T
0.4095528650291471	0.4527852111276925	0.3117183509141408	T	T	T
0.0643888499714805	0.6273317810685417	0.0783177046555809	T	T	T
0.0836153121362035	0.4959638971515637	0.0731880166231948	T	T	T
0.1175804797710245	0.3663339451604228	0.0664563756289193	T	T	T
0.3050661275210916	0.6384112989053231	0.1105969260485487	T	T	T
0.3119781623776489	0.5056617360088309	0.0800672803495503	T	T	T
0.2949104617720211	0.3734583077713966	0.0620458706235512	T	T	T
0.5093863212474069	0.5401976576842901	0.2918496152806676	T	T	T
0.5102628373931015	0.3669208461806959	0.2782655574537651	T	T	T
0.4336089321606718	0.7522189428416048	0.6385666085951505	T	T	T
0.1677056341059474	0.7468471432671743	0.6216562263528147	T	T	T
0.2752910844699387	0.7509524955873000	0.0184731992347154	T	T	T
0.1036977443751082	0.7510030124060710	0.0436378717336003	T	T	T
0.0654959479152491	0.2531678944570386	0.1308622594145519	T	T	T

Structure files (CONTCAR) involved in this work:

0.3109120876075434	0.2511425228039668	0.1304437245561522	T	T	T
0.2227658155771504	0.2505933610438137	0.5097272152791242	T	T	T
0.3933138076361043	0.2511616013595387	0.5445948893271838	T	T	T
0.5536957547779147	0.2500981046772082	0.3501429855769321	T	T	T
0.8120914304902684	0.2519987690625189	0.3438492063983617	T	T	T
0.7283895941296931	0.2515206839567380	0.9409406469171792	T	T	T
0.8922231272051037	0.2512669913679161	0.9462019566180938	T	T	T
0.9425923241692936	0.7519038909961108	0.8556184449616141	T	T	T
0.6858809488329642	0.7537619941972946	0.8435305110243165	T	T	T
0.7963984036106355	0.7412435004335878	0.4684161474939070	T	T	T
0.6010153722940301	0.7517548705616225	0.4463059727882033	T	T	T
0.9365183623792952	0.4921127608600709	0.5136949846764910	T	T	T
0.9700059637371579	0.7266153972367050	0.5759011915129539	T	T	T
0.9281138930320644	0.3942859938989216	0.4542634931937545	T	T	T
0.8986952068741298	0.5764706775555241	0.5517519330681286	T	T	T
0.8824003272552327	0.7565129825130904	0.6045992981081284	T	T	T
0.0512319854814360	0.7550598691598831	0.6337439241686985	T	T	T
0.9833949550140642	0.4916707611399662	0.5337693076499453	T	T	T
0.9498604253816514	0.6519367049800644	0.5590217069143826	T	T	T
0.0552655701777414	0.3888651623146471	0.4664345869717444	T	T	T
0.0179694343139504	0.3560540637389266	0.5784579082082342	T	T	T
0.0196475026273454	0.3061468405509044	0.4657054828364276	T	T	T
0.0150939723553867	0.3570796624383603	0.4965754325710843	T	T	T

Figure S11(d) TS2

Si Al O Zn H C

1.0000000000000000

20.0219999999999985 0.0000000000000000 0.0000000000000000

0.0000000000000000 19.8990000000000009 0.0000000000000000

0.0000000000000000 0.0000000000000000 13.3829999999999991

92 4 194 4 5 1

Selective dynamics

Direct

0.4230851885589463	0.0612017679378882	0.6484592903901717	T	T	T
0.3023124192988709	0.0347006807760070	0.7891016097304064	T	T	T
0.2837627817680732	0.0553089968016056	0.0165567771366484	T	T	T
0.1235045247314780	0.0634035565323433	0.0104856581312603	T	T	T
0.0688673493439595	0.0322531031291601	0.7934903574585295	T	T	T
0.1815032295367662	0.0742112405408189	0.6621059821903125	T	T	T
0.4147051458652753	0.8303814732716586	0.6737819799257156	T	T	T
0.2928158520541291	0.8761959407940698	0.7993523686035900	T	T	T
0.2680357078897864	0.8329461157904544	0.0159317871458472	T	T	T
0.1104746688824256	0.8288627642275893	0.0117333748232618	T	T	T
0.0621013077969180	0.8755496590432102	0.7951678084493119	T	T	T
0.0772532813002096	0.9426412650777783	0.1503769555868846	T	T	T
0.1976605583034612	0.9740061759093624	0.2865676123015368	T	T	T
0.2174905878258911	0.9514005288481933	0.5141384750504714	T	T	T
0.3777312448182203	0.9370548688571594	0.5133692110694439	T	T	T
0.4348236721518386	0.9685565089005791	0.3010313067073185	T	T	T
0.3215635467721596	0.9339254224367779	0.1645611595197012	T	T	T
0.0831979475743976	0.1756010008419437	0.1612638106826506	T	T	T
0.2020812844626050	0.1302874533267862	0.2910579745132006	T	T	T
0.2310739473400837	0.1707105803565001	0.5079412882798849	T	T	T
0.3869411702099527	0.1741434869577665	0.5067556109841561	T	T	T

Structure files (CONTCAR) involved in this work:

0.4360573568230546	0.1265002527133005	0.2938012326107701	T	T	T
0.3234091683308324	0.1736695073028044	0.1601023965807507	T	T	T
0.5756749698154039	0.5596064559816701	0.3589607942147885	T	T	T
0.6901903634831190	0.5269137127128480	0.2121635974908841	T	T	T
0.7151849557758547	0.5660023475297411	0.9926274793220562	T	T	T
0.8735879930531033	0.5712870536754193	0.9875126146984373	T	T	T
0.8139972411253259	0.5508256338171391	0.3494074607302289	T	T	T
0.5755287198467807	0.3277400300775126	0.3295418928716985	T	T	T
0.6930839857849245	0.3739013723663321	0.1912205329692175	T	T	T
0.7303913234663434	0.3294251035527968	0.9744602174663005	T	T	T
0.8857907605687493	0.3266894348581967	0.9880919613612752	T	T	T
0.9397385449402048	0.3763764834822333	0.1891467130312504	T	T	T
0.9218340432217432	0.4469506213141635	0.8586718217747082	T	T	T
0.8006137725374605	0.4725003913285047	0.7172252426778770	T	T	T
0.7795479841581310	0.4342418166645504	0.4944717133482566	T	T	T
0.6203900524614210	0.4312713030912586	0.4871502717949678	T	T	T
0.5689005772053966	0.4707472490585847	0.6977982816502175	T	T	T
0.6765056961004271	0.4496482852360414	0.8536184905961320	T	T	T
0.9195727870239008	0.6772017246795249	0.8338486970453834	T	T	T
0.7655548590078965	0.6737384498602468	0.4655431239108099	T	T	T
0.6135805973510079	0.6759419485095549	0.4932663223871922	T	T	T
0.5601370673976059	0.6287822353870700	0.7011738557071816	T	T	T
0.6743708471291141	0.6693352899006796	0.8328852585396285	T	T	T
0.5794789991146058	0.9455120105775663	0.3584710073351732	T	T	T
0.6996252939663984	0.9729031092132189	0.2128233972031990	T	T	T
0.7196334367112758	0.9337573259102967	0.9936617523830343	T	T	T
0.8794891795749465	0.9337119921913215	0.9984529384944132	T	T	T
0.9330888459513040	0.9757253908707627	0.2043306846711796	T	T	T
0.8237013997883397	0.9525527344663978	0.3540109276162550	T	T	T
0.5776693063306616	0.1722054230134716	0.3345034630890502	T	T	T
0.6988116433421535	0.1289469733613099	0.1976924717392614	T	T	T
0.7316594934736819	0.1729250719482886	0.9783775738204252	T	T	T
0.8875007798912822	0.1746831501452877	0.9843776331431643	T	T	T
0.9381859576524906	0.1320703834266926	0.1958664731305981	T	T	T
0.8212965436488671	0.1716243865569841	0.3311258126300163	T	T	T
0.9234012225233876	0.0526080296025911	0.8563136649129468	T	T	T
0.8006426743945460	0.0243796755530794	0.7106680880485295	T	T	T
0.7811392549254484	0.0713020801528720	0.4937670414184153	T	T	T
0.6206546362113782	0.0706756795104493	0.4934112967250856	T	T	T
0.5681206057404093	0.0320510134759525	0.7038766306066057	T	T	T
0.6781768577975988	0.0521624490870111	0.8549134430335358	T	T	T
0.9211834155479196	0.8307122479937363	0.8450927615397416	T	T	T
0.8010329317393020	0.8665995646804443	0.6985106555561366	T	T	T
0.6130958884956383	0.8303207594603361	0.4953134462962928	T	T	T
0.5589258336843087	0.8741380866326034	0.7028219869764079	T	T	T
0.6768966851805333	0.8293297016162395	0.8319425669574106	T	T	T
0.4223002166895292	0.4424482199183998	0.6434268630473428	T	T	T
0.3030214395937936	0.4662297605409885	0.7872535477362500	T	T	T
0.2804278054557860	0.4476543989837588	0.0134533325313024	T	T	T
0.1224783596475898	0.4406463086450425	0.0106106001020456	T	T	T
0.0653594054020630	0.4683016493208251	0.7942102733008407	T	T	T
0.1790621140425781	0.4270034096574797	0.6625787266050467	T	T	T
0.4149528556617048	0.6750015467873047	0.6688775912402979	T	T	T

Structure files (CONTCAR) involved in this work:

0.2929187780075680	0.6254053472361507	0.7923474121008531	T	T	T
0.2673035163168302	0.6722661388206617	0.0135214835083619	T	T	T
0.1112152146593791	0.6732783227089270	0.0124841685751067	T	T	T
0.0630545029778064	0.6261975009110848	0.7956669617518501	T	T	T
0.1726148812960502	0.6709412755882220	0.6537919616532517	T	T	T
0.0722110172991971	0.5597393361808964	0.1509315047750749	T	T	T
0.1950531648975353	0.5305892362283665	0.2852011567287819	T	T	T
0.2124574815715312	0.5509062116539979	0.5167135126402869	T	T	T
0.3730325180356627	0.5686323270415674	0.5147005323628506	T	T	T
0.4291801007900666	0.5335608470192461	0.3027325707784502	T	T	T
0.3198720405674520	0.5690103388413495	0.1593162194495066	T	T	T
0.0852760918723240	0.3291576986914822	0.1585811412575582	T	T	T
0.2007942934872452	0.3733792575630614	0.2933169000194749	T	T	T
0.2303749334585738	0.3313387808255902	0.5088587171420451	T	T	T
0.3853435992389292	0.3285149959641668	0.5032831814267931	T	T	T
0.4327627669926032	0.3752056246938309	0.2910938376272738	T	T	T
0.3193565635364197	0.3294681873438934	0.1581134913601776	T	T	T
0.9258567271545592	0.5311046309477963	0.1947705656022360	T	T	T
0.8199003205321492	0.3344586416952931	0.3227195704474355	T	T	T
0.7991042828025261	0.6331335051700711	0.6924991047324160	T	T	T
0.1778537810835820	0.8283803655512362	0.6558465851791037	T	T	T
0.7675059545710848	0.8305589261453682	0.4750221941802821	T	T	T
0.0034035522215989	0.5508339103385199	0.2141013604597689	T	T	T
0.3597483380869118	0.0707029294278873	0.7225009608544991	T	T	T
0.3164292897333892	0.0503429673975042	0.9060938042478895	T	T	T
0.2030862708089755	0.0503006184274652	0.0089655610598581	T	T	T
0.0951702809147290	0.0640148709337574	0.8974524384284107	T	T	T
0.1041966453362624	0.0704493158634429	0.7003597085510131	T	T	T
0.2300247250758222	0.0668852737383418	0.7594721979567051	T	T	T
0.3537622806137395	0.8319766365247231	0.7530152120025831	T	T	T
0.2988297908383193	0.8720087236630182	0.9206095878008426	T	T	T
0.1883925749914402	0.8490184699084490	0.0243133172792277	T	T	T
0.0868833392246997	0.8404931593031619	0.8970604897935618	T	T	T
0.0898623547340521	0.8306143498832934	0.6989517264067374	T	T	T
0.2220836681375423	0.8471371678199435	0.7630114982860662	T	T	T
0.3033035622149128	0.9545491994225320	0.7659413382158612	T	T	T
0.0878556571817630	0.9521618039260796	0.7866619397553581	T	T	T
0.4320529767987401	0.1287847052042571	0.5811733681490071	T	T	T
0.4139661373122397	0.9975288476550245	0.5742901009553826	T	T	T
0.3927826235766120	0.8664865190726870	0.5699600371781920	T	T	T
0.1924698696213243	0.1471729804549279	0.6087524393137833	T	T	T
0.1969923643935137	0.0155854536610872	0.5827770774652521	T	T	T
0.1887696940887265	0.8829847887851220	0.5587447487259369	T	T	T
0.9884864103792056	0.0412587778510513	0.7858040206849927	T	T	T
0.9806606929531028	0.8720688950983795	0.7883555805646690	T	T	T
0.1414535143151016	0.9335627092764471	0.2228183191115472	T	T	T
0.18479377371113814	0.9647287058681195	0.4042666546882816	T	T	T
0.2985786895803536	0.9510500408328280	0.5044969140471729	T	T	T
0.4102475677857114	0.9321126079610438	0.4028330970933783	T	T	T
0.3979319968828769	0.9342193871033442	0.2053388058560629	T	T	T
0.2713719190438682	0.9454789518358580	0.2588390221091004	T	T	T
0.1435879096882930	0.1759930739365589	0.2420011565261052	T	T	T
0.1973003538596694	0.1343331734227411	0.4117072401566402	T	T	T

Structure files (CONTCAR) involved in this work:

0.3094269428091133	0.1496156278945325	0.5140291530449710	T	T	T
0.4130854423153273	0.1679032298693270	0.3926637879652440	T	T	T
0.3996909074342103	0.1592521527593249	0.1962562915790896	T	T	T
0.2743554083641273	0.1588289173388149	0.2551373805845364	T	T	T
0.1923378638046182	0.0531330004714576	0.2541557413235024	T	T	T
0.4149579668062218	0.0481210827058873	0.3053959333360339	T	T	T
0.0656334299356455	0.8737689834249722	0.0870014192533793	T	T	T
0.0868202865347373	0.0037454912612059	0.0715079659059736	T	T	T
0.1050311759193223	0.1353886861125999	0.0608376095858629	T	T	T
0.3059545135321598	0.8609889857383739	0.1146495237008216	T	T	T
0.3117951767597247	0.9939473100751264	0.0837765850288510	T	T	T
0.3043679152738563	0.1271680964812965	0.0650839295385159	T	T	T
0.5148657222663927	0.9593924669773034	0.2874512104035101	T	T	T
0.5163764181237465	0.1332555155574786	0.2790056930761479	T	T	T
0.6376151751630741	0.5671461549314454	0.2816507302901822	T	T	T
0.7021797915413828	0.5707846597501085	0.1117849406280851	T	T	T
0.7949208032856013	0.5557964615278251	0.9708126207005691	T	T	T
0.8920314797157377	0.5756220485704429	0.1059138949787702	T	T	T
0.8880735575680621	0.5422054298699226	0.3016585766933746	T	T	T
0.7605849729656003	0.5202194842221445	0.2727504002761485	T	T	T
0.6400536600541724	0.3307219627930250	0.2571803007616711	T	T	T
0.6916049962873936	0.3436141879031994	0.0781839369704239	T	T	T
0.8086556972616417	0.3517873596987010	0.9842763375351543	T	T	T
0.9107678029902055	0.3264759905494820	0.1040651913759088	T	T	T
0.9059543241039389	0.3580946632398694	0.2974834443114990	T	T	T
0.7668560408218418	0.3712469887341359	0.2379240250718855	T	T	T
0.6650807874426563	0.4514967446622984	0.1869858391542092	T	T	T
0.9205079656378951	0.4531298282001786	0.1595220256601797	T	T	T
0.5670735811803714	0.6284502576043454	0.4224540474282172	T	T	T
0.5882087268372876	0.4974319104025986	0.4359055554577317	T	T	T
0.5910949714449173	0.3635212181611293	0.4369428595936701	T	T	T
0.8007862844391257	0.6277924408539319	0.3788800751288677	T	T	T
0.8103988610249452	0.5090539223860221	0.4582932836397150	T	T	T
0.8229004495534378	0.3766090132680590	0.4404946558122225	T	T	T
0.0198795601481500	0.3689018724059007	0.2006508906217291	T	T	T
0.8554657269309932	0.4381840716049288	0.7891605647454559	T	T	T
0.7946767245085338	0.4295893320359818	0.6140398307264076	T	T	T
0.7012706063197466	0.4322291169066974	0.4690680392920102	T	T	T
0.6049952303343554	0.4307373141198800	0.6059664366765734	T	T	T
0.6034176850355861	0.4478747157156668	0.8023497546746546	T	T	T
0.7294444274978187	0.4797359283782040	0.7708572499860938	T	T	T
0.8615857522292608	0.6806869266814700	0.7498332378342855	T	T	T
0.8101646002371675	0.6645157914683072	0.5697263271891386	T	T	T
0.6901630627669971	0.6460537381066269	0.4889169686815082	T	T	T
0.5863723676045242	0.6730532077936768	0.6073296559040094	T	T	T
0.5965258140273669	0.6544242497109796	0.8029870850915545	T	T	T
0.7228742244110870	0.6383936172222752	0.7480145088351480	T	T	T
0.8295427112535388	0.5474411482650471	0.6801714985205696	T	T	T
0.5787917597184747	0.5505677532413291	0.6791366419242152	T	T	T
0.9316663287087901	0.3787799993691808	0.9235994890266926	T	T	T
0.9158695462176061	0.5116987594331540	0.9324399080183507	T	T	T
0.8928031225428629	0.6429580098873572	0.9367313668923907	T	T	T
0.6973763565949296	0.3739915125214053	0.8851440704126802	T	T	T

Structure files (CONTCAR) involved in this work:

0.6765318308397795	0.4999767357662468	0.9491253281391772	T	T	T
0.6890178606738444	0.6346182418258096	0.9414438727824974	T	T	T
0.4904914196389527	0.4519272807448904	0.7070144465835514	T	T	T
0.4798204314523564	0.6365485522206351	0.7151909200287688	T	T	T
0.6453191373390470	0.9405290402611828	0.2883344884132802	T	T	T
0.7006376575147455	0.9279375092787315	0.1109552076529620	T	T	T
0.8001115652015343	0.9433541827086821	0.9789076578262833	T	T	T
0.8978851449925889	0.9318889361447726	0.1158535691784706	T	T	T
0.8994837944664632	0.9609081959433748	0.3111781837285973	T	T	T
0.7731138044354865	0.9727598833554310	0.2627789301842503	T	T	T
0.6435044761384766	0.1675888664391911	0.2647874848299887	T	T	T
0.6984913040254079	0.1640232218445409	0.0879676217740062	T	T	T
0.8099375549918999	0.1505386187667338	0.9833247067321886	T	T	T
0.9155400970919767	0.1748634909317835	0.0979083714018615	T	T	T
0.8982452028174136	0.1565038946960863	0.2948035923067255	T	T	T
0.7719388176907378	0.1353748907310530	0.2494672700677264	T	T	T
0.6791476946872932	0.0501123806574279	0.1857820824973869	T	T	T
0.9240610307089892	0.0537759517924915	0.1714983956572605	T	T	T
0.5686090758433689	0.8752186519231657	0.4177043970058352	T	T	T
0.5861941040353887	0.0063658201171278	0.4394359567591947	T	T	T
0.5918925145755536	0.1395471636203863	0.4437867248556738	T	T	T
0.8130415176202052	0.8782841024186518	0.3939782290255271	T	T	T
0.8155564356710634	0.0057904968382530	0.4454270732220090	T	T	T
0.8101220279620943	0.1392114070400667	0.4421057071867046	T	T	T
0.0114919000850228	0.9567885814499004	0.2170130496330852	T	T	T
0.0177797670519113	0.1433317715405806	0.2146993879638771	T	T	T
0.8580649939217072	0.0516803596949473	0.7855389717860530	T	T	T
0.7995793126523620	0.0719939478155098	0.6124559351787568	T	T	T
0.7007875913637293	0.0674164496181058	0.4777466998793738	T	T	T
0.6023076569962300	0.0724955521518598	0.6113930736769446	T	T	T
0.6033897150742338	0.0531763248617733	0.8086125567264032	T	T	T
0.7292039744883827	0.0284400764382056	0.7671317252262519	T	T	T
0.8556845105627351	0.8337719908200816	0.7744746381319759	T	T	T
0.8120220873630847	0.8226952251407219	0.5951381980892410	T	T	T
0.6880464010943964	0.8587309777600769	0.5032029092372604	T	T	T
0.5772336115575191	0.8302915180166366	0.6047967119883638	T	T	T
0.6005880989804024	0.8470348965587623	0.7997832977658831	T	T	T
0.7268066923433960	0.8556930503553474	0.7433545638618740	T	T	T
0.8152017876095956	0.9459458945993399	0.6798352487860249	T	T	T
0.5775297591228982	0.9523254781911228	0.6830609585171366	T	T	T
0.9302381094911516	0.1250680207142537	0.9122477556137099	T	T	T
0.9195432421290390	0.9935086120565177	0.9405618020456546	T	T	T
0.9043425156626792	0.8614669578198345	0.9536963495939584	T	T	T
0.6946784456513464	0.1273438764150834	0.8949128139939824	T	T	T
0.6822204917184493	0.9991950746206595	0.9471021061749739	T	T	T
0.6958833294807478	0.8656286330718741	0.9369710306711109	T	T	T
0.4897815969147675	0.0512290134758988	0.7153750550210342	T	T	T
0.4793138201351614	0.8666173400656917	0.7249843352418492	T	T	T
0.3606970524428289	0.4306324200011719	0.7204977990089548	T	T	T
0.3156743668979728	0.4494194744131214	0.9042277415860603	T	T	T
0.2005614010759647	0.4606585242018298	0.0013640881906740	T	T	T
0.0889256516104528	0.4384798302201736	0.9007821323442906	T	T	T
0.1024834897918959	0.4287234303022244	0.7039981384748316	T	T	T

Structure files (CONTCAR) involved in this work:

0.2299113591699759	0.4366385496247568	0.7564382662896323	T	T	T
0.3535156050942448	0.6698928095299029	0.7479108009554213	T	T	T
0.2908784070639838	0.6349727330614675	0.9119643214264420	T	T	T
0.1888407333714760	0.6541842389549282	0.0320855370004315	T	T	T
0.0924226788090317	0.6595623086335758	0.8962271883125371	T	T	T
0.0942572299773302	0.6683752518803784	0.6998703946865448	T	T	T
0.2215712892174228	0.6488582923386572	0.7452539823931482	T	T	T
0.3053619164977760	0.5466740981513623	0.7659226411635798	T	T	T
0.0842111600667470	0.5479518248059482	0.7862327029071176	T	T	T
0.4317531682464272	0.3772564779541148	0.5714925330357192	T	T	T
0.4101607212892359	0.5082734504368425	0.5743304488891541	T	T	T
0.3924542378756338	0.6403234449635926	0.5640379484160982	T	T	T
0.1909000918363963	0.3545284560986491	0.6093517118601943	T	T	T
0.1901686258689798	0.4860766041137556	0.5813765386023784	T	T	T
0.1773076300026320	0.6174743694489853	0.5627244854501418	T	T	T
0.9848701873371795	0.4578152138717753	0.7834821191160006	T	T	T
0.9823888114645727	0.6332886009825620	0.7906722406633139	T	T	T
0.1340291832576955	0.5678973608359721	0.2278534561179279	T	T	T
0.1853296509288453	0.5415152618661117	0.4037304267421712	T	T	T
0.2928954290609243	0.5575583837081575	0.5183375301278310	T	T	T
0.3984319852879649	0.5702533320020290	0.4003053576419711	T	T	T
0.3950001723747744	0.5659652478384083	0.2039531604450927	T	T	T
0.2661305477640059	0.5618788882601193	0.2504164651771837	T	T	T
0.1397029662927362	0.3295661720930366	0.2481238893762849	T	T	T
0.1966546304028438	0.3699411177062961	0.4140741871908256	T	T	T
0.3082912534251961	0.3539746959226946	0.5156205475715898	T	T	T
0.4076885447097360	0.3317665185822133	0.3868849893292732	T	T	T
0.3954607729769792	0.3486075158755652	0.1903825277007683	T	T	T
0.2715268516484205	0.3427700786052424	0.2552787288113122	T	T	T
0.1927508570144333	0.4509219674877387	0.2563381149535868	T	T	T
0.4134538057130426	0.4535259561712605	0.3097584035919627	T	T	T
0.0643114833111926	0.6271485938885412	0.0835302745009154	T	T	T
0.0826209067737042	0.4955797260785426	0.0775666617414522	T	T	T
0.1144980346376921	0.3665955021206256	0.0599333947898254	T	T	T
0.3103631159417034	0.6413995525890909	0.1053097199311796	T	T	T
0.3109377125956231	0.5075820066831589	0.0808871693378278	T	T	T
0.2946834848521584	0.3749894726148512	0.0643129722483241	T	T	T
0.5088414987342708	0.5459230534535383	0.2942796483077567	T	T	T
0.5128217448196172	0.3660912753265594	0.2763791190626123	T	T	T
0.4326939301795582	0.7527293182916277	0.6476221314921227	T	T	T
0.1823405511549862	0.7457107956972522	0.6141507464865558	T	T	T
0.2792113822762572	0.7523305389474031	0.0065054887307862	T	T	T
0.0972537692123377	0.7508693781607750	0.0397832152345404	T	T	T
0.0669409716696343	0.2527201169969589	0.1286452962677757	T	T	T
0.3152836280369268	0.2514033850159333	0.1245959169035303	T	T	T
0.2231674638970796	0.2512794531357140	0.4951446217652819	T	T	T
0.3930096767416507	0.2519748942472641	0.5423783335498686	T	T	T
0.5569298023954949	0.2501704818573258	0.3518918365748483	T	T	T
0.8084594706611976	0.2505419787878965	0.3370326684681211	T	T	T
0.7249299565804800	0.2509352671833250	0.9433582737455931	T	T	T
0.8938807495290066	0.2515776307987583	0.9424188288028874	T	T	T
0.9459752033596835	0.7530806769591182	0.8574029614985663	T	T	T
0.6863093819367740	0.7493371826991959	0.8470176642315206	T	T	T

Structure files (CONTCAR) involved in this work:

0.7694701595903694	0.7493249345720100	0.4302540596560352	T	T	T
0.6104842598023308	0.7526321422789906	0.4543328922183316	T	T	T
0.9522137799436056	0.4715237219204499	0.5059290600391917	T	T	T
0.9646874616402740	0.7262316855355646	0.5789816234321399	T	T	T
0.9346992118704145	0.3937937424745134	0.4347420447018154	T	T	T
0.8914103752529301	0.5286684630845366	0.5682882843791909	T	T	T
0.8766973805240671	0.7457828548889838	0.6020330998459885	T	T	T
0.0341236533612220	0.7615170932564701	0.6437420334658415	T	T	T
0.9750480622441362	0.5547755315131385	0.5053293637570128	T	T	T
0.9673304626499977	0.5929467070631955	0.5233020987684562	T	T	T
0.0549039811583482	0.3535803910855496	0.4504664043079740	T	T	T
0.0100748951569088	0.3364728667667881	0.5668626353446696	T	T	T
0.9950040452692357	0.2832528653548722	0.4556096884617540	T	T	T
0.0101840637246107	0.3322178349556763	0.4854629913387368	T	T	T

Figure S12(a)

Si Al O Zn H C

1.0000000000000000		
20.0219999999999985	0.0000000000000000	0.0000000000000000
0.0000000000000000	19.8990000000000009	0.0000000000000000
0.0000000000000000	0.0000000000000000	13.3829999999999991
93	3	193
2	7	2

Selective dynamics

Direct

0.4230114341656075	0.0597070502721438	0.6484133753108697	T	T	T
0.3059182995586900	0.0316456076637529	0.7930111993076411	T	T	T
0.2826259140908105	0.0562486430377520	0.0172227649769738	T	T	T
0.1237284887142275	0.0615076950708991	0.0119683190752113	T	T	T
0.0685774191216119	0.0307790851916824	0.8006637586555602	T	T	T
0.1811553027024703	0.0641495440155324	0.6654284438208604	T	T	T
0.4187829167223883	0.8263590335251608	0.6676357943364536	T	T	T
0.3013397158330419	0.8724482329952060	0.8005730891625608	T	T	T
0.2671778690430208	0.8300672300763428	0.0199365180607289	T	T	T
0.1118961731806480	0.8267154670501320	0.0115939375282402	T	T	T
0.0665286523445335	0.8743487323629283	0.7974459649839355	T	T	T
0.1796808228458157	0.8285063285056591	0.6644522863812949	T	T	T
0.0759707763434043	0.9400979607628875	0.1489328578680149	T	T	T
0.1951482846426329	0.9693023806527329	0.2902595922383829	T	T	T
0.2169408024466144	0.9431570777815513	0.5160975678897907	T	T	T
0.3773915908021142	0.9352270670479710	0.5132770686080893	T	T	T
0.4338662900572869	0.9683536283395238	0.3010508045036063	T	T	T
0.3207261926236206	0.9353199806309965	0.1641222835611908	T	T	T
0.0829382924930432	0.1710850475640966	0.1662669082159890	T	T	T
0.1981045502921533	0.1278693985788999	0.3024994810957291	T	T	T
0.2324705175731546	0.1684725333472443	0.5193350403878433	T	T	T
0.3878854072824773	0.1732715568175021	0.5086130291510323	T	T	T
0.4354173812726996	0.1268836032957976	0.2946359434618946	T	T	T
0.3181689507763975	0.1723214107546495	0.1671553215372965	T	T	T
0.5785294039130003	0.5560185477339457	0.3536814438946844	T	T	T
0.6923819038646083	0.5256206646538624	0.2043356036682616	T	T	T
0.7189909876727701	0.5671851246920802	0.9860149359139800	T	T	T
0.8772517442963932	0.5734452555356353	0.9853715343677306	T	T	T
0.8131730913697880	0.5483629571555433	0.3488275197823259	T	T	T
0.5748111121441544	0.3281718946774420	0.3305119210307043	T	T	T

Structure files (CONTCAR) involved in this work:

0.6929133578032435	0.3720760978635626	0.1881944237211953	T	T	T
0.7318785589647462	0.3270988694643759	0.9763216240352556	T	T	T
0.8867591787697832	0.3238818099355968	0.9919996875410865	T	T	T
0.9435441850954857	0.3708268751997733	0.1892884513630701	T	T	T
0.9211256527747417	0.4447161398571873	0.8623328880948939	T	T	T
0.8030454165471269	0.4715521844612406	0.7184558670993051	T	T	T
0.7799785851390765	0.4346402231624475	0.4976613238890219	T	T	T
0.6204162298914716	0.4293011671279086	0.4897301714012799	T	T	T
0.5691914304242532	0.4687564337321429	0.7024367452281078	T	T	T
0.6790906487015710	0.4473774503285887	0.8525766919275831	T	T	T
0.9222018876325777	0.6780859384297363	0.8285407183574183	T	T	T
0.7706889650960048	0.6682953163150182	0.4663844712468421	T	T	T
0.6154623754894611	0.6725740687671086	0.4881973408358470	T	T	T
0.5617652451980583	0.6269955968626090	0.6982531168351322	T	T	T
0.6737281382746221	0.6714977523752350	0.8285050947464987	T	T	T
0.5785836981840307	0.9443089289113750	0.3579588567769357	T	T	T
0.6983595671201377	0.9720997135553633	0.2132457498986751	T	T	T
0.7201178184622361	0.9353562617498699	0.9923850979903901	T	T	T
0.8800969264043790	0.9328368143229026	0.9943476340160173	T	T	T
0.9311015596031113	0.9701881237345349	0.2043861347708296	T	T	T
0.8219841949478816	0.9460877654438604	0.3544965386287935	T	T	T
0.5782010678511181	0.1728381432113054	0.3296949700318594	T	T	T
0.6982653468122232	0.1294645404183759	0.1933150817558687	T	T	T
0.7322978682871311	0.1707644221013024	0.9724312968640334	T	T	T
0.8869859635655789	0.1722727779916252	0.9813517939628742	T	T	T
0.9358456648753526	0.1281544731469453	0.1953739049071969	T	T	T
0.8203685536529612	0.1714291785272583	0.3289187818000809	T	T	T
0.9235676299000818	0.0529453986961454	0.8551789670000047	T	T	T
0.8018711548666809	0.0257737487995091	0.7091099897614077	T	T	T
0.7814796075705013	0.0660328826227743	0.4914036972180090	T	T	T
0.6209619012820938	0.0694891936162864	0.4901618468336900	T	T	T
0.5683558835260656	0.0308144406820831	0.6993071308206875	T	T	T
0.6784625312881497	0.0522042363752486	0.8503281826312884	T	T	T
0.9243523564999688	0.8307929188942674	0.8357316123402171	T	T	T
0.8029453939187009	0.8685485476870056	0.6945836955514503	T	T	T
0.7705431269699275	0.8257547325475143	0.4776011453144952	T	T	T
0.6155525117560355	0.8260275453193874	0.4898818753650243	T	T	T
0.5638482687923757	0.8734252622675117	0.6979381168823373	T	T	T
0.6791098298256093	0.8309221051041984	0.8318037264781579	T	T	T
0.4233788921005350	0.4412939061478875	0.6482406319109671	T	T	T
0.3044777296861784	0.4694261325048927	0.7904606223668641	T	T	T
0.2791679090869185	0.4453211223798481	0.0170704017676826	T	T	T
0.1208001509016904	0.4375549185372234	0.0166307439712038	T	T	T
0.0641065218648732	0.4684651595368816	0.8020021224106006	T	T	T
0.1775144546865251	0.4351732900743306	0.6638602484234429	T	T	T
0.4158831218340988	0.6726733413309062	0.6670679573015920	T	T	T
0.3020422003110673	0.6281140565607948	0.8037213503195052	T	T	T
0.2668969869340240	0.6686050314745412	0.0211327884100321	T	T	T
0.1119889552576991	0.6725209099836645	0.0077554041165234	T	T	T
0.0632521224643186	0.6273192560335917	0.7932047846403336	T	T	T
0.1816089861950152	0.6715187573445733	0.6664325657695779	T	T	T
0.0785097512313940	0.5599125146224677	0.1496689105058606	T	T	T
0.1959981725308064	0.5286765176461709	0.2922135734358665	T	T	T

Structure files (CONTCAR) involved in this work:

0.2155155968354223	0.5549566963790202	0.5176600089588244	T	T	T
0.3739913071164149	0.5639068189077897	0.5155175046817700	T	T	T
0.4305406047638674	0.5314776654561437	0.3046522896824903	T	T	T
0.3204219074542656	0.5634585549493643	0.1648184623745232	T	T	T
0.0870125838491093	0.3232329631081828	0.1635545994176865	T	T	T
0.1990211186332716	0.3706232801152840	0.3021722150848550	T	T	T
0.2306653277828214	0.3298851086729377	0.5198422716746839	T	T	T
0.3856710340089471	0.3275825351012668	0.5077235319665099	T	T	T
0.4319557836204018	0.3740315219240007	0.2943637739462743	T	T	T
0.3175319976722498	0.3298467628949074	0.1652248551589122	T	T	T
0.9240842712699818	0.5270483424208455	0.1936653239206366	T	T	T
0.8192483213256192	0.3330711478933311	0.3224572151964715	T	T	T
0.7997527892541724	0.6338803835764375	0.6956368065001096	T	T	T
0.0110610861852885	0.5573714710568393	0.2268270568622245	T	T	T
0.3594650910194075	0.0702186182735298	0.7223530460629891	T	T	T
0.3175386496278589	0.0550198518116405	0.9077388532132252	T	T	T
0.2028089320680674	0.0449839267505697	0.0059670956674682	T	T	T
0.0925904892675332	0.0694434259145846	0.9011467502273035	T	T	T
0.1043249937092112	0.0646751831717721	0.7040582210492027	T	T	T
0.2300269759246766	0.0509877535387027	0.7607541424877859	T	T	T
0.3594510667892212	0.8272361482274854	0.7502052817218627	T	T	T
0.3019187514331401	0.8588156582963169	0.9195017725969479	T	T	T
0.1889215689214776	0.8520898726702391	0.0213095998656261	T	T	T
0.0878889564888196	0.8323570451488700	0.8965489078148139	T	T	T
0.1028074830244897	0.8403221146701095	0.7007368170386677	T	T	T
0.2286921693567653	0.8516768820993018	0.7555887085074848	T	T	T
0.3169868456377675	0.9511119364444153	0.7785829173430392	T	T	T
0.0905224058266818	0.9520167670301861	0.8090616064269167	T	T	T
0.4334500612921400	0.1272940049890059	0.5818322989434171	T	T	T
0.4124296240530109	0.9962059938687783	0.5740166771555103	T	T	T
0.3939740745252781	0.8640061534255949	0.5666166381716577	T	T	T
0.1976405213061643	0.1374061465318804	0.6182338740597532	T	T	T
0.1899734698973878	0.0051834886961068	0.5829498865955787	T	T	T
0.1946290557642950	0.8715476539286039	0.5640031552347202	T	T	T
0.9885311970469747	0.0381729528791543	0.7859682537232657	T	T	T
0.9859473231711906	0.8717996230545282	0.7835074481126633	T	T	T
0.1403028565872213	0.9309888342341498	0.2216572357083494	T	T	T
0.1836271067703435	0.9486719443748278	0.4059685052789055	T	T	T
0.2975078953499419	0.9478096921423078	0.5089344408911005	T	T	T
0.4074766636505934	0.9314964306131716	0.4015583706877874	T	T	T
0.3969735510282148	0.9351767149168170	0.2048614588711318	T	T	T
0.2702502915648532	0.9474960448896445	0.2578856166535198	T	T	T
0.1388374968266858	0.1723315426572319	0.2539904230594635	T	T	T
0.1951126474657146	0.1370932896209504	0.4224452993215802	T	T	T
0.3108256510871564	0.1473311795521272	0.5150996075341460	T	T	T
0.4138672632266045	0.1680541338073318	0.3943836879032335	T	T	T
0.3954287283161396	0.1581813248203907	0.1991895476926027	T	T	T
0.2706445346631868	0.1529443310111957	0.2620526963082701	T	T	T
0.1859705291558277	0.0496840956485000	0.2726828169254988	T	T	T
0.4160575422168101	0.0480741574162745	0.3076361604016896	T	T	T
0.0652577973215237	0.8712176076134287	0.0852933381080096	T	T	T
0.0858552240319766	0.0011746363454998	0.0701655330728712	T	T	T
0.1117349478309609	0.1318262656778507	0.0695281465555225	T	T	T

Structure files (CONTCAR) involved in this work:

0.3053595401556639	0.8623041753323084	0.1151344525698526	T	T	T
0.3128599999502006	0.9949057522060839	0.0824604291043776	T	T	T
0.2982330293316341	0.1281690605924342	0.0696437707347205	T	T	T
0.5134537476020198	0.9560439855945649	0.2878404390374772	T	T	T
0.5154062515164139	0.1343080152844038	0.2767626224197676	T	T	T
0.6372517058734564	0.5644722513224208	0.2716006750624362	T	T	T
0.7074013935195242	0.5708349589673792	0.1061473107409300	T	T	T
0.7981072096152271	0.5626628947808979	0.9591106139972759	T	T	T
0.8910455476864968	0.5779195822345421	0.1033021088887622	T	T	T
0.8873680265162822	0.5322117675622355	0.3109261927771871	T	T	T
0.7597668042382241	0.5183071207351195	0.2713931279547790	T	T	T
0.6389246291833549	0.3333381245715158	0.2583760374393886	T	T	T
0.6893711748537474	0.3373545099931641	0.0780050613719499	T	T	T
0.8094859603982035	0.3492985342047161	0.9942614869134306	T	T	T
0.9159204253967413	0.3186165515089333	0.1053926889585727	T	T	T
0.9048461186449730	0.3552336588411581	0.2954034874222929	T	T	T
0.7663866775858026	0.3672213888399382	0.2349457027868379	T	T	T
0.6680801389491922	0.4503432136426153	0.1762228484262262	T	T	T
0.9330515766652763	0.4464295782108951	0.1528666276213426	T	T	T
0.5704376415159654	0.6259752750412561	0.4149387791379996	T	T	T
0.5937258180719974	0.4963772835771006	0.4335909426333385	T	T	T
0.5888041219943057	0.3627053313910011	0.4390074702287368	T	T	T
0.8011787010496153	0.6281473147291208	0.3700925615360028	T	T	T
0.8042939897981198	0.5114535186781368	0.4611189041027403	T	T	T
0.8229114953620199	0.3806691191779454	0.4352731017856587	T	T	T
0.0224664518606547	0.3586243139008893	0.2137118758754672	T	T	T
0.8546297693483615	0.4351430022345346	0.7937656277944900	T	T	T
0.8010475033683623	0.4289711460757974	0.6143320274906900	T	T	T
0.7012820939545888	0.4264567676845929	0.4783366128213453	T	T	T
0.6007519580389750	0.4294043927368299	0.6068334858537618	T	T	T
0.6045608614657085	0.4439420265227372	0.8051771974065683	T	T	T
0.7289093127603986	0.4749724648258047	0.7650504224227698	T	T	T
0.8595508630918444	0.6799429879935853	0.7551707296364278	T	T	T
0.8152622243822287	0.6449737066413359	0.5637314222474464	T	T	T
0.6931270679583157	0.6469174898157328	0.4855576918065189	T	T	T
0.5872847059887660	0.6685938910280266	0.6011238176725038	T	T	T
0.5952349792681991	0.6587153414937276	0.7982390783193205	T	T	T
0.7201062262967406	0.6438049613493558	0.7389727480990114	T	T	T
0.8283553410238776	0.5477162016639222	0.6909421085380378	T	T	T
0.5816485818145882	0.5484381833940216	0.6850221973094278	T	T	T
0.9313228516162431	0.3763005057463862	0.9269194227533913	T	T	T
0.9165994105496624	0.5098015330068830	0.9344154935701666	T	T	T
0.9046808014250769	0.6421898868271175	0.9345842228979009	T	T	T
0.7007420885013205	0.3725671559085343	0.8870068876496422	T	T	T
0.6814407882402485	0.4995087821220430	0.9457405593464948	T	T	T
0.6875749244552306	0.6337898829582235	0.9348480144293749	T	T	T
0.4903661375519882	0.4513019525414385	0.7143311809503847	T	T	T
0.4809758310208287	0.6323278391248969	0.7069890740833090	T	T	T
0.6437294053589954	0.9384026493994251	0.2870126293818739	T	T	T
0.6998291250100158	0.9300401114577856	0.1094158148310211	T	T	T
0.8004536542148668	0.9435040429888034	0.9786803609468337	T	T	T
0.8986460479548823	0.9280767933881804	0.1120917298119504	T	T	T
0.8973051692317144	0.9482953819958958	0.3096359889689900	T	T	T

Structure files (CONTCAR) involved in this work:

0.7713428274158816	0.9676590633310147	0.2652982849601888	T	T	T
0.6419919059864055	0.1703525921068083	0.2556054674813451	T	T	T
0.6975520858035482	0.1585035529698403	0.0802976531404604	T	T	T
0.8099217709781295	0.1461499187005717	0.9771401283230347	T	T	T
0.9135720771150583	0.1682334711583047	0.0953500974294492	T	T	T
0.8974660473144132	0.1580573498863189	0.2922984264527692	T	T	T
0.7715051187309133	0.1388440362560376	0.2431710432345599	T	T	T
0.6788914727516854	0.0500330944749689	0.1922528818868598	T	T	T
0.9184694278922304	0.0491331254142785	0.1813661739688918	T	T	T
0.5702166556644206	0.8743202569715011	0.4196135933012923	T	T	T
0.5840957592539626	0.0058234447986376	0.4375402428449335	T	T	T
0.5964371746316888	0.1384279682828510	0.4366019030944276	T	T	T
0.8081653530780442	0.8700155234051284	0.3932339353981296	T	T	T
0.8153229018156257	0.9976592576778113	0.4477956023792331	T	T	T
0.8091880746571440	0.1318949355716406	0.4344810375871287	T	T	T
0.0102710382212321	0.9539416099815800	0.2162028469391884	T	T	T
0.0159927403702404	0.1366268183588822	0.2112270104582969	T	T	T
0.8580030819344722	0.0544972022184180	0.7847919895359942	T	T	T
0.8010824111923102	0.0718750848054195	0.6090060634158886	T	T	T
0.7009282866233888	0.0602675660274651	0.4775887398046178	T	T	T
0.6001800470284778	0.0738673270848061	0.6073322862695438	T	T	T
0.6034338915044373	0.0502424033878286	0.8046235943694693	T	T	T
0.7292359831258273	0.0287973243067980	0.7623215313718132	T	T	T
0.8600809206239731	0.8349281049023944	0.7631641804834303	T	T	T
0.8060613354477482	0.8322580273850095	0.5860570744212302	T	T	T
0.6932018524272261	0.8507017032829999	0.4859259870853116	T	T	T
0.5887388975921318	0.8279826474884585	0.6041645499011351	T	T	T
0.6031459725541751	0.8503987391353499	0.7984850843038654	T	T	T
0.7297329688024580	0.8573236527261244	0.7445068200116642	T	T	T
0.8178003637656511	0.9481549562419940	0.6802112120194698	T	T	T
0.5790876684355389	0.9517332392403942	0.6730748164173326	T	T	T
0.9325274427947475	0.1258728420951916	0.9084015160579983	T	T	T
0.9184599981212664	0.9958995749136097	0.9421998561878843	T	T	T
0.9051957614809705	0.8631957831551627	0.9436181959446839	T	T	T
0.6938404817249667	0.1283328404131335	0.8865704315617494	T	T	T
0.6838052315161101	0.0011992339044057	0.9448955677495825	T	T	T
0.6957638824950898	0.8670093077701099	0.9376674773600527	T	T	T
0.4895963583648803	0.0473490062717012	0.7144513522603182	T	T	T
0.4841792344857423	0.8626360998315167	0.7153185150298995	T	T	T
0.3599330441896439	0.4311434108381987	0.7228222409599868	T	T	T
0.3112801796082904	0.4457368427424555	0.9058943993891396	T	T	T
0.1989056964724129	0.4595891554973033	0.0135036398439975	T	T	T
0.0896893722970905	0.4351185729637446	0.9058306055019745	T	T	T
0.1022188308822500	0.4333087021631183	0.7084927049932029	T	T	T
0.2294062129272954	0.4506192462989208	0.7542563274657619	T	T	T
0.3604991234175263	0.6739253347016098	0.7556953198197043	T	T	T
0.3038328656565494	0.6379850908205583	0.9235683929637297	T	T	T
0.1886444539895923	0.6462255091008102	0.0170156918783238	T	T	T
0.0861196379045372	0.6667298564295812	0.8941299849368807	T	T	T
0.1045825534321771	0.6579972519317929	0.6990717457962113	T	T	T
0.2294762493969147	0.6508842420842674	0.7603180795530688	T	T	T
0.3163261068284081	0.5497989759249515	0.7769538114427839	T	T	T
0.0812467115996997	0.5481469924584410	0.8051884753223927	T	T	T

Structure files (CONTCAR) involved in this work:

0.4318622024970789	0.3750355774403955	0.5780954825923349	T	T	T
0.4144205842965227	0.5064062582606249	0.5762278160311879	T	T	T
0.3837173284839861	0.6363889222700415	0.5691005019068017	T	T	T
0.1934922008083695	0.3618821183323719	0.6163457183670769	T	T	T
0.1817119639850821	0.4939141967621047	0.5797452492761666	T	T	T
0.1995432272618773	0.6272570930823814	0.5679312426702680	T	T	T
0.9848405214252794	0.4542903885499242	0.7876396173250491	T	T	T
0.9840819785206629	0.6375117117147641	0.7744083775810477	T	T	T
0.1434394493051034	0.5686581838105303	0.2201918738171527	T	T	T
0.1832961485904858	0.5537748565611419	0.4057530239067795	T	T	T
0.2955082240135499	0.5430706992419192	0.5117887824987305	T	T	T
0.4034118328233662	0.5700895650418081	0.4033720130006577	T	T	T
0.3964619365459633	0.5648891668208006	0.2060414199281329	T	T	T
0.2715405565479729	0.5467270211354744	0.2593319077807126	T	T	T
0.1457704466613637	0.3224100420911371	0.2469011993689986	T	T	T
0.1936586444440508	0.3595023646115910	0.4213173153609104	T	T	T
0.3085344965499925	0.3529809693359423	0.5181794364602986	T	T	T
0.4087558971056584	0.3310994563548346	0.3917476049914667	T	T	T
0.3949203715202994	0.3455121679921982	0.1943744624596405	T	T	T
0.2734008457284198	0.3515935193682294	0.2629398903894704	T	T	T
0.1814631263654942	0.4489498500694932	0.2775434208039143	T	T	T
0.4112542212827562	0.4521819916729479	0.3122886229929711	T	T	T
0.0666488560836377	0.6255673009590803	0.0813804092078997	T	T	T
0.0790772073910595	0.4920678764541405	0.0845560808736217	T	T	T
0.1125199429159070	0.3636488430050884	0.0650717857476406	T	T	T
0.3017001592490181	0.6368197959913284	0.1198551782882617	T	T	T
0.3133986202412224	0.5054886371433427	0.0804443643260868	T	T	T
0.2940253595885750	0.3727558908265750	0.0679965373141029	T	T	T
0.5102825043116044	0.5402743451070275	0.2935423417176889	T	T	T
0.5117626421981047	0.3661137296161429	0.2776724683929920	T	T	T
0.4357946925922148	0.7491412892456004	0.6380557673375170	T	T	T
0.1920615887765068	0.7499250121598009	0.6374518517898881	T	T	T
0.2740022873166830	0.7492194845630121	0.0251232001337880	T	T	T
0.1057665892666516	0.7489809830738129	0.0471119849175531	T	T	T
0.0685509862952381	0.2475154368859284	0.1302251530843608	T	T	T
0.3079224255131126	0.2510068180441088	0.1385622160569681	T	T	T
0.2240503807931851	0.2492086885811865	0.5227400755300342	T	T	T
0.3927417747112094	0.2506395657303605	0.5459564531693906	T	T	T
0.5570357285891563	0.2500496941005251	0.3512321014340833	T	T	T
0.8066296025480958	0.2495452806655024	0.3445341273576245	T	T	T
0.7277088076564566	0.2492748496400489	0.9411030406589496	T	T	T
0.8920004668055296	0.2495270982193688	0.9423526148337386	T	T	T
0.9476545748400171	0.7540072555596835	0.8540914048622981	T	T	T
0.6861165808299691	0.7510353505972833	0.8480581187069209	T	T	T
0.7758841821888621	0.7476775573835966	0.4430577573502527	T	T	T
0.6103509045786262	0.7494825512890728	0.4486967674522566	T	T	T
0.9628536047020033	0.5383825960227474	0.5170261305081971	T	T	T
0.9280094204127544	0.4135924257351145	0.4132822507479008	T	T	T
0.8794886330928242	0.5621533396901411	0.5614078663355951	T	T	T
0.0496465517347801	0.6627804728524740	0.5094756225493242	T	T	T
0.0337727443232807	0.4714050099009484	0.4702927296282091	T	T	T
-0.0127208759459282	0.4434120655346269	0.5754082887590364	T	T	T
-0.0040017566103006	0.5791534584107906	0.3794555027290611	T	T	T

Structure files (CONTCAR) involved in this work:

0.9790122125589270	0.6478113232671533	0.2943068659589664	T	T	T
0.0638904237157549	0.6239906827405065	0.3211348616598083	T	T	T
0.0618261751983786	0.6928884661147753	0.4807091159789444	T	T	T
-0.0167235746620892	0.4707163303839845	0.5038750275815626	T	T	T
0.0126332398324275	0.6060117294465684	0.3122368901647176	T	T	T

Figure S12(b) IS

Si Al O Zn H C

1.0000000000000000

20.0219999999999985 0.0000000000000000 0.0000000000000000

0.0000000000000000 19.8990000000000009 0.0000000000000000

0.0000000000000000 0.0000000000000000 13.3829999999999991

93 3 193 2 7 2

Selective dynamics

Direct

0.4222067175631574	0.0602533794655352	0.6483057002513969	T	T	T
0.3049194054487585	0.0320196651881667	0.7923139190313880	T	T	T
0.2820111566058360	0.0564380017233989	0.0169412806390379	T	T	T
0.1226593436530254	0.0622794242341283	0.0115847650518041	T	T	T
0.0678555588360534	0.0313746096418582	0.8004515024649252	T	T	T
0.1802768422558360	0.0647350103349935	0.6647362852250699	T	T	T
0.4184716993746637	0.8274208800564982	0.6688622981400412	T	T	T
0.3008164388820078	0.8730342137516161	0.8011233884922979	T	T	T
0.2668551518103774	0.8303557916462204	0.0204160664997467	T	T	T
0.1109210763363140	0.8265823546277674	0.0131555578574450	T	T	T
0.0660723767465495	0.8747830469223347	0.7987999398880240	T	T	T
0.1791164908128816	0.8289393591589982	0.6650858617615530	T	T	T
0.0754798738540452	0.9408990725152949	0.1487362697017846	T	T	T
0.1945769891542780	0.9700031639585456	0.2903714239817343	T	T	T
0.2165073939849809	0.9435689460208929	0.5160059994155543	T	T	T
0.3768714988356281	0.9355951450606741	0.5135720772921690	T	T	T
0.4331598926523171	0.9687570027030412	0.3014359615934468	T	T	T
0.3200153388722137	0.9356225470731749	0.1642583255118815	T	T	T
0.0817062361875334	0.1723101121846436	0.1665924326307036	T	T	T
0.1977067775430061	0.1287225033467225	0.3017866244853402	T	T	T
0.2314314437537468	0.1694066256382821	0.5191445012075137	T	T	T
0.3868776802445141	0.1738835126396178	0.5088888819987962	T	T	T
0.4347948207539715	0.1271513229079912	0.2955411276149876	T	T	T
0.3183416828671587	0.1724157476464499	0.1665661574124447	T	T	T
0.5780928075841857	0.5556818837067566	0.3563941200628010	T	T	T
0.6906781535892274	0.5274202976998063	0.2035119606534775	T	T	T
0.7157943517034024	0.5684601612788691	0.9870052970530165	T	T	T
0.8747407782785186	0.5735570389041030	0.9866723241268304	T	T	T
0.8114981521000315	0.5514854980222323	0.3457711076131131	T	T	T
0.5729325474488974	0.3293441528687356	0.3328414747455128	T	T	T
0.6935938216582115	0.3735531470176158	0.1946276803067736	T	T	T
0.7319639054591807	0.3280152962382016	0.9802536562596164	T	T	T
0.8869488558896290	0.3254195584271908	0.9888858317855836	T	T	T
0.9423064756849563	0.3719715712821995	0.1881554369793852	T	T	T
0.9202988600005245	0.4466265262020760	0.8599995100829678	T	T	T
0.7998376700967638	0.4746363608910410	0.7203450673537209	T	T	T
0.7795654065543145	0.4371812818127015	0.4962023723329531	T	T	T
0.6220819224696574	0.4288389104982129	0.4902946601778969	T	T	T
0.5701756915829610	0.4693690971790422	0.7021163330224420	T	T	T

Structure files (CONTCAR) involved in this work:

0.6760334851530608	0.4477350491715867	0.8572698551355867	T	T	T
0.9206490658948759	0.6790561635065542	0.8297774645631726	T	T	T
0.7672563458492908	0.6704768766663681	0.4649875127868227	T	T	T
0.6125146642382084	0.6735802189961895	0.4882848346241643	T	T	T
0.5601051998105446	0.6277283323416871	0.6990176216013091	T	T	T
0.6710610833790533	0.6748701001543861	0.8294103908813021	T	T	T
0.5776024199572557	0.9458077027835238	0.3581603309536684	T	T	T
0.6981664616598516	0.9748372830144058	0.2154518250354783	T	T	T
0.7192969399033059	0.9390489068782201	0.9934783252260251	T	T	T
0.8792246478619974	0.9347236721152464	0.9949028970255861	T	T	T
0.9308364313244432	0.9719012437796146	0.2051091900400352	T	T	T
0.8221440693665535	0.9471072957352346	0.3549702544220709	T	T	T
0.5776817385174376	0.1744088142276372	0.3297086769005257	T	T	T
0.6974342737596839	0.1330522044919646	0.1938231748555559	T	T	T
0.7323119789852895	0.1717624327779996	0.9721999282587738	T	T	T
0.8869222966478209	0.1735506415737052	0.9819488761424030	T	T	T
0.9347694376494468	0.1303905673186885	0.1974820439903701	T	T	T
0.8192414876170951	0.1752727694522518	0.3321145018086580	T	T	T
0.9231913309710531	0.0540398316626656	0.8554683548126937	T	T	T
0.8015090724046787	0.0261136104612232	0.7098271521640240	T	T	T
0.7809121000606102	0.0661443145990738	0.4921184782096636	T	T	T
0.6206822313667101	0.0701742488205254	0.4900057180223962	T	T	T
0.5676295369262204	0.0327234750100606	0.6988974928608588	T	T	T
0.6781348615172732	0.0544346367472568	0.8494687243394322	T	T	T
0.9233533971558388	0.8312674304534857	0.8372139823721455	T	T	T
0.8024317310410151	0.8685758795216637	0.6955505111764402	T	T	T
0.7687360530657464	0.8275433648697681	0.4779236488763970	T	T	T
0.6138449362933338	0.8273415341693384	0.4901756038784644	T	T	T
0.5632180506450861	0.8755434598390062	0.6981787360655297	T	T	T
0.6779219094079896	0.8333514068260038	0.8340604875893550	T	T	T
0.4234238645933638	0.4419376307391308	0.6452257599939152	T	T	T
0.3049229124806316	0.4694230006556326	0.7884723277160987	T	T	T
0.2795405473627597	0.4455733467388659	0.0150560462272199	T	T	T
0.1216926927790067	0.4375696999235209	0.0154337693874267	T	T	T
0.0641757239161369	0.4700738036590759	0.8021843006386733	T	T	T
0.1771829877658224	0.4362703130670341	0.6625078097895825	T	T	T
0.4150382498790786	0.6735914407980577	0.6665146346976567	T	T	T
0.3003927755156314	0.6278684463408438	0.8007477398255406	T	T	T
0.2668960574356557	0.6690118817338051	0.0197193451773274	T	T	T
0.1114185059151549	0.6728766666975176	0.0085534756879274	T	T	T
0.0627819410052662	0.6287662398367145	0.7941566217086944	T	T	T
0.1793869608988084	0.6717531567629333	0.6641842997317341	T	T	T
0.0781445980475199	0.5592278163213533	0.1487745880084385	T	T	T
0.1964358668024521	0.5288700671432361	0.2895798939890176	T	T	T
0.2145271843820749	0.5561174169155866	0.5156225779774161	T	T	T
0.3734787364824140	0.5655410761385702	0.5142201040843191	T	T	T
0.4299995576900916	0.5308920738265200	0.3045430192237456	T	T	T
0.3215517960734680	0.5634187402272594	0.1626533059861502	T	T	T
0.0866488089716589	0.3244812566890094	0.1610526149959561	T	T	T
0.1984192575145597	0.3707629948606999	0.3004436559811411	T	T	T
0.2299620512345812	0.3307156802277611	0.5192432399185984	T	T	T
0.3847066707278354	0.3278372372373979	0.5066230176529294	T	T	T
0.4300272620938265	0.3740553040629229	0.2935660404918913	T	T	T

Structure files (CONTCAR) involved in this work:

0.3168819475194928	0.3298299340082491	0.1628974073635915	T	T	T
0.9225895109860800	0.5278998117385618	0.1950008440390011	T	T	T
0.8228901266860480	0.3358286502177132	0.3273536245499019	T	T	T
0.7972581625296269	0.6384834678111621	0.6970343731501436	T	T	T
0.0112049084016119	0.5565396085749823	0.2274097297317550	T	T	T
0.3584512299702654	0.0706007541492670	0.7217631422492073	T	T	T
0.3165120160488584	0.0547830801799931	0.9072094489637229	T	T	T
0.2019819215174627	0.0468064107737051	0.0066212571364699	T	T	T
0.0922814217241209	0.0704411040720530	0.9003230368092235	T	T	T
0.1035044071602485	0.0645656029083600	0.7032966510901322	T	T	T
0.2292411261558119	0.0518088052794697	0.7599629288962826	T	T	T
0.3595175909216841	0.8279435843581031	0.7521014032302238	T	T	T
0.3007064089529471	0.8609565553051783	0.9204384565207011	T	T	T
0.1882519222739611	0.8508967128970676	0.0234681420553443	T	T	T
0.0878702248595417	0.8327998004551154	0.8977057347386639	T	T	T
0.1024040540351406	0.8410595025989089	0.7018594433188700	T	T	T
0.2285648856649031	0.8510648564207579	0.7560775272811850	T	T	T
0.3157846821070509	0.9515627396984901	0.7772617533606165	T	T	T
0.0895504942924561	0.9525966503293062	0.8098272093983404	T	T	T
0.4325899213026571	0.1277531339916678	0.5816361471908993	T	T	T
0.4119130362906415	0.9965926413130136	0.5741477124891058	T	T	T
0.3929599458716683	0.8645151073670186	0.5677995627507476	T	T	T
0.1961366880238633	0.1380580056693732	0.6174251745524639	T	T	T
0.1897201725616989	0.0059478006954262	0.5822327615398869	T	T	T
0.1942712304974952	0.8722997899136129	0.5650477406931561	T	T	T
0.9878607290415395	0.0391709658584004	0.7856550587185326	T	T	T
0.9854925995323855	0.8716016292895123	0.7854714418552955	T	T	T
0.1398525385875929	0.9318919905682077	0.2213515389146470	T	T	T
0.1831685646233294	0.9486161988068584	0.4058393307024862	T	T	T
0.2970562588040976	0.9481251855233945	0.5085497615573328	T	T	T
0.4073187109253275	0.9315317713732608	0.4020016882674705	T	T	T
0.3962420696666720	0.9358866633019201	0.2050522561736327	T	T	T
0.2697433234177550	0.9483835011598031	0.2580432823032197	T	T	T
0.1389026096455500	0.1733249872219669	0.2524947636905587	T	T	T
0.1946401229823603	0.1384085524060207	0.4216061323712266	T	T	T
0.3098061030683783	0.1481582900509106	0.5159616583782445	T	T	T
0.4126851658214091	0.1685789597157328	0.3946390352288368	T	T	T
0.3954632842075185	0.1584092532952780	0.1994466254611502	T	T	T
0.2704437516868033	0.1530516481049105	0.2610361640872415	T	T	T
0.1851453428406377	0.0503774447039059	0.2734504180539941	T	T	T
0.4151958391529380	0.0484189722757747	0.3088767682897626	T	T	T
0.0644000026913287	0.8715053216821195	0.0864201663966616	T	T	T
0.0854136195423936	0.0009673646593417	0.0683402599034568	T	T	T
0.1088640619772981	0.1319116161576198	0.0698222601353748	T	T	T
0.3048742160164893	0.8622453121132300	0.1160885835393123	T	T	T
0.3116446560225526	0.9945541166420159	0.0816712798863749	T	T	T
0.2991586134834312	0.1279999267904193	0.0690831551061758	T	T	T
0.5127533841462274	0.9569006281738307	0.2872312028541955	T	T	T
0.5148707489184614	0.1346007574867171	0.2790325579774084	T	T	T
0.6368838755521570	0.5647626953144489	0.2748334537735925	T	T	T
0.7013570425307105	0.5743824704421394	0.1060388769640290	T	T	T
0.7952584749753905	0.5614926852869435	0.9637377537728578	T	T	T
0.8908671057672815	0.5793156141512295	0.1038002973065789	T	T	T

Structure files (CONTCAR) involved in this work:

0.8869079487552028	0.5366515500071510	0.3128697282113228	T	T	T
0.7608869466192655	0.5224031133150870	0.2639385938312668	T	T	T
0.6375001873684140	0.3357051647875808	0.2621420478283992	T	T	T
0.6939393579754677	0.3361298225073850	0.0862293990150205	T	T	T
0.8097363895161124	0.3515989422802708	0.9905333132964393	T	T	T
0.9165262013812602	0.3205590967176434	0.1012187523857533	T	T	T
0.9055095066998963	0.3534734036586053	0.2922815464811115	T	T	T
0.7650628613841262	0.3710345996028631	0.2477041389322482	T	T	T
0.6682839405640553	0.4513380724094970	0.1766728086054243	T	T	T
0.9295899449652467	0.4477680702841270	0.1528134582714910	T	T	T
0.5677368982690300	0.6262448362485481	0.4155806061773575	T	T	T
0.5963839782489435	0.4975542211556228	0.4374179527718018	T	T	T
0.5856141893295724	0.3640342044683323	0.4418178456458359	T	T	T
0.7991283712684335	0.6310756812157875	0.3692610812042606	T	T	T
0.7972065306617411	0.5151606699857350	0.4574564148054012	T	T	T
0.8314932436632967	0.3869494264912477	0.4401366724279813	T	T	T
0.0224344601872861	0.3624069395880495	0.2059054293685959	T	T	T
0.8546783063182812	0.4376255666678728	0.7894739682928001	T	T	T
0.7954212894409172	0.43444404558527324	0.6144721900239610	T	T	T
0.7025002623200038	0.4207752941274136	0.4714611718560971	T	T	T
0.6064457417920454	0.4310428427114242	0.6089618698153971	T	T	T
0.6023658272178970	0.4442850412114339	0.8069591925305750	T	T	T
0.7272011099878920	0.4748455827108125	0.7714741445656839	T	T	T
0.8598278513279287	0.6826783063750678	0.7529873004241380	T	T	T
0.8115678192607443	0.6479499041628245	0.5637137937402770	T	T	T
0.6902192207125756	0.6480296360872885	0.4842846679754910	T	T	T
0.5848224664848177	0.6692800976065509	0.6013545186010089	T	T	T
0.5929434951485140	0.6608807574463619	0.7985358884099277	T	T	T
0.7177239191676330	0.6512852789399116	0.7377354867491868	T	T	T
0.8228929805241760	0.5517693359978112	0.6950285141530045	T	T	T
0.5816045577576039	0.5494866810003929	0.6868637086938224	T	T	T
0.9310713785675999	0.3772173594998633	0.9216827022990826	T	T	T
0.9142848862544829	0.5105567384528031	0.9340704277356554	T	T	T
0.9000231567233020	0.6425002818322714	0.9337757357255769	T	T	T
0.6961658475675143	0.3733332934601736	0.8947678987068587	T	T	T
0.6770665488956239	0.5010643258162696	0.9487511582589642	T	T	T
0.6867266514565048	0.6348457762660796	0.9328463028419786	T	T	T
0.4913479951815010	0.4512241620400507	0.7090197709429298	T	T	T
0.4791639194208189	0.6320786180813578	0.7077414454459436	T	T	T
0.6435040885816751	0.9404479230616773	0.2886154270799631	T	T	T
0.6986518167413052	0.9341869031744829	0.1103529336971363	T	T	T
0.7996864273729370	0.9469033909860302	0.9802709357590371	T	T	T
0.8984106548345838	0.9301690529611607	0.1123846681468613	T	T	T
0.8973728022581340	0.9482670049257638	0.3098487811932633	T	T	T
0.7715368904120155	0.9690212414656735	0.2659514251682857	T	T	T
0.6396320599828678	0.1743679794004454	0.2522634860738647	T	T	T
0.6963855238274453	0.1577013031948968	0.0785908459237359	T	T	T
0.8098723926284185	0.1472158417005248	0.9782285500548485	T	T	T
0.9134918425876485	0.1695160656178148	0.0960208036493989	T	T	T
0.8957758954339550	0.1607715089942107	0.2935394966464439	T	T	T
0.7698907247773612	0.1468816398126059	0.2435931097465190	T	T	T
0.6795400737985364	0.0533049197020831	0.1984867393449446	T	T	T
0.9176269574515394	0.0510732240027534	0.1845950113773802	T	T	T

Structure files (CONTCAR) involved in this work:

0.5688391978791943	0.8758098934272294	0.4197961662745883	T	T	T
0.5820045174312211	0.0074898796894561	0.4376018538544323	T	T	T
0.5993489081311911	0.1396026193608406	0.4348675320566027	T	T	T
0.8070518767010267	0.8713560882258322	0.3939378965586823	T	T	T
0.8164076214533907	0.9987243799948349	0.4482647875990468	T	T	T
0.8064422865032124	0.1324848249381658	0.4344793972942948	T	T	T
0.0100942467124538	0.9558822381637380	0.2161097317617783	T	T	T
0.0149277766958712	0.1389500932974848	0.2140943232595085	T	T	T
0.8572755165440437	0.0551954845691989	0.7857346410886460	T	T	T
0.8010750616934571	0.0720159963728086	0.6095298390245374	T	T	T
0.7004090611989461	0.0576913420976432	0.4798548482656846	T	T	T
0.5987265441712430	0.0759968542313229	0.6065880967103754	T	T	T
0.6031137076931805	0.0526417416401435	0.8037198253335426	T	T	T
0.7285683913533619	0.0291001796566763	0.7622149218396792	T	T	T
0.8601544162804180	0.8343886219955555	0.7623462928496789	T	T	T
0.8044076002442657	0.8330948578587107	0.5863534975005655	T	T	T
0.6914092090038745	0.8522138577135591	0.4860338487393776	T	T	T
0.5877225634658207	0.8295166603761764	0.6048033913636078	T	T	T
0.6025458572463297	0.8534346810890563	0.7990150171683496	T	T	T
0.7296538239384558	0.8565024065791165	0.7463116873607701	T	T	T
0.8173801054631926	0.9482429624271010	0.6822841242976067	T	T	T
0.5785809293144875	0.9536833378075360	0.6724050685386207	T	T	T
0.9322770464046417	0.1267409524145089	0.9091638414599669	T	T	T
0.9186504796519733	0.9967627077753095	0.9421406888332254	T	T	T
0.9026178146622976	0.8645705454554631	0.9437796477709164	T	T	T
0.6947815509552604	0.1306528583174445	0.8838712772664247	T	T	T
0.6828905746878743	0.0046195907535887	0.9455079048219123	T	T	T
0.6950508577101946	0.8707629106356986	0.9385977474159184	T	T	T
0.4887531703211859	0.0485418095612376	0.7147042956791014	T	T	T
0.4836037675905384	0.8645959750055019	0.7157703934274960	T	T	T
0.3606922969940163	0.4312996630855604	0.7211089940151644	T	T	T
0.3117714967779857	0.4458060660284421	0.9038888887893387	T	T	T
0.1994465272283259	0.4611778597530318	0.0110081671371573	T	T	T
0.0897032060103893	0.4355139546057970	0.9049067514933714	T	T	T
0.1017771360700216	0.4358946192684839	0.7073298124888673	T	T	T
0.2297022440033779	0.4508003256780722	0.7524141397896039	T	T	T
0.3579007793623163	0.6748378332624854	0.7527025474853833	T	T	T
0.3013062240784107	0.6380252189215748	0.9204625637853331	T	T	T
0.1883167633773207	0.6477004038910510	0.0195438463741543	T	T	T
0.0872561331062016	0.6684536393946988	0.8937650745541723	T	T	T
0.1021483818875490	0.6589427581044951	0.6974389379716516	T	T	T
0.2274647494813313	0.6487239177936945	0.7565163582551047	T	T	T
0.3166386891914610	0.5498301365394155	0.7748398736974514	T	T	T
0.0815761662269610	0.5497515100187397	0.8062077998284911	T	T	T
0.4318294361340020	0.3761894867372037	0.5741611499294447	T	T	T
0.4134507475527009	0.5076394232547993	0.5747508074539833	T	T	T
0.3843035127919087	0.6382004918103801	0.5668341167183976	T	T	T
0.1919327934973334	0.3628458416755067	0.6149417100358707	T	T	T
0.1814064943960692	0.4951116196104252	0.5785286800751116	T	T	T
0.1956842226193161	0.6284682644213493	0.5639814020552577	T	T	T
0.9846421527531984	0.4578644007522212	0.7864585567336304	T	T	T
0.9832457427761120	0.6381079682698377	0.7775562684733390	T	T	T
0.1434108347441233	0.5690378176658388	0.2182908252866828	T	T	T

Structure files (CONTCAR) involved in this work:

0.1834279971037967	0.5537944590660564	0.4031755594666538	T	T	T
0.2947102391960974	0.5459682753645300	0.5119697613556640	T	T	T
0.4022624237324258	0.5709045698338744	0.4016508863275005	T	T	T
0.3975119124227846	0.5645525760267922	0.2047921889748404	T	T	T
0.2718495574248556	0.5475547539980830	0.2566275205662326	T	T	T
0.1439733049362067	0.3231536143753839	0.2469061019232127	T	T	T
0.1948096228217485	0.3605269623812077	0.4197071398194872	T	T	T
0.3079239246105190	0.3534650455060370	0.5198324770368032	T	T	T
0.4059528887503563	0.3303522894573951	0.3897487817484507	T	T	T
0.3941486625396535	0.3461320539886183	0.1923188737917347	T	T	T
0.2723935546316004	0.3510670343538220	0.2601995798610448	T	T	T
0.1821297882075730	0.4492579916191684	0.2745213628644462	T	T	T
0.4088418625032342	0.4520795980040006	0.3122973821535055	T	T	T
0.0656745796768105	0.6242909444470929	0.0792865014617044	T	T	T
0.0793044376150474	0.4911867316906681	0.0841309643915423	T	T	T
0.1157308360015713	0.3631437958642991	0.0627353347831362	T	T	T
0.3034650430262025	0.6366433266872875	0.1165604223649648	T	T	T
0.3148064073912289	0.5050074348806597	0.0788406926378788	T	T	T
0.2934869086782154	0.3726609188616324	0.0654696280809469	T	T	T
0.5102662354063180	0.5371723336065992	0.2968362011023298	T	T	T
0.5100513815862567	0.3667522286439284	0.2787634393800401	T	T	T
0.4361321140242563	0.7501619865665204	0.6400137957398472	T	T	T
0.1907259680950214	0.7503026638128991	0.6373449753965899	T	T	T
0.2752283033667982	0.7495423642350468	0.0231538589441386	T	T	T
0.1033021110103396	0.7489363842164477	0.0489119059736602	T	T	T
0.0677869463103160	0.2484893327068629	0.1292924937655028	T	T	T
0.3079739106211909	0.2508503494329999	0.1367075118220775	T	T	T
0.2230669386515430	0.2500884057284731	0.5227068548721507	T	T	T
0.3923309955687155	0.2512555446256301	0.5461243077785322	T	T	T
0.5553509275755774	0.2510787517077243	0.3532910345540637	T	T	T
0.8074608549543364	0.2530291101680068	0.3548535001292986	T	T	T
0.7276146222692516	0.2506051963939072	0.9432695465507765	T	T	T
0.8914728695792909	0.2503728369447566	0.9409922670398334	T	T	T
0.9463871123414628	0.7545139668799097	0.8578221462232096	T	T	T
0.6823378652355229	0.7537663986314100	0.8544328848849611	T	T	T
0.7729395910531174	0.7496745023654520	0.4424594281381964	T	T	T
0.6077759930281910	0.7506545327369164	0.4493990581554784	T	T	T
0.9381717549009261	0.5101832422247410	0.5182130112893981	T	T	T
0.9332460234961040	0.4090072727180496	0.4380393655360493	T	T	T
0.8683813527881403	0.5645004729765184	0.5590639521429739	T	T	T
0.0515196453619661	0.4154966417951995	0.5146664608631289	T	T	T
0.0507265214955417	0.4287906506705968	0.3826101300054970	T	T	T
0.0444426978868192	0.3457014612527247	0.4306386662327720	T	T	T
0.0057153844040879	0.5637269978232144	0.3835798285674921	T	T	T
0.9771385559454685	0.6367344467597768	0.3163672830304416	T	T	T
0.0652456090656182	0.6197002316344101	0.3254537904359033	T	T	T
0.9715574352357328	0.5022261823293417	0.5699893168167425	T	T	T
0.0301210598115785	0.3981539462819395	0.4437573315556639	T	T	T
0.0153853293139317	0.5974788533506860	0.3204858257282036	T	T	T

Figure S12(b) TS

Si Al O Zn H C

1.0000000000000000

20.0219999999999985 0.0000000000000000 0.0000000000000000

Structure files (CONTCAR) involved in this work:

0.0000000000000000 19.8990000000000009 0.0000000000000000
0.0000000000000000 0.0000000000000000 13.3829999999999991
93 3 193 2 7 2

Selective dynamics

Direct

0.4227161185310807	0.0605556253372160	0.6476430717757068	T	T	T
0.3050857792747533	0.0323112324174673	0.7909638345858440	T	T	T
0.2826342388294759	0.0554825846281743	0.0163250327048317	T	T	T
0.1235548307199126	0.0625437033079469	0.0117745503947066	T	T	T
0.0682905730403666	0.0315290062438205	0.8011229851287209	T	T	T
0.1801546186964050	0.0657338060159645	0.6643724034239599	T	T	T
0.4183773518854101	0.8280316057288062	0.6683551236741861	T	T	T
0.3006590222047803	0.8735149062722172	0.7996799523401392	T	T	T
0.2672196693429940	0.8307477837324209	0.0189387268345903	T	T	T
0.1113208817621313	0.8259468304641605	0.0127141107270102	T	T	T
0.0667212947515893	0.8750045665830055	0.7987937823903202	T	T	T
0.1788746920730471	0.8291712536312964	0.6631799162328026	T	T	T
0.0759893507496330	0.9408808467299791	0.1480897777802005	T	T	T
0.1952356370063383	0.9703695051648172	0.2892868904819006	T	T	T
0.2164067741772544	0.9445405346347774	0.5154037469299744	T	T	T
0.3766166738403754	0.9360724712233741	0.5132911328952238	T	T	T
0.4335936731541731	0.9687612825309873	0.3014881254894768	T	T	T
0.3206556745521033	0.9349279842325988	0.1641215721087926	T	T	T
0.0828258219238715	0.1728292286759149	0.1655791484772933	T	T	T
0.1986961583180916	0.1290339837443014	0.2999858843733384	T	T	T
0.2312147773574052	0.1699954266491179	0.5177614099356269	T	T	T
0.3870898604138699	0.1743916821980313	0.5085083423001731	T	T	T
0.4349281002414413	0.1272994511689809	0.2950332454978264	T	T	T
0.3192109234295619	0.1724049229082716	0.1642253805930981	T	T	T
0.5773741633595096	0.5551529513365873	0.3567185332286865	T	T	T
0.6914642777445149	0.5272878138810499	0.2039433965132044	T	T	T
0.7137616238695486	0.5692386747914555	0.9873067314445504	T	T	T
0.8717240489173014	0.5749901293594990	0.9890836426572365	T	T	T
0.8117331688586611	0.5496068741752148	0.3498958172149879	T	T	T
0.5730425378527367	0.3303923772561383	0.3350778001029555	T	T	T
0.6960315509851098	0.3729951544919728	0.1983247051236198	T	T	T
0.7299798603660043	0.3273856268865048	0.9838370495585345	T	T	T
0.8845033090115834	0.3259717880210142	0.9931891888246611	T	T	T
0.9408822474434386	0.3757273579841857	0.1856980854267732	T	T	T
0.9189219356593513	0.4473958081339725	0.8650563437884836	T	T	T
0.7970728609953738	0.4739861081951893	0.7262475379694714	T	T	T
0.7774077127288544	0.4359952760621463	0.5003962359394081	T	T	T
0.6193933387981638	0.4292948634195067	0.4939109181950168	T	T	T
0.5675801029598724	0.4699223007689901	0.7060527783210480	T	T	T
0.6723769279564358	0.4469389455584429	0.8617505681965394	T	T	T
0.9205349114791087	0.6796055233520588	0.8334239295483723	T	T	T
0.7701602982974177	0.6702629855885965	0.4659467530220425	T	T	T
0.6143614169136631	0.6731283289070488	0.4865601466073979	T	T	T
0.5604810760208192	0.6285192932266783	0.6988003910271768	T	T	T
0.6691030879664642	0.6766447050381291	0.8317056137522483	T	T	T
0.5781740160984317	0.9462349559708262	0.3592310493458639	T	T	T
0.6991054131101553	0.9755918398030646	0.2177856036071866	T	T	T
0.7191329927840190	0.9401249324800255	0.9947730944864697	T	T	T

Structure files (CONTCAR) involved in this work:

0.8791460051458952	0.9353475466674828	0.9959330856758443	T	T	T
0.9314168523109621	0.9712702150011957	0.2052720986896808	T	T	T
0.8235597934924918	0.9478840876074333	0.3568936104667197	T	T	T
0.5776250793248312	0.1753211704612548	0.3300768274151546	T	T	T
0.6984936542671651	0.1344275060007901	0.1961233404465356	T	T	T
0.7319284839448438	0.1716161528375697	0.9730320872557134	T	T	T
0.8865660521099258	0.1738793459726043	0.9819966867205804	T	T	T
0.9358964459303443	0.1293395313765480	0.1962917273301500	T	T	T
0.8221849576526949	0.1768742031994345	0.3323689770934252	T	T	T
0.9231914274254593	0.0544226900188441	0.8560640814871920	T	T	T
0.8014218061869692	0.0266267513204076	0.7093379022001801	T	T	T
0.7818265439817172	0.0684540889256499	0.4918621530503850	T	T	T
0.6215549985742503	0.0712040163762083	0.4898364221414747	T	T	T
0.5684296164773269	0.0329109720007659	0.6982875912056481	T	T	T
0.6780959763420262	0.0550313802656469	0.8497439126339115	T	T	T
0.9238680315304431	0.8321267912861229	0.8380514486996289	T	T	T
0.8019320173963204	0.8690693940626805	0.6972873595338673	T	T	T
0.7701351047539426	0.8271458808148547	0.4793825231271150	T	T	T
0.6148023841300411	0.8271311587789282	0.4903378003613181	T	T	T
0.5637401759783967	0.8758386850047700	0.6975939495764005	T	T	T
0.6771178190948577	0.8344285584382369	0.8365188116930877	T	T	T
0.4223946505984000	0.4428177799753424	0.6440831117303948	T	T	T
0.3034595674462217	0.4693722941345856	0.7859757779930480	T	T	T
0.2814203870711366	0.4456345130822469	0.0120328543364355	T	T	T
0.1234772637494354	0.4377726211166850	0.0132010845677591	T	T	T
0.0629039363943231	0.4694638171483948	0.8018523170107449	T	T	T
0.1755231035079435	0.4357756057749282	0.6623559262835823	T	T	T
0.4148668182233234	0.6741486755633714	0.6642844846238198	T	T	T
0.2993061359509509	0.6279194963487716	0.7975325064294437	T	T	T
0.2674516966597457	0.6695143063198425	0.0170723991878101	T	T	T
0.1116882390833093	0.6717409244470472	0.0094628562004669	T	T	T
0.0627042909462191	0.6285599570670137	0.7946685252614812	T	T	T
0.1777449435508545	0.6720571867877965	0.6619307979812723	T	T	T
0.0737785428884185	0.5583612130514812	0.1511253037688546	T	T	T
0.1959508789179638	0.5305357446689994	0.2865125045388340	T	T	T
0.2143000999795078	0.5556505023411941	0.5159382733316137	T	T	T
0.3731527250541299	0.5659630572027743	0.5134461307379968	T	T	T
0.4290470462949444	0.5307312880874218	0.3034858408789501	T	T	T
0.3217330726151635	0.5647492128870558	0.1598543733672584	T	T	T
0.0865613509893398	0.3258148656492944	0.1580720023115839	T	T	T
0.1991023163810293	0.3718264763289196	0.2971368285683099	T	T	T
0.2297830621051377	0.3313483111370540	0.5167917759426416	T	T	T
0.3851693590272563	0.3281490925348106	0.5062151187409201	T	T	T
0.4305574627832028	0.3740576507352190	0.2930208726520743	T	T	T
0.3182948769576210	0.3293413030734699	0.1599600552306415	T	T	T
0.9241847467459454	0.5295708938049288	0.1923856561445069	T	T	T
0.8267529072011088	0.3395646331071633	0.3319844680976222	T	T	T
0.7961813424705770	0.6396349654128995	0.7019360520490444	T	T	T
0.0075485911186913	0.5522802196327640	0.2203974812727147	T	T	T
0.3593382956160878	0.0710384304923696	0.7217661168890660	T	T	T
0.3170293499411368	0.0531265045487813	0.9065747810882182	T	T	T
0.2025893154418666	0.0456891288656837	0.0061704392229209	T	T	T
0.0928186160941099	0.0708186767378487	0.9007394349613075	T	T	T

Structure files (CONTCAR) involved in this work:

0.1035355533676105	0.0650147462306442	0.7037758128690608	T	T	T
0.2297770921886347	0.0539636552259439	0.7592163676999565	T	T	T
0.3604166004703714	0.8285631589422280	0.7531309879756470	T	T	T
0.2998694181470895	0.8632865512552143	0.9193204483365346	T	T	T
0.1885345649992461	0.8505120521170468	0.0240616094921321	T	T	T
0.0888717399821136	0.8325070205098444	0.8969002054432572	T	T	T
0.1025062931016975	0.8419321875480222	0.7009359657894217	T	T	T
0.2291052502571580	0.8500016190198948	0.7538769903668974	T	T	T
0.3146466761483673	0.9519033041784697	0.7732639668708191	T	T	T
0.0902471704258130	0.9528192609963555	0.8104374768018596	T	T	T
0.4328842900276886	0.1278492711921469	0.5804887673548131	T	T	T
0.4120963051778314	0.9967281260959356	0.5739895332180275	T	T	T
0.3918204923915924	0.8649328062605361	0.5677859935884364	T	T	T
0.1951099739710567	0.1389386669812675	0.6156969340740972	T	T	T
0.1897118862298570	0.0063522312886762	0.5828769756385968	T	T	T
0.1941963032528941	0.8729384486886809	0.5634965765733470	T	T	T
0.9881707801005611	0.0388456720682455	0.7872740926734580	T	T	T
0.9860863247742702	0.8719564100954853	0.7857794616865676	T	T	T
0.1403336849898082	0.9321148763832404	0.2208126306885654	T	T	T
0.1831361207769373	0.9506990557285768	0.4052941235551508	T	T	T
0.2969429933908830	0.9492239120464007	0.5076826602251998	T	T	T
0.4075088368298037	0.9317173520775170	0.4020454560219400	T	T	T
0.3968609075713238	0.9354773153627407	0.2052353149329176	T	T	T
0.2701480728199037	0.9471874987638523	0.2578496785188568	T	T	T
0.1393013174002553	0.1738948901384809	0.2525711694245673	T	T	T
0.1960234897951177	0.1374824617585225	0.4200157630532379	T	T	T
0.3098104081766012	0.1495771589343262	0.5171924823408565	T	T	T
0.4119545077172139	0.1686761289710179	0.3938045765372152	T	T	T
0.3960577080194349	0.1580619784256181	0.1982224572705641	T	T	T
0.2708774359852021	0.1546740327154189	0.2589274470224098	T	T	T
0.1870444770009731	0.0507628183033699	0.2701230057604577	T	T	T
0.4156795436387916	0.0484670975885389	0.3083496546744809	T	T	T
0.0649441517666039	0.8718506843168649	0.0849892664155933	T	T	T
0.0854486709796436	0.0020610066010372	0.0692979475671548	T	T	T
0.1113290873074652	0.1329046618153116	0.0691526385420142	T	T	T
0.3057666366696716	0.8618031428193326	0.1148990304087682	T	T	T
0.3123975251217912	0.9942354678273784	0.0821255301012333	T	T	T
0.2997278596104286	0.1273322234524726	0.0676088554932538	T	T	T
0.5133067301162115	0.9570906281046860	0.2882468856869924	T	T	T
0.5150437586628828	0.1352577121025535	0.2792678290222699	T	T	T
0.6363553462996729	0.5625401597410579	0.2750784056300799	T	T	T
0.7017819010576876	0.5747698131089011	0.1070572669320644	T	T	T
0.7928252609405555	0.5634941868905803	0.9596855381234561	T	T	T
0.8826132408303926	0.5798368320248871	0.1077997295631521	T	T	T
0.8875667932030417	0.5274159343598653	0.3180337252962380	T	T	T
0.7616132497051703	0.5249305373678356	0.2653902527590942	T	T	T
0.6396832628683977	0.3379486469615284	0.2689185970945020	T	T	T
0.6939757380551237	0.3332576094899876	0.0916953403071448	T	T	T
0.8074697883988403	0.3523082409382618	0.9908055983886167	T	T	T
0.9106428483854495	0.3200317633500426	0.1081812621232756	T	T	T
0.9094633614771094	0.3658058245567803	0.2981728365921647	T	T	T
0.7683786486505823	0.3708464245088745	0.2485019089824824	T	T	T
0.6716814207733498	0.4507159411956917	0.1766525892604498	T	T	T

Structure files (CONTCAR) involved in this work:

0.9242450959946812	0.4492665200652177	0.1454172500019751	T	T	T
0.5686317472754913	0.6266159867357001	0.4141208505971763	T	T	T
0.5943699367132138	0.4978690117477992	0.4396233189989883	T	T	T
0.5831739143333371	0.3643782375528609	0.4451540373565572	T	T	T
0.8064962817324299	0.6299218323443184	0.3736493262240853	T	T	T
0.7943096856561144	0.5151644547839045	0.4610526556505450	T	T	T
0.8284026272441041	0.3880257919983804	0.4430632733742834	T	T	T
0.0212068960925480	0.3648633871450966	0.1976562653962700	T	T	T
0.8532178283795667	0.4378456193821356	0.7942471415082509	T	T	T
0.7935634898598303	0.4355344761052333	0.6189641214560417	T	T	T
0.6997309460500233	0.4216682590612790	0.4773267638102763	T	T	T
0.6026956953257406	0.4315884425196074	0.6121445150368832	T	T	T
0.5989444287204130	0.4434580589868748	0.8107711366458107	T	T	T
0.7242469516574547	0.4723260861814465	0.7758377791119448	T	T	T
0.8597211389111453	0.6829455656865490	0.7563301926801917	T	T	T
0.8112982260663408	0.6471910248947540	0.5677669594057502	T	T	T
0.6924083318852701	0.6481320551571331	0.4787804354098595	T	T	T
0.5882311434075813	0.6672402369043716	0.6003036126976949	T	T	T
0.5913151801453993	0.6641653895562354	0.7979024056155845	T	T	T
0.7165610240349061	0.6534967714443010	0.7406283711935087	T	T	T
0.8191102405406347	0.5519500812573468	0.7027251933982223	T	T	T
0.5814113043594755	0.5498130984528956	0.6926786951767181	T	T	T
0.9297824183099781	0.3786999322586894	0.9288980955796607	T	T	T
0.9127783865941883	0.5125281671321543	0.9367674164072934	T	T	T
0.8993515824293215	0.6438352913945861	0.9379196958884007	T	T	T
0.6914519917374747	0.3728585729361451	0.9013726007052102	T	T	T
0.6743143258925335	0.5017273823204363	0.9511915150783813	T	T	T
0.6827088702867045	0.6352933402648815	0.9346337525742447	T	T	T
0.4884536104744797	0.4529156920642827	0.7119749120114323	T	T	T
0.4795276188923709	0.6330066531738480	0.7040600644441760	T	T	T
0.6440233516854292	0.9408265062842115	0.2897097669497985	T	T	T
0.6988753546104916	0.9362610882609638	0.1117252350369536	T	T	T
0.7995315838713362	0.9465651738365350	0.9805043507096534	T	T	T
0.8978092866231827	0.9295952403343001	0.1134856078308188	T	T	T
0.8985140470594896	0.9487445977326284	0.3109006153063825	T	T	T
0.7723872091250552	0.9677015182306993	0.2676660364189625	T	T	T
0.6399574380378578	0.1756769074252647	0.2531929801280549	T	T	T
0.6970038775174638	0.1569231453694910	0.0799278424711577	T	T	T
0.8096254737048119	0.1472940180961725	0.9773689298131578	T	T	T
0.9133455056378195	0.1688529966910557	0.0958182700284812	T	T	T
0.8977950518532967	0.1583940722565078	0.2938370992188565	T	T	T
0.7707507814479428	0.1503929409717921	0.2450825032424132	T	T	T
0.6817199772134072	0.0545608927039691	0.2037027412824402	T	T	T
0.9186891727098574	0.0502220091583341	0.1828050436881574	T	T	T
0.5696765136463259	0.8762354497297491	0.4210895786663047	T	T	T
0.5829496349764527	0.0081701807759054	0.4381741960242053	T	T	T
0.5990040880781726	0.1405128872225583	0.4354094793793523	T	T	T
0.8096229604630643	0.8725720136441506	0.3987793331203488	T	T	T
0.8179133424976853	1.0014662386934690	0.4476244679318714	T	T	T
0.8072467016945754	0.1354873491816255	0.4356087866727922	T	T	T
0.0105347317310492	0.9548747094035511	0.2157424854223384	T	T	T
0.0160946483577311	0.1383616559674402	0.2113231933872967	T	T	T
0.8577963805008041	0.0543680328065174	0.7852751811159580	T	T	T

Structure files (CONTCAR) involved in this work:

0.8012159775286873	0.0732754194362298	0.6097435633235426	T	T	T
0.7013903147108019	0.0598332926414636	0.4781342644983746	T	T	T
0.6005157685823677	0.0763532817361206	0.6069087990077934	T	T	T
0.6031621010906270	0.0523144660496648	0.8038888692233670	T	T	T
0.7288084399061041	0.0302415966772169	0.7625773998373414	T	T	T
0.8604561547207989	0.8360746938985195	0.7637089601593910	T	T	T
0.8032333137276524	0.8314962958643236	0.5896170872868461	T	T	T
0.6925600620010306	0.8511982199160019	0.4845478844091827	T	T	T
0.5893911363226115	0.8292636645947987	0.6053670604283550	T	T	T
0.6020755263909012	0.8540411501839443	0.7994296012986043	T	T	T
0.7296833444820606	0.8573791158325131	0.7498145635218265	T	T	T
0.8159454314890299	0.9486382974642511	0.6802872570751843	T	T	T
0.5793685950462477	0.9538809263603354	0.6714055756553116	T	T	T
0.9318128990264217	0.1279374035742744	0.9077227464356342	T	T	T
0.9179632785218703	0.9983714801021205	0.9445031115987902	T	T	T
0.9035656603158615	0.8658202950107708	0.9443412780497379	T	T	T
0.6938182405753678	0.1313747580705276	0.8844238718919226	T	T	T
0.6834280106154197	0.0058121130290328	0.9462574377748050	T	T	T
0.6931859946509188	0.8720880950334577	0.9411192583925064	T	T	T
0.4895859527917731	0.0489894113141357	0.7132748833506626	T	T	T
0.4839975730249372	0.8651861641774469	0.7135999645388094	T	T	T
0.3578937871425628	0.4315198443338184	0.7160163272375677	T	T	T
0.3143240662419918	0.4468416770235119	0.9011619915907545	T	T	T
0.2015433324749791	0.4592869459620995	0.0043006747570883	T	T	T
0.0895652176625273	0.4349127812901205	0.9035704231947116	T	T	T
0.0995001927172188	0.4349112531168076	0.7057807260797846	T	T	T
0.2277915091158770	0.4491627958465914	0.7531810370094211	T	T	T
0.3577371010960266	0.6742206237317933	0.7503829714323700	T	T	T
0.3001609582214145	0.6375659518243252	0.9171324016855282	T	T	T
0.1891503018368969	0.6480807448097627	0.0214503638589827	T	T	T
0.0896063709507900	0.6675164219708213	0.8931954422391190	T	T	T
0.1007204981064161	0.6588670407200620	0.6964550319467918	T	T	T
0.2267434121513244	0.6498707906173052	0.7533917484293970	T	T	T
0.3139908431652102	0.5497700835102706	0.7703109822263056	T	T	T
0.0804996980533416	0.5490821672603424	0.8037314724712018	T	T	T
0.4321005351816136	0.3771658466224339	0.5731317500321007	T	T	T
0.4144083170476536	0.5086828136477626	0.5733108223034807	T	T	T
0.3844867605392203	0.6391440875441783	0.5640997784547613	T	T	T
0.1906795032237621	0.3631699561746852	0.6119938039160782	T	T	T
0.1800413006560679	0.4956642105010916	0.5798925580431255	T	T	T
0.1935254309947547	0.6283358890233700	0.5616960263196235	T	T	T
0.9827544273720642	0.4572635348356046	0.7892891136627257	T	T	T
0.9828654665686373	0.6383307520653733	0.7812972391201558	T	T	T
0.1388732470238371	0.5699586709745877	0.2232723772941085	T	T	T
0.1849042890879073	0.5513626440073472	0.4028355511024806	T	T	T
0.2944729202963680	0.5459370665988904	0.5151200912219637	T	T	T
0.4000548647029477	0.5705716397669048	0.3998771915848330	T	T	T
0.3973824883306112	0.5642771616332973	0.2033402273457705	T	T	T
0.2703899158611600	0.5521283950655628	0.2527234925634788	T	T	T
0.1413767253002042	0.3259376880843727	0.2477374240173731	T	T	T
0.1960076513785261	0.3627688337550039	0.4169952505779677	T	T	T
0.3080402088396484	0.3529581990776637	0.5194138825171457	T	T	T
0.4063923826186536	0.3305374490580217	0.3893232484208528	T	T	T

Structure files (CONTCAR) involved in this work:

0.3951496586684300	0.3452821216263971	0.1920711373977378	T	T	T
0.2718469263301034	0.3489444263167502	0.2559890315343559	T	T	T
0.1855291358626236	0.4503509184182019	0.2691435089845940	T	T	T
0.4081971563543630	0.4518329278675876	0.3108431239366102	T	T	T
0.0655225045294621	0.6231997806148031	0.0778682252796050	T	T	T
0.0843458153760590	0.4917743778944053	0.0825277649233807	T	T	T
0.1179114974612803	0.3628236807891119	0.0603317682518038	T	T	T
0.3066672376115756	0.6380940929837432	0.1122168550560012	T	T	T
0.3145186884450832	0.5055495377288599	0.0774070365510327	T	T	T
0.2966059186699698	0.3730204978975197	0.0626660804147082	T	T	T
0.5093592821998586	0.5372647155096349	0.2974611908228686	T	T	T
0.5108458970224876	0.3677704881938779	0.2788594568694062	T	T	T
0.4357322205364959	0.7508749862273568	0.6388362792458554	T	T	T
0.1887707174244226	0.7505052171055387	0.6339759040636079	T	T	T
0.2763269565902889	0.7500643872190322	0.0182071013329621	T	T	T
0.1031347934160005	0.7484465667291267	0.0480643777660971	T	T	T
0.0680169421656329	0.2491337398371933	0.1293045370235042	T	T	T
0.3100352402021372	0.2505548928079412	0.1320954262931083	T	T	T
0.2217128238439961	0.2507011458679111	0.5185963131340577	T	T	T
0.3935621118868778	0.2516770026930317	0.5458332827052025	T	T	T
0.5549039902482331	0.2519541687995734	0.3531912228831052	T	T	T
0.8160335291258676	0.2553149556638271	0.3531902646202111	T	T	T
0.7268127288429700	0.2504883716440920	0.9447973586029592	T	T	T
0.8908881709604893	0.2514559953259694	0.9439456732959833	T	T	T
0.9463409547162699	0.7553175969271688	0.8594444619440272	T	T	T
0.6814545320131598	0.7550326309662194	0.8585993932356591	T	T	T
0.7764350900573426	0.7493570493854638	0.4428659271015621	T	T	T
0.6083982077274427	0.7504960581541197	0.4495134420821210	T	T	T
0.9301492955359267	0.4995271289345117	0.5361154116709738	T	T	T
0.9380169429827325	0.4484600638910656	0.3970104692540281	T	T	T
0.8617592193051503	0.5602889446006030	0.5670374396887463	T	T	T
0.0507348404878294	0.4384270710846674	0.4907341190233390	T	T	T
0.0746546478000656	0.4598766538859557	0.3646505870385359	T	T	T
0.0362549702255933	0.3805170042688487	0.3862489659328928	T	T	T
0.0104943643300619	0.5502858909335597	0.4684585790020195	T	T	T
0.9852860425445109	0.6122467606324646	0.3701734097074358	T	T	T
0.0740848779406134	0.5836727515742612	0.3768201260094582	T	T	T
0.9461549503834448	0.4748929098506766	0.5945008061526678	T	T	T
0.0389308697442301	0.4331080182984320	0.4112117877619281	T	T	T
0.0225430414149224	0.5783200739692032	0.4010028776329020	T	T	T

Figure S12(b) FS

Si Al O Zn H C

1.0000000000000000		
20.0219999999999985	0.0000000000000000	0.0000000000000000
0.0000000000000000	19.8990000000000009	0.0000000000000000
0.0000000000000000	0.0000000000000000	13.3829999999999991
93	3	193
2	7	2

Selective dynamics

Direct

0.4238319728443616	0.0593900567187360	0.6475177094328433	T	T	T
0.3058870389143714	0.0296037345879500	0.7905525355170347	T	T	T
0.2835772210546737	0.0559011823480334	0.0154568482892769	T	T	T
0.1241205372115358	0.0615638719527922	0.0118567970183750	T	T	T

Structure files (CONTCAR) involved in this work:

0.0685254063806313	0.0303810312769803	0.8001421218457857	T	T	T
0.1807231563958441	0.0636787754990723	0.6640221673256413	T	T	T
0.4196388668467449	0.8271583710950829	0.6666450132718664	T	T	T
0.3026821322660797	0.8704717322427736	0.8009237106772753	T	T	T
0.2677521388986702	0.8314238143092180	0.0205127219305880	T	T	T
0.1131115229284241	0.8262328332632080	0.0107123033743087	T	T	T
0.0666710732151879	0.8734758498613147	0.7965415038853110	T	T	T
0.1809514157245683	0.8266674746883038	0.6653132154517395	T	T	T
0.0777269987960003	0.9393185513012658	0.1487623502374456	T	T	T
0.1955547388999212	0.9692664077548907	0.2915077165566315	T	T	T
0.2173438984436477	0.9425632078804402	0.5164753255486656	T	T	T
0.3772085985688654	0.9360136760979414	0.5127068403775142	T	T	T
0.4343365454268121	0.9680410834920807	0.3012527356480784	T	T	T
0.3210997569548529	0.9365759151845064	0.1650802840746263	T	T	T
0.0832904189752788	0.1722532489626512	0.1645679549459991	T	T	T
0.1984237770635324	0.1282290385519704	0.3010516206458441	T	T	T
0.2327389704798944	0.1696325044494387	0.5194653175847870	T	T	T
0.3883358970617294	0.1734449710165173	0.5086972803901102	T	T	T
0.4355796535553683	0.1266295929039565	0.2945349479081678	T	T	T
0.3190564177426636	0.1713354030997029	0.1644000246733041	T	T	T
0.5761134599720346	0.5549415621299407	0.3534575133199785	T	T	T
0.6905752285925842	0.5248904348864419	0.2010535564956887	T	T	T
0.7145303283200668	0.5687047565983638	0.9846046384466245	T	T	T
0.8718600273370350	0.5732851211182054	0.9874625169676489	T	T	T
0.8109182931404417	0.5486967626655226	0.3468359935358278	T	T	T
0.5741343019930486	0.3279685196204558	0.3323619200186760	T	T	T
0.6954684669593613	0.3704141908638646	0.1930080131347697	T	T	T
0.7306514539798078	0.3259120747500578	0.9806900154125155	T	T	T
0.8853246384628821	0.3247531729755957	0.9956154327173561	T	T	T
0.9428694918767258	0.3743179921027183	0.1874992739163671	T	T	T
0.9205995311690950	0.4449530098705938	0.8647880337233956	T	T	T
0.8007546208161941	0.4698909703090025	0.7227853964733306	T	T	T
0.7746855852433773	0.4346849935938946	0.4987666712955752	T	T	T
0.6165790517967957	0.4288645411940087	0.4910227020677653	T	T	T
0.5669062398935837	0.4691780920925591	0.7045377856514514	T	T	T
0.6748791392571933	0.4465541664409884	0.8572782853993632	T	T	T
0.9217845365170192	0.6773374186816405	0.8324133879864279	T	T	T
0.7719343855693778	0.6679271470036097	0.4662617303532005	T	T	T
0.6162246881151852	0.6718554688779051	0.4858512259704813	T	T	T
0.5611538934638955	0.6278549108860769	0.6978595641665969	T	T	T
0.6724806148584783	0.6740905881531513	0.8278710094326848	T	T	T
0.5790692420828411	0.9444908808288286	0.3587411328653176	T	T	T
0.7000257525500679	0.9732629408617808	0.2156419047077108	T	T	T
0.7206832089353344	0.9367335752185342	0.9937671823788988	T	T	T
0.8809234882921044	0.9335621990182660	0.9952412855864977	T	T	T
0.9331502334325822	0.9694181941822905	0.2048994605146990	T	T	T
0.8242690066760666	0.9456781460932958	0.3557470724345742	T	T	T
0.5785921574123418	0.1727686976913218	0.3293200728219049	T	T	T
0.6994056436519124	0.1318188184514109	0.1938968607887491	T	T	T
0.7330253364848478	0.1704909324839255	0.9719156019230433	T	T	T
0.8876171112139397	0.1727835708553666	0.9832512309231040	T	T	T
0.9373724831461748	0.1273939715291906	0.1964437935224461	T	T	T
0.8226856352546988	0.1724366544175730	0.3310773094230068	T	T	T

Structure files (CONTCAR) involved in this work:

0.9239109434559959	0.0540803022994521	0.8562799251464044	T	T	T
0.8029769989920156	0.0258810108880750	0.7099880090000478	T	T	T
0.7821384448930134	0.0653481879314959	0.4919301619838954	T	T	T
0.6219015447114790	0.0690509147106415	0.4901789112332190	T	T	T
0.5694020494306731	0.0312155307321757	0.6986914521665647	T	T	T
0.6793948881599442	0.0523846657928673	0.8498084531062526	T	T	T
0.9246637334991716	0.8301902436994970	0.8368066520890718	T	T	T
0.8036574908705485	0.8691051971227827	0.6967967393012184	T	T	T
0.7720850179493968	0.8258152476459321	0.4790810327055552	T	T	T
0.6168918057395957	0.8258341307319648	0.4897708237101885	T	T	T
0.5650715989210517	0.8742292408112375	0.6969291707752524	T	T	T
0.6791982272120236	0.8329568608243588	0.8329459263249873	T	T	T
0.4236669815349348	0.4432625307077649	0.6384492850652500	T	T	T
0.3033687144858916	0.4701570744718288	0.7795933483329082	T	T	T
0.2834876163239517	0.4411640923667960	0.0029851475529286	T	T	T
0.1249906644272704	0.4367470103486377	0.0101428171966623	T	T	T
0.0655663480424139	0.4690735951977436	0.8001165143104072	T	T	T
0.1751894713628603	0.4402984460774677	0.6520757024179639	T	T	T
0.4175465909153879	0.6737911759126833	0.6564267998902594	T	T	T
0.3012877427847049	0.6286252173972975	0.7938701045799441	T	T	T
0.2693553918935850	0.6709423274237681	0.0134987955559631	T	T	T
0.1148287099476349	0.6719535722598334	0.0043136182632642	T	T	T
0.0641687948226147	0.6280383012643468	0.7931333925128137	T	T	T
0.1787841389725334	0.6690153804313893	0.6592008390151139	T	T	T
0.0743802747969172	0.5585965561175246	0.1452200569511477	T	T	T
0.1971713103650164	0.5283795425846651	0.2781852789333857	T	T	T
0.2177105442057589	0.5569248645347621	0.5088349454394591	T	T	T
0.3755714785377133	0.5649825810634667	0.5082105079613417	T	T	T
0.4270135736982442	0.5283642094464289	0.2972392371330465	T	T	T
0.3240252577064201	0.5587113122509956	0.1439880859430207	T	T	T
0.0871151621005266	0.3247665050155628	0.1580732474951173	T	T	T
0.1988060362305502	0.3708255340797335	0.2969570927469692	T	T	T
0.2316500537015594	0.3306017902806065	0.5172804655187876	T	T	T
0.3869471943197867	0.3270913967642780	0.5041964379697752	T	T	T
0.4323648151468056	0.3709972130688310	0.2901091990296994	T	T	T
0.3184864601808061	0.3288192194711961	0.1593125955748909	T	T	T
0.9263937121340822	0.5299427299691051	0.1906007737800578	T	T	T
0.8238231945950948	0.3341512917843125	0.3258931420476253	T	T	T
0.7995877992697268	0.6338962861334327	0.6986505824706464	T	T	T
0.0083658460816516	0.5532948425451566	0.2121397434837392	T	T	T
0.3599588395693915	0.0683470900502653	0.7210461838402087	T	T	T
0.3175475478609348	0.0518488156495209	0.9056157498006095	T	T	T
0.2034545192509895	0.0462659393820460	0.0066022936353597	T	T	T
0.0932289063312620	0.0681818827314451	0.9007854896739607	T	T	T
0.1041887685062088	0.0646747851429200	0.7038367420788805	T	T	T
0.2304037204503937	0.0502391047093767	0.7582785087329758	T	T	T
0.3620402830801939	0.8260109334191786	0.7519645079047230	T	T	T
0.3041120561684368	0.8593897540165026	0.9204929990134550	T	T	T
0.1896234817737488	0.8537847673651543	0.0179321091166167	T	T	T
0.0875010762467296	0.8324652154881133	0.8964228444004378	T	T	T
0.1041399825349768	0.8398876117573362	0.7006072012077249	T	T	T
0.2304483732175089	0.8467969027441311	0.7574677992052433	T	T	T
0.3159956988566003	0.9491048958513685	0.7746461845580938	T	T	T

Structure files (CONTCAR) involved in this work:

0.0896877458749363	0.9514823947391671	0.8069319966870917	T	T	T
0.4338301157690274	0.1275068567051627	0.5820561250088095	T	T	T
0.4140059912604054	0.9965577518265879	0.5718643788787738	T	T	T
0.3919183240385777	0.8650607745613043	0.5677287502769521	T	T	T
0.1970086472761962	0.1366798873251136	0.6161556513318527	T	T	T
0.1884775389651781	0.0045042352353021	0.5817659419086521	T	T	T
0.1979154922892647	0.8708904976377343	0.5666341898856668	T	T	T
0.9884286737501909	0.0386519345260411	0.7865769526411116	T	T	T
0.9861255520806717	0.8695033416942296	0.7815599275016879	T	T	T
0.1423234872941311	0.9303210896334059	0.2209152354011653	T	T	T
0.1839495758380433	0.9460806726381672	0.4062022700021458	T	T	T
0.2977000730910425	0.9503383303242652	0.5084872817146743	T	T	T
0.4075504544086794	0.9308108387569686	0.4012139240307878	T	T	T
0.3976814753945342	0.9353946344699818	0.2045946494910113	T	T	T
0.2715099185676808	0.9502571291935744	0.2594485490012818	T	T	T
0.1405955016215071	0.1734797880959992	0.2502155443998791	T	T	T
0.1962690432996146	0.1407059704356096	0.4203149060790886	T	T	T
0.3111004788266972	0.1483019030356293	0.5160674736362343	T	T	T
0.4138386223098987	0.1676698192601208	0.3942354469062935	T	T	T
0.3961570490452032	0.1580324015651434	0.1986009212534335	T	T	T
0.2713339009562781	0.1498511108104753	0.2579635796567900	T	T	T
0.1837879801050374	0.0496193584413835	0.2768287042203639	T	T	T
0.4166530208248144	0.0477936699172692	0.3080417490045430	T	T	T
0.0666369079896993	0.8705778745486127	0.0851438905077637	T	T	T
0.0870353021278174	0.0011809828449747	0.0709887708921820	T	T	T
0.1106116453848942	0.1324617729776348	0.0672827442682669	T	T	T
0.3044715077145545	0.8638704499151205	0.1167564534383029	T	T	T
0.3136530124656076	0.9956852198727200	0.0827825160142632	T	T	T
0.3013037501293440	0.1281866897258807	0.0649905633109649	T	T	T
0.5139885078084255	0.9556109081010041	0.2884615690234237	T	T	T
0.5157377483709764	0.1339675736144649	0.2773742167148998	T	T	T
0.6341303737380274	0.5598626047157523	0.2698144903757632	T	T	T
0.7030009043150064	0.5722672079576314	0.1047611154904762	T	T	T
0.7932197632408982	0.5632332713806190	0.9553822091691203	T	T	T
0.8804448073359857	0.5768865552374427	0.1065040065713321	T	T	T
0.8863970926829015	0.5254509166330092	0.3151385970809445	T	T	T
0.7591327632902601	0.5214692863727529	0.2666195645398078	T	T	T
0.6416543484576012	0.3354815621002610	0.2678260472653899	T	T	T
0.6912600119332442	0.3313085291556007	0.0861984115214705	T	T	T
0.8079936784951048	0.3502640442553911	0.9940345783230893	T	T	T
0.9117897306531841	0.3187187605334948	0.1109320466723447	T	T	T
0.9092002136618714	0.3623831798059269	0.3005288325134285	T	T	T
0.7691635982350175	0.3667993582540285	0.2395861230796811	T	T	T
0.6714613379995998	0.4482387208639722	0.1729603471690965	T	T	T
0.9246692823431892	0.4476192838316301	0.1499836399161663	T	T	T
0.5711579679862432	0.6264356335907996	0.4112242422928393	T	T	T
0.5919318846068604	0.4969489015697227	0.4358920126936470	T	T	T
0.5826368612116484	0.3630079420912430	0.4420076121111237	T	T	T
0.8049351856263549	0.6285172687640035	0.3702432845048591	T	T	T
0.7967213490442779	0.5125941711694358	0.4595290050381807	T	T	T
0.8232377334119070	0.3855245949581255	0.4361599053480774	T	T	T
0.0225934094012567	0.3633569695897218	0.2038307114561657	T	T	T
0.8557437598173383	0.4331889670531043	0.7919845140517182	T	T	T

Structure files (CONTCAR) involved in this work:

0.7941895217025543	0.4307197770669485	0.6156616286623920	T	T	T
0.6973966729463085	0.4225203372202276	0.4755644814701211	T	T	T
0.5998413558543586	0.4308000646773216	0.6088537867290600	T	T	T
0.6014215940159159	0.4417649361805208	0.8064390108735380	T	T	T
0.7277282584320697	0.4721389600795809	0.7723735088963036	T	T	T
0.8606110877561394	0.6791108307652469	0.7557091800360634	T	T	T
0.8153910904085829	0.6420329678733682	0.5644618757729126	T	T	T
0.6942407529689829	0.6460761309272711	0.4816332582021093	T	T	T
0.5881461248147830	0.6658631605823634	0.5983518583257021	T	T	T
0.5942775105308971	0.6632223714092870	0.7952978635447512	T	T	T
0.7197257022128040	0.6457916030722888	0.7394413904037740	T	T	T
0.8258435010843641	0.5466062712890076	0.6955098722015127	T	T	T
0.5812833301051152	0.5489068922910902	0.6917498943879894	T	T	T
0.9306580270187059	0.3773231288130997	0.9316422514675053	T	T	T
0.9118772434517476	0.5101546364059387	0.9354526838709092	T	T	T
0.9014942400991588	0.6416771872382100	0.9374998440386660	T	T	T
0.6950902771571308	0.3726798095049976	0.8969400635839555	T	T	T
0.6750410035274640	0.5016364795518654	0.9463893637769621	T	T	T
0.6836994364562415	0.6357705468700098	0.9342835003341967	T	T	T
0.4875975710288047	0.4528066741849449	0.7117536445043540	T	T	T
0.4803847707769607	0.6338941473617896	0.7053577820538334	T	T	T
0.6446981304702093	0.9399686504287852	0.2885832028944513	T	T	T
0.7002415099849838	0.9324323679272915	0.1107541067383915	T	T	T
0.8010873377069296	0.9435880204299366	0.9801134967379678	T	T	T
0.8998052793426468	0.9278585619230013	0.1127779774904091	T	T	T
0.8993198891146768	0.9478813137637020	0.3103423510003242	T	T	T
0.7730400664254943	0.9663900827797314	0.2669101581292236	T	T	T
0.6415734247162016	0.1722642566675011	0.2535921263406189	T	T	T
0.6978228677098117	0.1576239698449882	0.0792142883568873	T	T	T
0.8106715805638968	0.1463408189555159	0.9779456665293728	T	T	T
0.9139534360284449	0.1678344458670853	0.0972537100356147	T	T	T
0.8988608671527082	0.1555987082873622	0.2943791287873855	T	T	T
0.7720472792214002	0.1459794487762892	0.2431762344301298	T	T	T
0.6826332618548748	0.0519143896907545	0.1974434442484390	T	T	T
0.9207784007552440	0.0483713843321373	0.1815897488984290	T	T	T
0.5714334627347677	0.8741274569613148	0.4198228146116190	T	T	T
0.5836116907888677	0.0057535832034483	0.4389332315159589	T	T	T
0.5989364615258197	0.1379938758646029	0.4350608818950378	T	T	T
0.8108112056323921	0.8697382097425499	0.3956599417894186	T	T	T
0.8176159177083797	0.9978394793261263	0.4483654604843396	T	T	T
0.8079548087944470	0.1318387443721879	0.4345870573817859	T	T	T
0.0121586641888151	0.9529745484250869	0.2165964040298322	T	T	T
0.0172795356846030	0.1372515029684333	0.2120065584095943	T	T	T
0.8581723494444292	0.0558334864646826	0.7860402842879889	T	T	T
0.8018100272178659	0.0715926609459398	0.6094369572644193	T	T	T
0.7017131864012981	0.0577086266687396	0.4781535300964705	T	T	T
0.6012395327854417	0.0748910247906484	0.6072764304940800	T	T	T
0.6043276643015620	0.0504074313608028	0.8042895343015490	T	T	T
0.7299346829711643	0.0277685547233562	0.7622194026129595	T	T	T
0.8596571735842109	0.8337053040797451	0.7653489069240164	T	T	T
0.8059853800269248	0.8324889455531581	0.5884634609180819	T	T	T
0.6945890049152084	0.8501746413578293	0.4844236625605214	T	T	T
0.5910218039687245	0.8279133038108789	0.6045515888275171	T	T	T

Structure files (CONTCAR) involved in this work:

0.6032583576397476	0.8516662022107205	0.7987179384321491	T	T	T
0.7300790436015652	0.8599875503091410	0.7464135454228860	T	T	T
0.8204354503384284	0.9483399190526735	0.6822962034128351	T	T	T
0.5810567064481501	0.9523527500753952	0.6715731419421245	T	T	T
0.9332155827729898	0.1271362136736222	0.9092537176512240	T	T	T
0.9184188336589048	0.9973636601272621	0.9436668341477356	T	T	T
0.9065007382355035	0.8645832118734529	0.9434776173456719	T	T	T
0.6953142839702859	0.1286789144785358	0.8847082533282955	T	T	T
0.6849134436578497	0.0026710872452899	0.9457645223706699	T	T	T
0.6951904577222054	0.8686637529162484	0.9392872229990800	T	T	T
0.4905241841561220	0.0472268039750705	0.7135596069628056	T	T	T
0.4852168909997135	0.8642530370912039	0.7122963221603069	T	T	T
0.3563921259597776	0.4345150426432706	0.7048251912262882	T	T	T
0.3090575833588161	0.4346462549037233	0.8882927334311425	T	T	T
0.2038156278357179	0.4565083613952520	0.0079065732878502	T	T	T
0.0967187941696687	0.4315551868884014	0.8967611079394637	T	T	T
0.0996157914006201	0.4397778031413986	0.6978648430278782	T	T	T
0.2272564932661880	0.4610365555630345	0.7397877065970079	T	T	T
0.3553940135440927	0.6730694356019202	0.7335969151200383	T	T	T
0.3050018110920076	0.6507581001920437	0.9094090623934653	T	T	T
0.1919936891950702	0.6462017993912440	0.0115672842144734	T	T	T
0.0910294085207016	0.6705174773963218	0.8883369135887250	T	T	T
0.1015778604869016	0.6554374838978148	0.6925281364029701	T	T	T
0.2268832059056529	0.6426227566248987	0.7494591384646945	T	T	T
0.3207301743731150	0.5497391929732612	0.7843478736393296	T	T	T
0.0813916513613954	0.5488782724999418	0.8083369493060416	T	T	T
0.4341006740433542	0.3761447197310754	0.5708031029470700	T	T	T
0.4202327245613480	0.5078460730344917	0.5637407339931478	T	T	T
0.3944705484169166	0.6385550776435004	0.5522168259006924	T	T	T
0.1931484736382799	0.3657017364430590	0.6105911080729476	T	T	T
0.1779332804852628	0.4948662705465565	0.5613532719155969	T	T	T
0.1945929565197557	0.6282836978213271	0.5565690536689983	T	T	T
0.9855385832204435	0.4550210967355962	0.7923817157016240	T	T	T
0.9841796292517744	0.6369839510663782	0.7792743339889887	T	T	T
0.1405952680973464	0.5683564156529161	0.2158440724965713	T	T	T
0.1997083671533119	0.5575808887147810	0.3912525568810186	T	T	T
0.2973879704154505	0.5467213424053147	0.5272574142146085	T	T	T
0.3917734899593056	0.5671466562455740	0.3899425520037418	T	T	T
0.3981763568264386	0.5584283065255471	0.1932205292430320	T	T	T
0.2705516113307329	0.5377374269316442	0.2295823205398425	T	T	T
0.1443200070709142	0.3227069252072534	0.2438216467558329	T	T	T
0.1963587523150583	0.3566765562074373	0.4156417747958815	T	T	T
0.3099046674779330	0.3526099420283103	0.5153414594604449	T	T	T
0.4094020428785571	0.3282499330225426	0.3877684526369467	T	T	T
0.3960887014090297	0.3413731132620239	0.1906676919684773	T	T	T
0.2726972065014865	0.3538986964219718	0.2532509591697770	T	T	T
0.1786031003428154	0.4487039777017974	0.2770634899047389	T	T	T
0.4105255653826086	0.4487152977240965	0.3071453233867123	T	T	T
0.0681959290742954	0.6239120409097535	0.0718479181753130	T	T	T
0.0842784612453985	0.4924815672134544	0.0735724660948023	T	T	T
0.1154586089090598	0.3626242135230333	0.0593290150016360	T	T	T
0.3086957208123165	0.6339784045220390	0.1039525670334172	T	T	T
0.3224724816336267	0.5042980106653011	0.0533771007082884	T	T	T

Structure files (CONTCAR) involved in this work:

0.3001655972282201	0.3708620544877030	0.0592444735559018	T	T	T
0.5068494891560376	0.5397013274374154	0.2968573289067785	T	T	T
0.5125669298139268	0.3643906759986464	0.2737369469147846	T	T	T
0.4383718409796687	0.7509377268082975	0.6338975675506294	T	T	T
0.1910274490450945	0.7480839805791604	0.6365726102344207	T	T	T
0.2744126648684516	0.7509649813110800	0.0297636015856387	T	T	T
0.1091785075642708	0.7484268054359129	0.0454811525175922	T	T	T
0.0668716685785723	0.2484482640075446	0.1289251774985667	T	T	T
0.3068641203013555	0.2497291946429011	0.1363666791017851	T	T	T
0.2244768565918337	0.2501894986175698	0.5273795242045922	T	T	T
0.3943971651123983	0.2509008899633254	0.5454615446627648	T	T	T
0.5569091041430355	0.2496980125656661	0.3522127665921567	T	T	T
0.8149264477134541	0.2510685179068541	0.3515225399234590	T	T	T
0.7278922053732683	0.2490948406766134	0.9409598071961839	T	T	T
0.8918902948115685	0.2504886068914453	0.9460471581576465	T	T	T
0.9467101004592019	0.7533372209700960	0.8580726105428418	T	T	T
0.6867286303659028	0.7530718154754545	0.8484682633544786	T	T	T
0.7782076552250069	0.7472773427309106	0.4460364169339411	T	T	T
0.6115455742109606	0.7492060437141942	0.4488145228696069	T	T	T
0.9304597742335515	0.4848042200819392	0.5212096627818238	T	T	T
0.9116998997075677	0.4382525618433687	0.3960129778921712	T	T	T
0.8688160884432646	0.5546810485444496	0.5605555133938017	T	T	T
0.0541410228097639	0.5754212374953561	0.5208953840302381	T	T	T
0.0628517860587865	0.5473866526545982	0.3952159543338554	T	T	T
-0.0150103218694603	0.5776092065579310	0.4356754612711689	T	T	T
0.0353287678751574	0.6938394279622123	0.4619961906094291	T	T	T
0.0381814004724032	0.6666453653211014	0.3352480195629715	T	T	T
0.1114339288436574	0.6642443984845682	0.4099386497316924	T	T	T
0.9766966946662020	0.4894928227803843	0.5428713388992472	T	T	T
0.0391118752885458	0.5854360058387639	0.4429932767632623	T	T	T
0.0571700334614655	0.6566011467286149	0.4108171556556146	T	T	T

Figure S13 IS

Si Al O Ga H C

1.0000000000000000		
20.0219999999999985	0.0000000000000000	0.0000000000000000
0.0000000000000000	19.8990000000000009	0.0000000000000000
0.0000000000000000	0.0000000000000000	13.3829999999999991

93 3 192 1 8 2

Selective dynamics

Direct

0.4217625114217803	0.0571316731531257	0.6480159568529367	T	T	T
0.3008518239840862	0.0268975960406150	0.7894533968336082	T	T	T
0.2793276416556988	0.0606232001702559	0.0125809973617153	T	T	T
0.1195796408997815	0.0638885128318348	0.0130419328983896	T	T	T
0.0669355439722228	0.0297679133138491	0.7999277749528817	T	T	T
0.1761350388175154	0.0558977702568951	0.6514200176988807	T	T	T
0.4193210260267908	0.8271594521925392	0.6706409602374770	T	T	T
0.3014602216172268	0.8685188677495121	0.8097206713209699	T	T	T
0.2668662879468039	0.8283937237389981	0.0299015682814601	T	T	T
0.1118542383068504	0.8265991156279878	0.0171362476460018	T	T	T
0.0615138223938569	0.8707576220033258	0.8028182026453696	T	T	T
0.1788854757316222	0.8278750700878068	0.6736658263832743	T	T	T
0.0750031613111867	0.9429380944475266	0.1506888906834130	T	T	T

Structure files (CONTCAR) involved in this work:

0.1958285221899793	0.9730827983537143	0.2933117607621503	T	T	T
0.2165954473035920	0.9369094961735681	0.5145343763150737	T	T	T
0.3762150969996130	0.9338017747038828	0.5155881386099957	T	T	T
0.4297966725928468	0.9694515459250157	0.3045135695330739	T	T	T
0.3202064744015302	0.9450091006429359	0.1553444878884861	T	T	T
0.0780922381494142	0.1730862017300949	0.1653067122787588	T	T	T
0.1955079224221746	0.1304323198821972	0.3075107415479221	T	T	T
0.2307064936064978	0.1731724075205135	0.5247209757699981	T	T	T
0.3852952509712743	0.1737404411126145	0.5122357798188041	T	T	T
0.4363432105333241	0.1277907988876602	0.3018406490218481	T	T	T
0.3183743154602628	0.1674986274176007	0.1714794209709753	T	T	T
0.5834991385718369	0.5544523200863286	0.3500941573982955	T	T	T
0.6960133056305616	0.5278876008440769	0.1882349915907507	T	T	T
0.7145003204283353	0.5657141880992582	0.9757413231573598	T	T	T
0.8728151348129400	0.5645671496524511	0.9852862940486656	T	T	T
0.9331281298019087	0.5315155663128673	0.1918221485438411	T	T	T
0.5760601710460881	0.3298347319064399	0.3343510319999389	T	T	T
0.7007361441839693	0.3737871741829705	0.2019514407397402	T	T	T
0.7302239156479061	0.3259705772680557	0.9880571202542413	T	T	T
0.8822636863116101	0.3277035128889537	0.9860829632330312	T	T	T
0.9350962403119467	0.3738479701900479	0.1975464403577158	T	T	T
0.9293160783832016	0.4425552192684211	0.8574788959362852	T	T	T
0.7820155874403817	0.4384819782044380	0.4905840323370984	T	T	T
0.6227231249826489	0.4309961994265287	0.4926946182225249	T	T	T
0.5675194463158876	0.4680955701340466	0.7060183502094138	T	T	T
0.6703780383318920	0.4364505132815189	0.8571398269062245	T	T	T
0.9182327148380869	0.6727882090580583	0.8305684143536137	T	T	T
0.8001435368066917	0.6344588733046471	0.6936045819485870	T	T	T
0.7667068054626879	0.6694368701805137	0.4769087068507850	T	T	T
0.6114964450454282	0.6711205847992198	0.4868084242125444	T	T	T
0.5631710290397195	0.6264016229428481	0.7031817107420947	T	T	T
0.6818276525854132	0.6811090512292955	0.8223700690525123	T	T	T
0.5742186443466795	0.9431949170466482	0.3647225902834073	T	T	T
0.6932420218691090	0.9725924140154841	0.2206153524801653	T	T	T
0.7176823593696399	0.9409581326140425	0.9995583420224631	T	T	T
0.8775327883627706	0.9340484684838251	0.9953415969363263	T	T	T
0.9305703368332807	0.9695540695513584	0.2057433535455162	T	T	T
0.8190171701190273	0.9432692714552592	0.3545177325550762	T	T	T
0.5803178663150107	0.1745485687569756	0.3346596692537022	T	T	T
0.6960521222537985	0.1286515437821219	0.1973445987949862	T	T	T
0.7308234567046197	0.1706471552762025	0.9768111897983718	T	T	T
0.8851135927136776	0.1734263153033387	0.9938814570473402	T	T	T
0.9338750396114495	0.1276855348405718	0.2047380116837487	T	T	T
0.8168162617309065	0.1660228014034935	0.3350678968229260	T	T	T
0.9228750821093865	0.0576169158869177	0.8619550217351069	T	T	T
0.8038351611530357	0.0284969431034033	0.7213367768260680	T	T	T
0.7797176624737213	0.0596274110460457	0.4971044099838492	T	T	T
0.6200511444177181	0.0676995082721609	0.4939234465975104	T	T	T
0.5667289402471734	0.0318196936436277	0.7020062483368258	T	T	T
0.6769769161823950	0.0548834133680885	0.8537694265308161	T	T	T
0.9174497303029259	0.8256970131720556	0.8390968082417550	T	T	T
0.8024344314791688	0.8728180402008539	0.7028062035388203	T	T	T
0.7663755145418857	0.8303545742086892	0.4848714361747349	T	T	T

Structure files (CONTCAR) involved in this work:

0.6116768805128765	0.8258516101784532	0.4974686849720733	T	T	T
0.5619611908174859	0.8754040040685038	0.7036334507678144	T	T	T
0.6779567926327662	0.8372837152315811	0.8369342973446436	T	T	T
0.4223031725780143	0.4452286822130092	0.6403688127002886	T	T	T
0.3036154587841733	0.4740397863808065	0.7889712580901731	T	T	T
0.2860437581141956	0.4341293092621578	0.0084805954183628	T	T	T
0.1295374899917464	0.4325925919646468	0.0061242430696074	T	T	T
0.0770131515221750	0.4725495239501168	0.8000942514476024	T	T	T
0.1817397271591458	0.4497587521202127	0.6460352778276252	T	T	T
0.4230143101433802	0.6723579290862542	0.6646425005555329	T	T	T
0.3008408349485358	0.6305144936521080	0.7999302264787955	T	T	T
0.2695180657996878	0.6724235427748673	0.0188381084458909	T	T	T
0.1154318304126699	0.6738092931493876	0.0082025964287717	T	T	T
0.0655979570561262	0.6296500745727344	0.7999670761899056	T	T	T
0.1786932026075987	0.6692525480319481	0.6634687656736865	T	T	T
0.0793774892745572	0.5539556048172022	0.1351323144072342	T	T	T
0.2003952124495957	0.5285383845910858	0.2804898739509322	T	T	T
0.2214348085142087	0.5677051552298762	0.5020736207644027	T	T	T
0.3823873291479920	0.5698845806638482	0.5046696790353936	T	T	T
0.4346295964867440	0.5280727410584491	0.2964792111256764	T	T	T
0.3283192199289402	0.5530552103143682	0.1432494190715018	T	T	T
0.0810967566171372	0.3281481234037653	0.1569345114360831	T	T	T
0.1958489426237780	0.3701925265474387	0.3039341098219019	T	T	T
0.2314848306629194	0.3300550246561881	0.5231241479963814	T	T	T
0.3857375967867488	0.3271600716730514	0.5097772345957680	T	T	T
0.4331989240262367	0.3710640434037332	0.2961243597372128	T	T	T
0.3171120545079662	0.3260431392878906	0.1668241603428840	T	T	T
0.8101021350608136	0.5596476623559010	0.3329203387329285	T	T	T
0.8230753903915393	0.3254073643380351	0.3272452761571265	T	T	T
0.7957242781003959	0.4729192272065367	0.7261657018228767	T	T	T
0.3563607834810450	0.0622954830238318	0.7190315847121644	T	T	T
0.2993776079575198	0.0659945900138036	0.8956948465105760	T	T	T
0.1991758429067987	0.0513944578053835	0.0271898377059136	T	T	T
0.1001187146336434	0.0670840291924913	0.8958758868417556	T	T	T
0.1013178619541824	0.0574194993381639	0.6980475992485348	T	T	T
0.2276179923555721	0.0325736770472301	0.7385432602098780	T	T	T
0.3571239708493272	0.8265299538664900	0.7482467473628107	T	T	T
0.3039330842596917	0.8433797960749848	0.9246123137508718	T	T	T
0.1891381863359141	0.8519972961105988	0.0206161974419188	T	T	T
0.0837261276294928	0.8321132722367951	0.9042267426598881	T	T	T
0.1014870968899403	0.8380109375961073	0.7084354771746517	T	T	T
0.2275480520561063	0.8546903811220877	0.7629292350333703	T	T	T
0.3192246476187917	0.9480394128494962	0.8044382180108520	T	T	T
0.0803146882181888	0.9496593928129481	0.8118320680964003	T	T	T
0.4296807085342577	0.1266391964629304	0.5852950169371706	T	T	T
0.4161066488117119	0.9948313922231355	0.5696874121772089	T	T	T
0.3969525203577314	0.8627614797245136	0.5664779207769348	T	T	T
0.1936959108360338	0.1307911329776689	0.6117974729032976	T	T	T
0.1786294579729420	0.0025506165597299	0.5594402997510355	T	T	T
0.1926288986819947	0.8686453250466671	0.5705875176823810	T	T	T
0.9877674791200007	0.0460115070526322	0.7913776294932984	T	T	T
0.9815175816443742	0.8620887310928651	0.7864579152889389	T	T	T
0.1410209870458380	0.9390290731496788	0.2203376727829210	T	T	T

Structure files (CONTCAR) involved in this work:

0.1972602645853440	0.9308651494923577	0.3971593638678459	T	T	T
0.2965825029914771	0.9468195538322270	0.5293318766313246	T	T	T
0.3957930459781276	0.9301226652953111	0.3982954206284768	T	T	T
0.3952048096569464	0.9451643962920364	0.2008931282105763	T	T	T
0.2691664853143994	0.9702492363460939	0.2420625993584609	T	T	T
0.1412837450757899	0.1707162092100550	0.2408383220557327	T	T	T
0.1931739255620447	0.1624693608323793	0.4185904764119042	T	T	T
0.3078858583158404	0.1481561644464656	0.5147962331877709	T	T	T
0.4133423989282779	0.1708885270530099	0.3989227144954871	T	T	T
0.3957499099329163	0.1553016878976275	0.2044171352988571	T	T	T
0.2699134883930028	0.1391451585153819	0.2600496598477774	T	T	T
0.1761578484443134	0.0512198795097824	0.3131775919138109	T	T	T
0.4182122539300246	0.0494708901223999	0.3212301985100586	T	T	T
0.0668139369241867	0.8717265498648343	0.0921694107605409	T	T	T
0.0800383031030326	0.0028931301870796	0.0681811563627100	T	T	T
0.0974592755512924	0.1350956765442151	0.0618909207226370	T	T	T
0.3024291402604641	0.8691873397607650	0.1199456185327847	T	T	T
0.3166104704630736	0.9953691028635426	0.0598247708583942	T	T	T
0.3034225776042753	0.1292028184455612	0.0669445922324480	T	T	T
0.5086467492113212	0.9524002313440855	0.2948534924974733	T	T	T
0.5161410197284142	0.1369204516766787	0.2839402519267000	T	T	T
0.6451525413430973	0.5573455976182553	0.2727608614832548	T	T	T
0.6839254005590828	0.5726219902339739	0.0874845569095255	T	T	T
0.7942025101501938	0.5467352654234492	0.9822386631917249	T	T	T
0.9006680835530081	0.5720587074268597	0.0996029982710959	T	T	T
0.9017011580766389	0.5648577175199361	0.2990292971311539	T	T	T
0.7722551967174657	0.5359967289166256	0.2242488617697273	T	T	T
0.6405965500429894	0.3384973965046862	0.2643066346639538	T	T	T
0.7143843921172794	0.3250099361416479	0.1064123854574534	T	T	T
0.8061962079899012	0.3544026226168720	0.9676357800077686	T	T	T
0.9021229099103095	0.3351444065753669	0.1026770922064974	T	T	T
0.9066710203248847	0.3412264641951607	0.2986076169274482	T	T	T
0.7673919180642523	0.3771453026468419	0.2682114933853272	T	T	T
0.6781295741657458	0.4488867054363566	0.1656746184129798	T	T	T
0.9135744552512071	0.4535088327794943	0.1906620956227571	T	T	T
0.5723296325151940	0.6273142266580019	0.4025186404287308	T	T	T
0.6001026110755048	0.4999774909271099	0.4378220404200882	T	T	T
0.5865168521360874	0.3670278818995116	0.4416099784794064	T	T	T
0.7964605612156277	0.6396351934591757	0.3751885832021805	T	T	T
0.8061115453616066	0.5014943298948408	0.4284689999574703	T	T	T
0.8272361099684225	0.3696439796983494	0.4503710540217505	T	T	T
0.0126182212782042	0.5435189841382556	0.2031438680283874	T	T	T
0.0162808141002814	0.3710606967136169	0.1923961775287616	T	T	T
0.8739494583297989	0.4381236814559888	0.7677063291348141	T	T	T
0.8103271761515262	0.4399132044212448	0.6046525091437753	T	T	T
0.7038713734491022	0.4207542279807568	0.4844574141222932	T	T	T
0.6012776667235148	0.4330475902854258	0.6087021645432198	T	T	T
0.5963912738359248	0.4335135894007430	0.8064324422098074	T	T	T
0.7278342430166473	0.4335050606162137	0.7740066014962886	T	T	T
0.8635301670935434	0.6744808706095784	0.7421085961101392	T	T	T
0.8083251477719624	0.6403815710820776	0.5728990581099873	T	T	T
0.6888097044339305	0.6470283770827832	0.4921756590638689	T	T	T
0.5772210271770349	0.6601013663481176	0.5950876185042557	T	T	T

Structure files (CONTCAR) involved in this work:

0.6050878868427776	0.6641956883434511	0.7906064154317021	T	T	T
0.7303295772928926	0.6715369763803195	0.7256023408570759	T	T	T
0.7997967050164511	0.5583199808613860	0.7325425178939335	T	T	T
0.5848206508010160	0.5479066065545600	0.7022947495587448	T	T	T
0.9333196378972449	0.3722443905773186	0.9180862627105760	T	T	T
0.9146612877684576	0.5035428351732153	0.9336203731362297	T	T	T
0.8893202076075388	0.6342537014739889	0.9286356194857680	T	T	T
0.6759597914401270	0.3723327453789175	0.9318412561797600	T	T	T
0.6745583150113121	0.5064986195727632	0.9193839157699045	T	T	T
0.7059627704552832	0.6360585634466596	0.9165156573647005	T	T	T
0.4873239963032256	0.4575973546373747	0.7088451450305536	T	T	T
0.4832771686102760	0.6348632575903737	0.7250124571489504	T	T	T
0.6396914465948996	0.9366567188142144	0.2940556578881401	T	T	T
0.6942074765890944	0.9330981898015196	0.1146630766038492	T	T	T
0.7981839558429960	0.9499745279203746	0.9904462205533255	T	T	T
0.9017213644983062	0.9278734421081087	0.1105479047219599	T	T	T
0.8938914665555336	0.9450189141809821	0.3075915525926574	T	T	T
0.7675198082953989	0.9686563000132588	0.2686781796603368	T	T	T
0.6424417986846274	0.1743890758784193	0.2572838669466519	T	T	T
0.6952027791850108	0.1541533210793287	0.0825982978719392	T	T	T
0.8086361007436134	0.1465986686187238	0.9841455431985530	T	T	T
0.9087812759233408	0.1720616453155484	0.1097292913003349	T	T	T
0.8950470091710371	0.1524415244436056	0.3044887167345397	T	T	T
0.7703526122007525	0.1346465395559311	0.2454583067809733	T	T	T
0.6720769695856560	0.0505530902801947	0.2038103916908784	T	T	T
0.9179822242058755	0.0488702097369061	0.1838938807965086	T	T	T
0.5651932622727813	0.8746452650767006	0.4294789970514000	T	T	T
0.5791528760890129	0.0068279576798643	0.4407161281948850	T	T	T
0.6020526786115361	0.1378820171039848	0.4383373766472756	T	T	T
0.8017836968816001	0.8670655799041379	0.3899374844403042	T	T	T
0.8155552999877121	0.9932810598582770	0.4504144584639940	T	T	T
0.8028201450781696	0.1273407813785168	0.4402416983750070	T	T	T
0.0099022768816215	0.9547382740613647	0.2205237133073369	T	T	T
0.0140683966983829	0.1382119302393647	0.2193738676192533	T	T	T
0.8571159016392667	0.0671997210201815	0.7923268357554676	T	T	T
0.8022292560585145	0.0652111787550650	0.6133158200091562	T	T	T
0.6991975262817821	0.0509204795014761	0.4866710643205174	T	T	T
0.5976242448414844	0.0754370112606970	0.6100657237321396	T	T	T
0.6023543883975297	0.0516306559499617	0.8068424829174637	T	T	T
0.7292475691148407	0.0304577154997730	0.7684143468346962	T	T	T
0.8549904724518279	0.8255602681162518	0.7621725262457004	T	T	T
0.8044690199855816	0.8530821492234125	0.5860830523860013	T	T	T
0.6883102700333303	0.8528907353324742	0.4914366232569742	T	T	T
0.5863183335529583	0.8269239529270247	0.6128670083277992	T	T	T
0.6012623032089509	0.8545091042535919	0.8052533137229420	T	T	T
0.7274730699106958	0.8626274166598759	0.7474996050298099	T	T	T
0.8268001767386070	0.9503382112739555	0.7143785109950844	T	T	T
0.5786115075721033	0.9529303706154296	0.6752060945948508	T	T	T
0.9336263757924668	0.1259581407837336	0.9268636048750466	T	T	T
0.9167107624825721	0.9943837579797854	0.9383677639268767	T	T	T
0.8959189398565085	0.8630612739355654	0.9420881933692143	T	T	T
0.6931147052703118	0.1313478100539858	0.8870534766587613	T	T	T
0.6815495982886461	0.0066141907351184	0.9515595023037866	T	T	T

Structure files (CONTCAR) involved in this work:

0.6953586788579367	0.8735515648382297	0.9416308752055358	T	T	T
0.4876405508084390	0.0473335714415134	0.7167607692257990	T	T	T
0.4819829016841165	0.8666290475782017	0.7214850207082498	T	T	T
0.3572651782446716	0.4425027283558998	0.7121676145020541	T	T	T
0.3030037240202230	0.4289978414664161	0.8901750693744176	T	T	T
0.2072176075902879	0.4514300496238374	0.0259750929140520	T	T	T
0.1146080901024864	0.4298590587088821	0.8869936969038428	T	T	T
0.1058961206333700	0.4535840690062268	0.6900961223897081	T	T	T
0.2304952409831792	0.4720639269911657	0.7368178149122560	T	T	T
0.3552238829918536	0.6672745146126096	0.7300852485773425	T	T	T
0.3004493950477229	0.6683946477929474	0.9069772747870127	T	T	T
0.1920623655038230	0.6468147445232024	0.0160475387660781	T	T	T
0.0918732050288227	0.6755996508158173	0.8922418784046637	T	T	T
0.1014766103460138	0.6551620569025991	0.6973906384628727	T	T	T
0.2274954594414158	0.6360134194010956	0.7476967907487071	T	T	T
0.3206079510716531	0.5519009619849927	0.8158766144646583	T	T	T
0.0858856403741280	0.5520242600263099	0.8232751611862902	T	T	T
0.4307802439200005	0.3742806970879528	0.5819349447295921	T	T	T
0.4156938274585267	0.5047671848194819	0.5579604097269131	T	T	T
0.4105366794005367	0.6380053324827106	0.5559571819151762	T	T	T
0.1954606869533597	0.3732163495707750	0.6107239831136899	T	T	T
0.1891180748437183	0.5001266146933413	0.5511206410325482	T	T	T
0.1911811767825039	0.6345766380679572	0.5550588890075666	T	T	T
0.9985541924776871	0.4526722888942999	0.7969366343972986	T	T	T
0.9851507893797161	0.6352403380885450	0.7882542613250537	T	T	T
0.1431970925585472	0.5607572697237654	0.2086148696151727	T	T	T
0.2010051237395983	0.5704117490256083	0.3847402800109023	T	T	T
0.3017492697722964	0.5654939536502251	0.5169483061118455	T	T	T
0.4033650716320086	0.5715679440594259	0.3880842381560416	T	T	T
0.4021398613155753	0.5565397711290935	0.1933046579302980	T	T	T
0.2730843700053135	0.5341695898819497	0.2282413753339252	T	T	T
0.1374034518741845	0.3315620178443393	0.2436375080343440	T	T	T
0.1934677711736134	0.3427076624185033	0.4176941940421220	T	T	T
0.3087942994838254	0.3541913078743555	0.5124674206927996	T	T	T
0.4123404876801630	0.3294099739998284	0.3956829826363897	T	T	T
0.3937808933449785	0.3404036410946206	0.2001557313111016	T	T	T
0.2683294771003236	0.3555413696423504	0.2540039288640676	T	T	T
0.1816660940237102	0.4505907300825051	0.3023113162116630	T	T	T
0.4136105733301498	0.4496485672168422	0.3118305899645116	T	T	T
0.0685829222017955	0.6228859307656924	0.0723329002114290	T	T	T
0.0844508359215198	0.4909460684117610	0.0584655215834390	T	T	T
0.1107283668371398	0.3599831745777354	0.0536231396866593	T	T	T
0.3117428224886464	0.6258028631774275	0.0948993845709071	T	T	T
0.3290461680973009	0.4948991537064945	0.0576861976171868	T	T	T
0.3027499968667277	0.3623258717213316	0.0600661576273280	T	T	T
0.5151874244417459	0.5348490773680975	0.2911522773823558	T	T	T
0.5125410386471636	0.3628413186620506	0.2759600115993435	T	T	T
0.4408860103190211	0.7505923859521166	0.6456101859649033	T	T	T
0.1930344692692127	0.7489080970485205	0.6523087193186650	T	T	T
0.2726317093400914	0.7493173608506709	0.0579420121157749	T	T	T
0.1078272770310566	0.7487856713822810	0.0539739349286961	T	T	T
0.0609519222261511	0.2505752627366118	0.1370145013385282	T	T	T
0.3040216995719193	0.2465431167326372	0.1526845132857654	T	T	T

Structure files (CONTCAR) involved in this work:

0.2268937861125329	0.2518720968382769	0.5554480721200327	T	T	T
0.3899415706808452	0.2507819829693970	0.5513590820455899	T	T	T
0.5608529391890117	0.2516614014725890	0.3594880455722098	T	T	T
0.8016447470688942	0.2441886588413892	0.3491983441766349	T	T	T
0.7259341434386508	0.2493560272205087	0.9476965647418778	T	T	T
0.8904311391767975	0.2499625615025153	0.9524813206315162	T	T	T
0.9369909378568514	0.7485381553487568	0.8655835082967465	T	T	T
0.6863854713331562	0.7582130328180334	0.8586348510989270	T	T	T
0.7726286051101825	0.7504746699310219	0.4721566405434944	T	T	T
0.6058543923688667	0.7497222090192723	0.4554567698558585	T	T	T
0.9035425616949683	0.3978841211053618	0.6355336517851264	T	T	T
0.8955807313124753	0.3204781048276556	0.6495629318875458	T	T	T
0.9323391108564297	0.5955231522959610	0.4409423506061270	T	T	T
0.9224802736963106	0.6620640949253009	0.3511020600698402	T	T	T
0.9935918413886697	0.6060286439351924	0.3436901200471855	T	T	T
0.9442639675249583	0.4613936692089805	0.4773447803806845	T	T	T
0.9549315583180291	0.5096774270681035	0.5880485245607036	T	T	T
0.0129341184960709	0.4437560274599214	0.5589913469246470	T	T	T
0.8752177542517867	0.3805393206383008	0.4505301860617608	T	T	T
0.9408174451728135	0.6108778985223774	0.3633131908743936	T	T	T
0.9604030741106337	0.4591125501610482	0.5559589947040053	T	T	T

Figure S13 TS

Si Al O Ga H C

1.0000000000000000

20.0219999999999985 0.0000000000000000 0.0000000000000000

0.0000000000000000 19.8990000000000009 0.0000000000000000

0.0000000000000000 0.0000000000000000 13.3829999999999991

93 3 192 1 8 2

Selective dynamics

Direct

0.4218236018994213	0.0575330081207144	0.6481654205290116	T	T	T
0.3007835090914465	0.0271995112423191	0.7892066939364143	T	T	T
0.2794850511091339	0.0608261543005436	0.0126398099977233	T	T	T
0.1197190906614236	0.0642222821392508	0.0135583259822297	T	T	T
0.0667754967608522	0.0300640649669712	0.8005468111467674	T	T	T
0.1757542832050679	0.0564611815727112	0.6517011372976466	T	T	T
0.4189497620850369	0.8272691005552802	0.6703293593553619	T	T	T
0.3013233353670636	0.8688034350872260	0.8093125510956324	T	T	T
0.2668194961889917	0.8287749041048872	0.0296573626779174	T	T	T
0.1118182686148666	0.8269976570429450	0.0171764073913414	T	T	T
0.0612678075823009	0.8709556566493509	0.8029215522793632	T	T	T
0.1786122212101706	0.8283287029309677	0.6735123063386379	T	T	T
0.0745476063394247	0.9431503882967857	0.1508362712128637	T	T	T
0.1954580824006394	0.9733320235461214	0.2930977421186820	T	T	T
0.2161867785247931	0.9376213079321610	0.5148352721226286	T	T	T
0.3756502661146155	0.9343582219531377	0.5160191788395005	T	T	T
0.4293542900715800	0.9698518581910920	0.3051267719865109	T	T	T
0.3200987514466170	0.9451519990947801	0.1552411925968426	T	T	T
0.0779319677472461	0.1734234834273937	0.1656140528176208	T	T	T
0.1954290172342651	0.1307013714349961	0.3072792365602827	T	T	T
0.2305883801566050	0.1734397134908627	0.5249398502780661	T	T	T
0.3851781303263416	0.1742813369952133	0.5128067179629668	T	T	T
0.4363064168228051	0.1281926823235613	0.3026391101163550	T	T	T

Structure files (CONTCAR) involved in this work:

0.3186295813175943	0.1677086605338473	0.1715452256030535	T	T	T
0.5818056337981434	0.5556199780192448	0.3487062601918549	T	T	T
0.6955045866215983	0.5277352754585521	0.1885595207958835	T	T	T
0.7120106619483145	0.5659512742312559	0.9758990326158359	T	T	T
0.8708941271871592	0.5630458637052285	0.9808143066753318	T	T	T
0.9337987571326700	0.5302791490899823	0.1889126736600926	T	T	T
0.5769294680488111	0.3299660678113206	0.3357898514165936	T	T	T
0.7038528350986025	0.3732623439971279	0.2080723950515460	T	T	T
0.7311718694255724	0.3268614986623497	0.9922656473515771	T	T	T
0.8829266264612612	0.3279873032846073	0.9843578612416866	T	T	T
0.9352649762260477	0.3730856768301113	0.1990786100274079	T	T	T
0.9272836698011838	0.4405455117990850	0.8485283524015323	T	T	T
0.7804782015943130	0.4371163802008807	0.4815716238085151	T	T	T
0.6196127929219296	0.4340140164786136	0.4925920033089681	T	T	T
0.5668435498523350	0.4684131566266859	0.7080479953739864	T	T	T
0.6700445896116831	0.4350687439062700	0.8581078310131860	T	T	T
0.9178756020383230	0.6731210248997513	0.8295026796331838	T	T	T
0.7992430624134506	0.6343648185309037	0.6961731652178086	T	T	T
0.7668325730978399	0.6681496821870887	0.4780938615054685	T	T	T
0.6110846457385509	0.6710712115161807	0.4858602537098888	T	T	T
0.5629076467253114	0.6265950172921941	0.7035595489130387	T	T	T
0.6804795028375884	0.6822423459590153	0.8236603024424241	T	T	T
0.5739858649113235	0.9435758085992968	0.3655665999237669	T	T	T
0.6938769858742098	0.9732563709612316	0.2229533113526009	T	T	T
0.7174462857664736	0.9417808145461104	0.0007779449642789	T	T	T
0.8772557419000364	0.9342433959048415	0.9961423228320975	T	T	T
0.9297569899220262	0.9702521608609226	0.2068182627649460	T	T	T
0.8195842552497123	0.9430378874198727	0.3579639106085650	T	T	T
0.5803229815807878	0.1750069702159543	0.3367918040344622	T	T	T
0.6966456959035364	0.1297596654886734	0.1999515862177849	T	T	T
0.7305422149350898	0.1715139417358523	0.9790926108459049	T	T	T
0.8847338820622238	0.1735986788657630	0.9950077553373111	T	T	T
0.9336468623961743	0.1283304433999672	0.2057980286219618	T	T	T
0.8177265670698721	0.1675550159909076	0.3378774859577661	T	T	T
0.9228171038261878	0.0578339088096162	0.8632484206502842	T	T	T
0.8032942759943030	0.0293028427298461	0.7231542945716136	T	T	T
0.7798527448578998	0.0595847594547031	0.4987201921471970	T	T	T
0.6202828725917500	0.0677315440703402	0.4949640913032050	T	T	T
0.5668490077849004	0.0321634253085879	0.7033464442147683	T	T	T
0.6764397441471275	0.0560330395484096	0.8562091116543686	T	T	T
0.9173277294257004	0.8259981264828815	0.8406210671049777	T	T	T
0.8016162399477383	0.8736137052758920	0.7051199043295823	T	T	T
0.7670024075680423	0.8293851767535800	0.4868376521188579	T	T	T
0.6119142714336150	0.8260830659990323	0.4981939423510894	T	T	T
0.5617145561081207	0.8755669959402350	0.7044747883949758	T	T	T
0.6769854188270796	0.8381785315216854	0.8389642180588190	T	T	T
0.4224213784403676	0.4459195245521294	0.6397563410219359	T	T	T
0.3034570462705214	0.4739841056627537	0.7878677916821528	T	T	T
0.2857003756835356	0.4333537045487607	0.0067220890324909	T	T	T
0.1281440541421828	0.4319868857840429	0.0037471900273055	T	T	T
0.0756383248235089	0.4731520179869380	0.7976604017309017	T	T	T
0.1816547694503957	0.4501891828649791	0.6446809423365355	T	T	T
0.4228880957375306	0.6723935116999286	0.6630475133688303	T	T	T

Structure files (CONTCAR) involved in this work:

0.3007425954335619	0.6305172415656088	0.7987547057840146	T	T	T
0.2693946742586369	0.6728089439204190	0.0171035315323483	T	T	T
0.1152218260317293	0.6742451066560936	0.0072301236696030	T	T	T
0.0651268734139272	0.6302833903718326	0.7988091797390401	T	T	T
0.1787657863566855	0.6696937091883581	0.6628124775492507	T	T	T
0.0796870973249524	0.5540203245904168	0.1337990618010806	T	T	T
0.2003634727669253	0.5287592450582549	0.2800309823578196	T	T	T
0.2218172437180279	0.5684397471655317	0.5010976827936368	T	T	T
0.3828236916864151	0.5701528555230134	0.5029288192603066	T	T	T
0.4346285807223227	0.5287176682588649	0.2935851091065980	T	T	T
0.3274001507404813	0.5531341246090242	0.1415956458003517	T	T	T
0.0806036286412858	0.3285297639306035	0.1568210168111868	T	T	T
0.1967729040572170	0.3705229698786426	0.3022050540912110	T	T	T
0.2316005329882179	0.3303004323992931	0.5218600379682602	T	T	T
0.3860144535048449	0.3278527122961759	0.5094320953906767	T	T	T
0.4342569627019430	0.3711656114559570	0.2952488771201427	T	T	T
0.3181396292883329	0.3262886372281162	0.1659481243023430	T	T	T
0.8109286174171617	0.5598730198675201	0.3288078034088014	T	T	T
0.8258435508477466	0.3281936387019280	0.3429122868309513	T	T	T
0.7919134019105153	0.47444444651021076	0.7258280615308373	T	T	T
0.3563323245597141	0.0627551522812778	0.7190293284715717	T	T	T
0.2993004237931623	0.0660390405954033	0.8956469745233755	T	T	T
0.1993393071502758	0.0518892476891433	0.0276791163415041	T	T	T
0.1003258078834535	0.0671913196182279	0.8963221069565706	T	T	T
0.1010205509906185	0.0578564486651080	0.6986326336800014	T	T	T
0.2275102804590814	0.0330994705693505	0.7384233122410516	T	T	T
0.3568780514585045	0.8263913130558875	0.7482257024675657	T	T	T
0.3037095757219757	0.8440864232395245	0.9243757589715006	T	T	T
0.1890703737316899	0.8524543308384530	0.0210105750711578	T	T	T
0.0838282512239084	0.8323885777660048	0.9041799743492210	T	T	T
0.1012166211582087	0.8382995322369116	0.7084272385204128	T	T	T
0.2273390482199333	0.8550049843199375	0.7627299520659007	T	T	T
0.3192006272056873	0.9482782523794788	0.8034618967034729	T	T	T
0.0798479860973935	0.9498923355948383	0.8119540315426963	T	T	T
0.4297697075118939	0.1271252012133137	0.5855713770199129	T	T	T
0.4160482188395502	0.9951791823012003	0.5698926423527404	T	T	T
0.3962647121405032	0.8631593406742012	0.5665608203258965	T	T	T
0.1931421399132923	0.1314130589895891	0.6120418044608935	T	T	T
0.1779915058368870	0.0031554224069499	0.5596374136860395	T	T	T
0.1921322251904000	0.8692178403068821	0.5704909266978109	T	T	T
0.9876495387561518	0.0465563487497193	0.7924452152219714	T	T	T
0.9812587111631722	0.8619203729404198	0.7868419820473904	T	T	T
0.1402842719798797	0.9389167150879251	0.2210898047324302	T	T	T
0.1973488626084943	0.9315722346259552	0.3973303904531102	T	T	T
0.2961043181839385	0.9476680260421226	0.5304951401555825	T	T	T
0.3947778322231856	0.9306200493193356	0.3985644050175342	T	T	T
0.3949601839956422	0.9456684499710883	0.2012933568710194	T	T	T
0.2686265726817970	0.9703184531848922	0.2413870562419959	T	T	T
0.1411247648433290	0.1713227288714050	0.2412535569149115	T	T	T
0.1933927376597145	0.1622398523909268	0.4187009724195466	T	T	T
0.3078284478945278	0.1485166872854944	0.5160494176078145	T	T	T
0.4127845692207206	0.1713745012912846	0.3993094059388677	T	T	T
0.3959502470311196	0.1555864534499339	0.2048855738244253	T	T	T

Structure files (CONTCAR) involved in this work:

0.2698225836189721	0.1393630777113475	0.2597168838974129	T	T	T
0.1757896064699549	0.0515378240973599	0.3122853107449662	T	T	T
0.4179908367265321	0.0498854820513498	0.3218326448396418	T	T	T
0.0665433278692789	0.8719715675799422	0.0920684324188981	T	T	T
0.0802025620959068	0.0031736425774883	0.0685674809598791	T	T	T
0.0976032034972013	0.1354594032415461	0.0622227482088646	T	T	T
0.3026460128299716	0.8692165164581338	0.1198356555563047	T	T	T
0.3166228489737476	0.9953673138604801	0.0595406712566235	T	T	T
0.3040072224879143	0.1293002099585091	0.0669523662707007	T	T	T
0.5081446714898018	0.9524560384434642	0.2961847428115913	T	T	T
0.5161821455863790	0.1372551952409087	0.2859004964475042	T	T	T
0.6459327983278098	0.5560552767564270	0.2758428180526902	T	T	T
0.6791299226130204	0.5698366750912575	0.0864198194507444	T	T	T
0.7918288614387924	0.5487464196785697	0.9845617307880584	T	T	T
0.9032834418630481	0.5674682334562807	0.0923998132724423	T	T	T
0.9019364962090883	0.5670292634687134	0.2931396095835226	T	T	T
0.7721438387743595	0.5406093578572121	0.2188919385459208	T	T	T
0.6420972477784532	0.3377010802489664	0.2670089776919568	T	T	T
0.7181101073248769	0.3255668434412171	0.1110884406040913	T	T	T
0.8067903432670868	0.3552539505401155	0.9682520224974294	T	T	T
0.9063930883899648	0.3372152540520189	0.0985700935458105	T	T	T
0.9071174818337842	0.3392746649450936	0.2983048916253869	T	T	T
0.7692612335728805	0.3769726821345760	0.2762543484959642	T	T	T
0.6804452021357261	0.4479146514169914	0.1702346778128012	T	T	T
0.9133819178202898	0.4527786098493052	0.1928747298619883	T	T	T
0.5717937330207341	0.6290670617076572	0.3998521641983182	T	T	T
0.5917072883302527	0.5014363173097408	0.4387467497237981	T	T	T
0.5862501940435032	0.3680410946995971	0.4425689183816619	T	T	T
0.7980209112914645	0.6385263748977267	0.3774678128814494	T	T	T
0.8091532656040995	0.4975815641028347	0.4172439834437128	T	T	T
0.8205976185718792	0.3663120365894526	0.4641758799277135	T	T	T
0.0131824811339560	0.5425717204334241	0.2016991827317803	T	T	T
0.0169262377079286	0.3714895965592319	0.1958166868458714	T	T	T
0.8728178395910567	0.4342008553072259	0.7550828795351503	T	T	T
0.8069398456151902	0.4516349843390751	0.5989874309097419	T	T	T
0.7003357494240683	0.4305482749141633	0.4827682482316031	T	T	T
0.5994689310051029	0.4345973853500515	0.6092960706671100	T	T	T
0.5963337554665088	0.4314964608784627	0.8065447913030039	T	T	T
0.7278721853690004	0.4299546692898888	0.7747227997482444	T	T	T
0.8630643989473724	0.6755350935852232	0.7410268915969804	T	T	T
0.8062223491510646	0.6369089220663007	0.5751090597314470	T	T	T
0.6884124729036432	0.6470843616036308	0.4902622097208803	T	T	T
0.5773087105368462	0.6578650674971007	0.5940091157303771	T	T	T
0.6038934119145606	0.6669722532590667	0.7895155310763474	T	T	T
0.7295397856347282	0.6714556071296803	0.7276777222504285	T	T	T
0.7998459975555090	0.5590688667615832	0.7405458036694360	T	T	T
0.5849972214513469	0.5481874304525698	0.7081516076779527	T	T	T
0.9317057773440724	0.3705344803171831	0.9090282289855410	T	T	T
0.9068714489039648	0.5010339543343501	0.9218371721931453	T	T	T
0.8889714557938586	0.6330087465742098	0.9260312753893006	T	T	T
0.6762641706201858	0.3734176071516284	0.9370433791331040	T	T	T
0.6748832651569511	0.5070644955287903	0.9146576300830790	T	T	T
0.7027171972512878	0.6368678731014091	0.9184535757574590	T	T	T

Structure files (CONTCAR) involved in this work:

0.4864743837028490	0.4587163616229630	0.7103001374790266	T	T	T
0.4828651362317308	0.6349749738967180	0.7240482902125889	T	T	T
0.6391516898721611	0.9372278731298312	0.2943281929933315	T	T	T
0.6961502485811287	0.9341015487836734	0.1167612440529594	T	T	T
0.7978898365057848	0.9495869455782725	0.9878185371670610	T	T	T
0.8996144743853881	0.9287722365776245	0.1122246744375354	T	T	T
0.8940698303990378	0.9458118042077588	0.3095793099317751	T	T	T
0.7673699571850967	0.9685383554076312	0.2732464503147563	T	T	T
0.6422449128929467	0.1748546989871029	0.2592509869641784	T	T	T
0.6953645209505317	0.1547722722626358	0.0849477257645492	T	T	T
0.8082476533422688	0.1468050473013544	0.9849151962313988	T	T	T
0.9083695768287215	0.1727633541034421	0.1108014787503876	T	T	T
0.8956967163144285	0.1528158383656931	0.3061555816048497	T	T	T
0.7707014621065709	0.1370910035927977	0.2479303097329368	T	T	T
0.6734400654204558	0.0513769730440387	0.2064247858738980	T	T	T
0.9174532188831561	0.0495242439842253	0.1847730548913304	T	T	T
0.5654680198919605	0.8750209372475194	0.4304400831828715	T	T	T
0.5789488459877135	0.0071574747728199	0.4416743727296246	T	T	T
0.6021285484804390	0.1381447860586410	0.4402921013083073	T	T	T
0.8033757350340565	0.8663438676827451	0.3927826775027058	T	T	T
0.8159859556073294	0.9925298749066683	0.4544953131788764	T	T	T
0.8038295926665477	0.1266579280022992	0.4415795558256918	T	T	T
0.0091421758734804	0.9549261881653150	0.2199241293008726	T	T	T
0.0140463152806993	0.1382232897559730	0.2193635667754691	T	T	T
0.8571657829788569	0.0676822400464762	0.7935554831805749	T	T	T
0.8011671912828843	0.0662774144251192	0.6154259775978643	T	T	T
0.6993565826617375	0.0506726282898339	0.4869674980360713	T	T	T
0.5982773622478456	0.0752672052841730	0.6113521296672445	T	T	T
0.6020513448644023	0.0523169308984116	0.8084024966265663	T	T	T
0.7291238728983177	0.0315197228857965	0.7714839357709180	T	T	T
0.8540583626924326	0.8266518801715166	0.7652917892391146	T	T	T
0.8036245773218861	0.8526514545089946	0.5889547522722584	T	T	T
0.6888563765583234	0.8520334655218844	0.4910484029567053	T	T	T
0.5869443117150391	0.8275673329831803	0.6137547933359293	T	T	T
0.6001863782101770	0.8541321512271078	0.8065435098242871	T	T	T
0.7266377879805423	0.8642929521480078	0.7502019674231003	T	T	T
0.8261097070561388	0.9511615843776748	0.7150831700685161	T	T	T
0.5786806773220263	0.9531829824889291	0.6772705803776872	T	T	T
0.9334913376938233	0.1260293408921820	0.9284510483279225	T	T	T
0.9168331761284501	0.9944658276464572	0.9394418063814449	T	T	T
0.8971864397020025	0.8631376987618329	0.9443976508769347	T	T	T
0.6920985827206103	0.1326649868412623	0.8894075505010458	T	T	T
0.6811206049005782	0.0078132546939970	0.9541176022829783	T	T	T
0.6931412087874103	0.8745720586927482	0.9439977878596278	T	T	T
0.4876625848668006	0.0477143459725037	0.7169943774203521	T	T	T
0.4816325740294679	0.8667130491785759	0.7210352853843190	T	T	T
0.3567419075397331	0.4429675275181258	0.7102234619952699	T	T	T
0.3035130457022919	0.4285639520304270	0.8886510655891721	T	T	T
0.2063548476099983	0.4488817242515907	0.0221958128747385	T	T	T
0.1113760603911280	0.4294197724323125	0.8849217942896227	T	T	T
0.1055780581401053	0.4545457014444605	0.6881696051167937	T	T	T
0.2300620036560744	0.4715243851161903	0.7363032889598307	T	T	T
0.3547295524970291	0.6666969962978458	0.7276058116740429	T	T	T

Structure files (CONTCAR) involved in this work:

0.3008629101689302	0.6688251171892897	0.9055128182954265	T	T	T
0.1919159364889615	0.6473043166125259	0.0134811884353676	T	T	T
0.0909846981670249	0.6759893442227506	0.8914891579662361	T	T	T
0.1014894220083687	0.6553770659946038	0.6964189428074832	T	T	T
0.2271482999912320	0.6361323324380784	0.7472437466375444	T	T	T
0.3200617089023114	0.5518448125358629	0.8152830736724117	T	T	T
0.0845730009360942	0.5523638313739384	0.8222444528330607	T	T	T
0.4312647620934753	0.3749494968076302	0.5814583523504041	T	T	T
0.4160106093738034	0.5052496469726413	0.5570052861603378	T	T	T
0.4111764072112165	0.6383473255253396	0.5539067856577428	T	T	T
0.1943170777484836	0.3737000527061203	0.6082223497893123	T	T	T
0.1895203744211624	0.5008741222015836	0.5503287661165364	T	T	T
0.1914987919884149	0.6352201428476789	0.5543062090915885	T	T	T
0.9967317503759692	0.4541391992950733	0.7904337601251632	T	T	T
0.9847841847126285	0.6361879060342022	0.7859354891696494	T	T	T
0.1434262077731591	0.5606122322388636	0.2074379388349542	T	T	T
0.2008714001862952	0.5710745257794054	0.3839336955940898	T	T	T
0.3021213241294819	0.5661076909694369	0.5155867600940144	T	T	T
0.4033558850681518	0.5713869342298132	0.3861798156433429	T	T	T
0.4013282552189373	0.5565803968163587	0.1907541042568488	T	T	T
0.2729363942250601	0.5343578245614189	0.2276332756731530	T	T	T
0.1391567736182669	0.3320233439779203	0.2402200357839087	T	T	T
0.1944071200647382	0.3420451720559617	0.4155060781092057	T	T	T
0.3089078949671895	0.3547152656950457	0.5127708045935778	T	T	T
0.4123180532139747	0.3303464707360631	0.3952059114777842	T	T	T
0.3948440241870542	0.3402069558534250	0.1993450212560894	T	T	T
0.2695299039485103	0.3570175484562660	0.2524835376906443	T	T	T
0.1818654468979763	0.4508533920701010	0.3026820605377391	T	T	T
0.4151529811494020	0.4499845212417437	0.3095107549600732	T	T	T
0.0687866475847631	0.6233570175919395	0.0720280137186927	T	T	T
0.0848980806719351	0.4917812981731011	0.0558279024255746	T	T	T
0.1078767179011333	0.3600283317198225	0.0516756869547319	T	T	T
0.3109953150516372	0.6259396868345605	0.0934805692893771	T	T	T
0.3272213529004623	0.4950331433875831	0.0561036537395312	T	T	T
0.3039115598051986	0.3620993441113957	0.0587500412078498	T	T	T
0.5147890655422126	0.5378159430416624	0.2853840505441692	T	T	T
0.5135908107718816	0.3622651726306540	0.2757696423773109	T	T	T
0.4405403117968188	0.7507735354673563	0.6448116762890320	T	T	T
0.1929232121512428	0.7493713673911002	0.6519968477126493	T	T	T
0.2725168936677563	0.7495483017217791	0.0567963843477329	T	T	T
0.1078607007597558	0.7490744221966844	0.0535154485727917	T	T	T
0.0605684232789011	0.2508422194579949	0.1374661945831568	T	T	T
0.3043006360313379	0.2468077092924961	0.1528552217880656	T	T	T
0.2267270328693140	0.2522824495877034	0.5550170169253014	T	T	T
0.3899866932050470	0.2514705865328147	0.5512554989687369	T	T	T
0.5609683201115916	0.2520419507844280	0.3620993903616535	T	T	T
0.8039217150406841	0.2451908454884945	0.3556762628065593	T	T	T
0.7260156506913956	0.2504382811264831	0.9509840772985889	T	T	T
0.8898952866379367	0.2498385021815425	0.9522445157165522	T	T	T
0.9363821999256239	0.7485082231665133	0.8662710613622542	T	T	T
0.6866686817476380	0.7591589809667028	0.8600872832145600	T	T	T
0.7740216201416877	0.7493272383284096	0.4756488785219511	T	T	T
0.6051685446061611	0.7499707783042949	0.4568732496113864	T	T	T

Structure files (CONTCAR) involved in this work:

0.8957259303521898	0.4158397923062843	0.6150349742156815	T	T	T
0.8702629077429244	0.3235188419826191	0.6188440284741411	T	T	T
0.9248751618251573	0.6019519611539442	0.4357791549784676	T	T	T
0.9319892383664901	0.6634061191469507	0.3382526698602862	T	T	T
0.9944613768023645	0.5982049594279724	0.3504069251390087	T	T	T
0.9624780231209720	0.4345716516422400	0.4602668415993139	T	T	T
0.9813617323530176	0.4962254236904573	0.5558745077116750	T	T	T
0.0183689432127272	0.4144176751603512	0.5627396800022950	T	T	T
0.8506719327368643	0.3323451764223325	0.5647647245460082	T	T	T
0.9416676362118175	0.6110413368664033	0.3589944953350332	T	T	T
0.9741928937157092	0.4426423792710883	0.5393933629506200	T	T	T

Figure S13 FS

Si Al O Ga H C

1.0000000000000000

20.0219999999999985 0.0000000000000000 0.0000000000000000

0.0000000000000000 19.8990000000000009 0.0000000000000000

0.0000000000000000 0.0000000000000000 13.3829999999999991

93 3 192 1 8 2

Selective dynamics

Direct

0.4218959965403347	0.0571604374946573	0.6480697267189638	T	T	T
0.3008711778155922	0.0268519207488102	0.7893279711360456	T	T	T
0.2794161262587918	0.0605598275263052	0.0125403472715371	T	T	T
0.1196908352032151	0.0640444046256397	0.0133482079899811	T	T	T
0.0669248311017852	0.0298516872082353	0.8004088122880630	T	T	T
0.1759725438860996	0.0559688118842651	0.6515773589940622	T	T	T
0.4193714268548998	0.8270422512285709	0.6705281480346464	T	T	T
0.3014699142839162	0.8684333452845905	0.8093896148719727	T	T	T
0.2669324562468228	0.8284576156717155	0.0297340154176974	T	T	T
0.1119736323657162	0.8267101306262868	0.0170569489673650	T	T	T
0.0615414623808983	0.8707557860165913	0.8028509953985739	T	T	T
0.1787853433523478	0.8279179872035000	0.6733567969738177	T	T	T
0.0747561782097112	0.9430076747606650	0.1506006860573870	T	T	T
0.1956361484139250	0.9731457828403665	0.2930647430481476	T	T	T
0.2165383022196578	0.9370670695770692	0.5145772130344068	T	T	T
0.3760869863856292	0.9338933388685839	0.5157547194854638	T	T	T
0.4295853504608779	0.9694502777084146	0.3047835491269489	T	T	T
0.3202070623895577	0.9449580604681872	0.1551972555507554	T	T	T
0.0779540714775661	0.1733241986245031	0.1655171918716689	T	T	T
0.1953579984596402	0.1305289993288371	0.3073757826884869	T	T	T
0.2306411875545721	0.1731393017064970	0.5248820907873903	T	T	T
0.3852282558465986	0.1738925396044073	0.5126778357400900	T	T	T
0.4359080929656122	0.1277183707997274	0.3022662885846079	T	T	T
0.3183138736940822	0.1675453277065221	0.1713602540426921	T	T	T
0.5821879356697351	0.5550372572350746	0.3506520105816392	T	T	T
0.6962160263612425	0.5280046385086340	0.1905867758547399	T	T	T
0.7109792852612521	0.5659851934390585	0.9780534865693801	T	T	T
0.8698764911205832	0.5607600352881879	0.9762961962602715	T	T	T
0.9334434022798314	0.5293976646481933	0.1873658892657112	T	T	T
0.5755364818853217	0.3295200880631587	0.3359293341970506	T	T	T
0.7060929038763157	0.3730670229760179	0.2156405283251977	T	T	T
0.7310693995626060	0.3273874630286978	0.9975709350954072	T	T	T
0.8823944298384763	0.3283977012522108	0.9839412989365542	T	T	T

Structure files (CONTCAR) involved in this work:

0.9352374869096814	0.3727954188879315	0.1993276136977715	T	T	T
0.9251423954868289	0.4380847638524820	0.8394570276955423	T	T	T
0.7763152990133746	0.4391102244789988	0.4806458369993097	T	T	T
0.6178794165845480	0.4318231245994649	0.4927243034096694	T	T	T
0.5679254158023798	0.4672675810574018	0.7089832497314743	T	T	T
0.6701858950380085	0.4351022807101360	0.8628555859780057	T	T	T
0.9178182913198031	0.6730007866313243	0.8299333056529090	T	T	T
0.8001033896399604	0.6334222286425296	0.6974985179083064	T	T	T
0.7671157697456999	0.6681405106851830	0.4794391803032554	T	T	T
0.6115920307362569	0.6707300111205886	0.4868441487075995	T	T	T
0.5632091154691171	0.6258206283905375	0.7041852410614270	T	T	T
0.6806261070690198	0.6813467203955098	0.8247032249552692	T	T	T
0.5742970915880473	0.9432342369807353	0.3649670821553640	T	T	T
0.6943994181212532	0.9732415646084246	0.2226256777471295	T	T	T
0.7175234776390412	0.9419230464155097	1.0000185860095183	T	T	T
0.8774366988304783	0.9344674671314761	0.9961966761923874	T	T	T
0.9301227208655802	0.9702010729578798	0.2071538155773141	T	T	T
0.8198333462771360	0.9422346920702555	0.3570915583281569	T	T	T
0.5795578575680213	0.1746034516355599	0.3359173794480526	T	T	T
0.6969986651113271	0.1307771855689889	0.2009442899091371	T	T	T
0.7302837857471338	0.1715949686168864	0.9796696637748947	T	T	T
0.8847703220705045	0.1738079400054704	0.9946402107560735	T	T	T
0.9335874522026522	0.1285902657529833	0.2060456239779582	T	T	T
0.8185177678063524	0.1696147914629006	0.3404972910566112	T	T	T
0.9228874887135790	0.0579262165599807	0.8628419619402158	T	T	T
0.8035347503485193	0.0291074950927296	0.7225318944516869	T	T	T
0.7798693923018897	0.0591303469480623	0.4980516381241606	T	T	T
0.6201823005765710	0.0675191474666349	0.4943700068501556	T	T	T
0.5669889806031762	0.0320549517410425	0.7029307108938012	T	T	T
0.6767609612266758	0.0564641752679117	0.8552906565919568	T	T	T
0.9175081546972478	0.8258097762263064	0.8407908663726168	T	T	T
0.8021723103394204	0.8733645548589939	0.7045832337870161	T	T	T
0.7670564996551189	0.8294549580884172	0.4869215081696834	T	T	T
0.6121552124433737	0.8258860004488715	0.4978568692224556	T	T	T
0.5620559162572132	0.8754037929190429	0.7043364360025332	T	T	T
0.6776497555068900	0.8377256971948427	0.8381952214525463	T	T	T
0.4229698429698784	0.4453168858356989	0.6406979890067154	T	T	T
0.3037940184681748	0.4739985327200484	0.7884262482607874	T	T	T
0.2856006617757767	0.4336953077541153	0.0072020511276910	T	T	T
0.1283603181993982	0.4320852160692652	0.0037917799709180	T	T	T
0.0751210476664104	0.4722050422069895	0.7974665226510064	T	T	T
0.1820637649010428	0.4498300354131207	0.6451448163986815	T	T	T
0.4231000720445000	0.6721630485653873	0.6638973945843765	T	T	T
0.3009135082097832	0.6304693345058581	0.7994553166281595	T	T	T
0.2694819892827932	0.6725105163718729	0.0181319886580826	T	T	T
0.1153705203588932	0.6737762845475177	0.0079205013921635	T	T	T
0.0651191557672920	0.6295654443769954	0.7992872498217203	T	T	T
0.1787648441324739	0.6691705225182294	0.6631955729394802	T	T	T
0.0794941929977074	0.5536137903909354	0.1341402128916182	T	T	T
0.2003618149755210	0.5285050677859509	0.2803334283504630	T	T	T
0.2219356630326239	0.5678298085183455	0.5015285703399029	T	T	T
0.3829523639690143	0.5696395680491463	0.5041148425801709	T	T	T
0.4349261085096665	0.5282040072394323	0.2947417092604808	T	T	T

Structure files (CONTCAR) involved in this work:

0.3278064902027000	0.5529668759835407	0.1423277192294876	T	T	T
0.0808155197039024	0.3284374791807891	0.1567139160891629	T	T	T
0.1962273657430542	0.3702165702425710	0.3032347449003415	T	T	T
0.2318091185879536	0.3299880266979595	0.5223328538382752	T	T	T
0.3862269582622906	0.3274411205248290	0.5092914250177647	T	T	T
0.4340725479439880	0.3706943738521122	0.2948464836380972	T	T	T
0.3172829334352034	0.3260157011563190	0.1662362959581243	T	T	T
0.8107365458290263	0.5619898458989664	0.3276587663033792	T	T	T
0.8298817006237329	0.3294942581598901	0.3528966853515909	T	T	T
0.7931388592375459	0.4737597575095220	0.7281678988845871	T	T	T
0.3564675240916012	0.0622323548992808	0.7190522776216223	T	T	T
0.2993548232260076	0.0658943032465807	0.8956036984100711	T	T	T
0.1992796482487013	0.0515007549577757	0.0274788011446782	T	T	T
0.1003596393426197	0.0671932291894682	0.8961050513913947	T	T	T
0.1012016351584825	0.0574156847999869	0.6983786138361872	T	T	T
0.2276316849597692	0.0326777590589822	0.7384636219007066	T	T	T
0.3571713327314246	0.8263227796449656	0.7481658623693817	T	T	T
0.3038612717351650	0.8434286255561917	0.9243541160723081	T	T	T
0.1892136224624575	0.8521848840697426	0.0208980556121137	T	T	T
0.0842256231657579	0.8320200513077559	0.9039201956488153	T	T	T
0.1014109682606434	0.8382902046750863	0.7081397466056303	T	T	T
0.2275758529904007	0.8545675923607112	0.7625422040367432	T	T	T
0.3191901103544069	0.9479580529029082	0.8040438204589663	T	T	T
0.0800896698173485	0.9497002442829676	0.8121483880784718	T	T	T
0.4297594373492042	0.1268067939966703	0.5856048014718248	T	T	T
0.4161618571971741	0.9949424578691660	0.5695672006149896	T	T	T
0.3968964472596411	0.8628377997421890	0.5665654012028332	T	T	T
0.1933611740085429	0.1309288814073927	0.6119286069995498	T	T	T
0.1784307486322117	0.0025963893569094	0.5596076659263666	T	T	T
0.1925702988661265	0.8686366516186407	0.5702469269698603	T	T	T
0.9877902771002746	0.0462996398225438	0.7922879458015644	T	T	T
0.9815335321017588	0.8616197648477718	0.7870686405574089	T	T	T
0.1405929628144939	0.9388786782249136	0.2206661019376785	T	T	T
0.1974062985839281	0.9311891967689933	0.3971355968953936	T	T	T
0.2964925171237860	0.9470263164280254	0.5298657817260068	T	T	T
0.3954156957573810	0.9300404952719097	0.3983755283402858	T	T	T
0.3951414827677515	0.9452279984924176	0.2010108499211936	T	T	T
0.2688845051759595	0.9702096308519168	0.2415293600105459	T	T	T
0.1411129746465430	0.1711247447267909	0.2412031286880027	T	T	T
0.1932594745586766	0.1621765954046852	0.4187277910859978	T	T	T
0.3078626098078033	0.1481910961284844	0.5156676165730451	T	T	T
0.4128449399952693	0.1708923780725635	0.3991775680390311	T	T	T
0.3956091983257963	0.1554159897391446	0.2046932182790410	T	T	T
0.2697283665669417	0.1392859996744326	0.2598188622022678	T	T	T
0.1759146190418248	0.0513209330228047	0.3125122176712450	T	T	T
0.4176728224198570	0.0494187701603078	0.3215106291719232	T	T	T
0.0667126362441395	0.8717951655358588	0.0918890335586080	T	T	T
0.0801345905175788	0.0029543453475805	0.0681691327002398	T	T	T
0.0975905673951273	0.1352325221707729	0.0622219971583345	T	T	T
0.3026783954947507	0.8690645037598128	0.1197993677725638	T	T	T
0.3166760163897110	0.9952031999579356	0.0595273001254324	T	T	T
0.3037006467618276	0.1290828760899809	0.0668684598857812	T	T	T
0.5084683561630777	0.9524296783402069	0.2955801483245351	T	T	T

Structure files (CONTCAR) involved in this work:

0.5157207784087933	0.1365769720032115	0.2849358144471740	T	T	T
0.6467818551669645	0.5556170269463004	0.2785728361370363	T	T	T
0.6781645636813627	0.5694784900906272	0.0887467464505388	T	T	T
0.7906445584308454	0.5482300011439531	0.9855956792559226	T	T	T
0.9047058791320426	0.5628010498207381	0.0867975940674911	T	T	T
0.9014461660710097	0.5679881324485826	0.2906669936139476	T	T	T
0.7730993324997840	0.5428943420214006	0.2172039777668489	T	T	T
0.6425173487622683	0.3381009840209621	0.2711428192051325	T	T	T
0.7224104924208102	0.3264343887156014	0.1179079740928006	T	T	T
0.8060523592951392	0.3551289691464116	0.9692173217092810	T	T	T
0.9056278514479531	0.3377088458114074	0.0987012986264623	T	T	T
0.9088109421406441	0.3391957437117866	0.3001669843673155	T	T	T
0.7693159135435652	0.3762633744373062	0.2897924380820493	T	T	T
0.6835522680075468	0.4474812323149465	0.1758369277148985	T	T	T
0.9124194991283026	0.4521920667934600	0.1959625119868457	T	T	T
0.5718212458382119	0.6285025164270062	0.4014623142257178	T	T	T
0.5926761220667177	0.5010080235813567	0.4410193562898678	T	T	T
0.5807543416435141	0.3677447170136603	0.4434602470629839	T	T	T
0.7990184677561186	0.6400769651723088	0.3782015058342465	T	T	T
0.8035986453523118	0.4993863827951515	0.4150855090308491	T	T	T
0.8292061449744353	0.3733014431322578	0.4750891930358100	T	T	T
0.0127232224559577	0.5418583478689983	0.2014795362958980	T	T	T
0.0167548615895632	0.3716060141478426	0.1938975800095273	T	T	T
0.8732369815699736	0.4292209177310002	0.7426462321978724	T	T	T
0.7985633606719261	0.4578355007225293	0.5978884264807505	T	T	T
0.6981186699691375	0.4225305842364580	0.4768350021461616	T	T	T
0.6013971367920038	0.4332791711340083	0.6105899243510569	T	T	T
0.5976417679681172	0.4304657508874284	0.8074590210888606	T	T	T
0.7302276766678519	0.4305162554315795	0.7831367080217937	T	T	T
0.8632421126471715	0.6763388379876344	0.7410888127905386	T	T	T
0.8064099908806122	0.6364059584958626	0.5761564398436548	T	T	T
0.6888250182530504	0.6462201479481963	0.4907000948531753	T	T	T
0.5779999480881873	0.6579486999832088	0.5952227478846456	T	T	T
0.6040287686541687	0.6657169628047996	0.7908034508707873	T	T	T
0.7296465043750308	0.6691342269596491	0.7291227257196756	T	T	T
0.8028684382796297	0.5585484626248215	0.7432213993585777	T	T	T
0.5851619781644584	0.5472587055681865	0.7076621800458923	T	T	T
0.9297506827374812	0.3705984457429953	0.9065435513433018	T	T	T
0.9013440394750544	0.4996798461056134	0.9098388667209139	T	T	T
0.8884462370329432	0.6320823277806101	0.9254681425076419	T	T	T
0.6754509832834522	0.3744492708651971	0.9442943367978452	T	T	T
0.6720722548421791	0.5077735779488979	0.9178386297032840	T	T	T
0.7022910005412897	0.6371078961153596	0.9209644696624226	T	T	T
0.4875963155670138	0.4570105746538709	0.7106012398806892	T	T	T
0.4831199074335388	0.6343004837743117	0.7242738572991493	T	T	T
0.6396008896063192	0.9372500621770515	0.2939158334983685	T	T	T
0.6950856486633641	0.9349424980075505	0.1156763015827861	T	T	T
0.7980513042121862	0.9499108356326351	0.9888029113567912	T	T	T
0.9002841181195630	0.9289940644795573	0.1120816692364197	T	T	T
0.8945830856337899	0.9450471017169076	0.3096724774184260	T	T	T
0.7683176578479641	0.9670347116123069	0.2710437483774066	T	T	T
0.6411362846302574	0.1753741333955203	0.2579047945040063	T	T	T
0.6952755329437642	0.1528988081435500	0.0848340713205728	T	T	T

Structure files (CONTCAR) involved in this work:

0.8081476312817021	0.1474430054761334	0.9845858105135220	T	T	T
0.9085478799057399	0.1723427436669744	0.1103442469150486	T	T	T
0.8958174948400218	0.1544202824879587	0.3058622208433659	T	T	T
0.7703772176838952	0.1427116739629069	0.2492868618700526	T	T	T
0.6755581541159340	0.0520364488234572	0.2097297352443335	T	T	T
0.9172955496792453	0.0496108208079804	0.1865763859880570	T	T	T
0.5658083437322519	0.8743736097336007	0.4291889847299710	T	T	T
0.5791727020023679	0.0065278678142566	0.4415908104682356	T	T	T
0.6017610645796069	0.1376827589032980	0.4391388313048069	T	T	T
0.8032943827273256	0.8656549790131185	0.3921095801998853	T	T	T
0.8154202814796351	0.9919872969496644	0.4532044180323938	T	T	T
0.8042585749578742	0.1260155815839781	0.4412257539390217	T	T	T
0.0095436452226375	0.9550170010329546	0.2200207456230075	T	T	T
0.0140206599259890	0.1383450599827662	0.2194516353712508	T	T	T
0.8573147262786027	0.0675302492193344	0.7929667710158915	T	T	T
0.8015363140963708	0.0656314671751996	0.6145406868635795	T	T	T
0.6993246170944255	0.0509637389624878	0.4864815142628316	T	T	T
0.5980427296974254	0.0751835553248955	0.6106581340370876	T	T	T
0.6023053605100757	0.0527977222402331	0.8076579661492579	T	T	T
0.7292689318538907	0.0317366165427005	0.7704970243534723	T	T	T
0.8545735024635490	0.8264463659174263	0.7648364601804545	T	T	T
0.8044925603117657	0.8529643871606638	0.5882162353091003	T	T	T
0.6889807745515344	0.8523576809073284	0.4913936674146778	T	T	T
0.5867463533563223	0.8274998804962708	0.6131706072127638	T	T	T
0.6008314132225836	0.8537999716969694	0.8060518256203629	T	T	T
0.7270738897227024	0.8635751465818647	0.7489945122601811	T	T	T
0.8263318867412354	0.9509557575317052	0.7150755454128757	T	T	T
0.5791253601473574	0.9530428047170760	0.6772941124862010	T	T	T
0.9333428506948622	0.1263446810758188	0.9275835485488327	T	T	T
0.9168361052340553	0.9948073940366424	0.9395187446042396	T	T	T
0.8970739774520835	0.8634017073864049	0.9441148860157013	T	T	T
0.6925483564102128	0.1331095731881061	0.8888434475333084	T	T	T
0.6813111586107425	0.0077818477372092	0.9526911464420508	T	T	T
0.6941986596230203	0.8743881890512315	0.9430010351554992	T	T	T
0.4877576684967797	0.0472597710386129	0.7168154762548790	T	T	T
0.4820123551002997	0.8665204726223565	0.7213691070534189	T	T	T
0.3574850506405247	0.4427524172068101	0.7115599433956863	T	T	T
0.3035536937617142	0.4285983917402063	0.8892312966805173	T	T	T
0.2063829084424649	0.4501513580650844	0.0220920086938380	T	T	T
0.1111598460329344	0.4289792553143421	0.8851970215662933	T	T	T
0.1060414709521078	0.4538646371073262	0.6884220536893092	T	T	T
0.2305997949417608	0.4718234553208286	0.7363103139351800	T	T	T
0.3551904054435914	0.6669516305766219	0.7291292667810337	T	T	T
0.3005563371859817	0.6685861540089065	0.9063244681442675	T	T	T
0.1920419307335106	0.6468398534215067	0.0152237141526019	T	T	T
0.0915380582020143	0.6749648768019576	0.8920139836229669	T	T	T
0.1015842369865493	0.6546998654311402	0.6969592604027128	T	T	T
0.2274758251592377	0.6359348051376824	0.7474853430867688	T	T	T
0.3205190019411521	0.5518415356619436	0.8157761855677893	T	T	T
0.0838947202655293	0.5514740545652459	0.8222141268692331	T	T	T
0.4311255181817166	0.3745016427221290	0.5818134876249281	T	T	T
0.4166440789238479	0.5050684248953774	0.5584972294616717	T	T	T
0.4108126598198205	0.6380904704475450	0.5549086393630800	T	T	T

Structure files (CONTCAR) involved in this work:

0.1954346495712425	0.3732756563395126	0.6095845106510634	T	T	T
0.1895266449213572	0.5001789414048501	0.5502623432058240	T	T	T
0.1915687678018490	0.6345742718732681	0.5547859463669222	T	T	T
0.9966865750317374	0.4528650292217403	0.7885834877076370	T	T	T
0.9848637065615453	0.6362858223663503	0.7864822601775625	T	T	T
0.1430367211273155	0.5601863306042839	0.2082182551515143	T	T	T
0.2012086017554791	0.5707746756588060	0.3842696066223903	T	T	T
0.3022387341606366	0.5652680506544910	0.5163971400457107	T	T	T
0.4036743774742426	0.5707810522389760	0.3873998925068457	T	T	T
0.4016535373242141	0.5563142930860657	0.1919878103202128	T	T	T
0.2728741302240530	0.5341397743918019	0.2276915359502264	T	T	T
0.1382048754072202	0.3318745104981972	0.2418704601724161	T	T	T
0.1937831619591251	0.3421536651180345	0.4167376843175916	T	T	T
0.3091041131319262	0.3542267574184760	0.5118703106793581	T	T	T
0.4130154919954899	0.3299120416656202	0.3952549713245734	T	T	T
0.3939517405407624	0.3400844956929817	0.1994860568007516	T	T	T
0.2687987948159646	0.3559703348769300	0.2534386884018781	T	T	T
0.1818925284363126	0.4506174381467529	0.3029837509693465	T	T	T
0.4152829918002072	0.4494919107343340	0.3101420219806149	T	T	T
0.0686981994282434	0.6231607332128851	0.0728663432307318	T	T	T
0.0846794713226661	0.4914584039984857	0.0560961474645097	T	T	T
0.1093991847221112	0.3599257732346753	0.0524171979863090	T	T	T
0.3115589782524896	0.6258256898720573	0.0942217902579469	T	T	T
0.3277989751744210	0.4948890545484205	0.0567361111086052	T	T	T
0.3027609047181986	0.3622679498677142	0.0595007118801734	T	T	T
0.5152717735708240	0.5368824508403965	0.2872555785784809	T	T	T
0.5132193225201450	0.3614376705336582	0.2731061744331618	T	T	T
0.4409763320402852	0.7504757494028077	0.6453738161667276	T	T	T
0.1927392719903085	0.7488823080474861	0.6521016680888599	T	T	T
0.2725589443982279	0.7493258153318153	0.0574984658581761	T	T	T
0.1079079343419020	0.7488105279260188	0.0534954536439794	T	T	T
0.0607305356554665	0.2507730174665382	0.1371768761665258	T	T	T
0.3038922605626805	0.2465516150345832	0.1522197303581928	T	T	T
0.2269734999554318	0.2519208164444922	0.5552373161959152	T	T	T
0.3901559562716935	0.2510654003210947	0.5511342991704925	T	T	T
0.5598858667280890	0.2515039643709788	0.3615364029965181	T	T	T
0.8070522815756668	0.2469094834138490	0.3660729322524059	T	T	T
0.7242364442203643	0.2510700042386105	0.9560079360581848	T	T	T
0.8899747581581063	0.2501419175856739	0.9527474322849974	T	T	T
0.9363012321503155	0.7483494628371601	0.8673631587789512	T	T	T
0.6871071818237612	0.7586761188586857	0.8591589165053420	T	T	T
0.7734039906530649	0.7493047415748998	0.4773602729075469	T	T	T
0.6060617236745320	0.7495391830524162	0.4570903506078322	T	T	T
0.8863559762553148	0.4176370836544784	0.5891440892465032	T	T	T
0.9943729366142092	0.2889153896297861	0.5308309020879921	T	T	T
0.9281142128915072	0.5979729010627384	0.4346854091265985	T	T	T
0.9283210945749431	0.6636038811774490	0.3428576512744482	T	T	T
0.9944741122853843	0.6015164932549835	0.3438884100464898	T	T	T
0.9683531536168364	0.4516766167015076	0.4583938474186687	T	T	T
0.9740682787843667	0.5039333333221584	0.5694193670614941	T	T	T
0.0141661986688072	0.4233922123398029	0.5674196504906789	T	T	T
0.9772658161064438	0.2913179635998431	0.4807845245012034	T	T	T
0.9415280541208173	0.6111458543373680	0.3576629406177917	T	T	T

Structure files (CONTCAR) involved in this work:

0.9715578393692503 0.4523808541243294 0.5401599264238000 T T T

Figure 4(a) Route(a)-Zn ①

Si Al O Zn H C

1.0000000000000000

20.0219999999999985 0.0000000000000000 0.0000000000000000

0.0000000000000000 19.8990000000000009 0.0000000000000000

0.0000000000000000 0.0000000000000000 13.3829999999999991

93 3 193 2 6 2

Selective dynamics

Direct

0.4220286184494478 0.0602459319619886 0.6482533681849786 T T T

0.3046437756275998 0.0319693037701075 0.7921428620614205 T T T

0.2818304766939824 0.0568346819876415 0.0168399819414755 T T T

0.1221790636780554 0.0629262540029749 0.0114214015584226 T T T

0.0674197380159968 0.0312081857589771 0.8002081787068092 T T T

0.1800114597873847 0.0646669792269655 0.6644608039541638 T T T

0.4185702166327666 0.8273948719990332 0.6690457997116546 T T T

0.3008570793684506 0.8729953652821695 0.8014550193429117 T T T

0.2669966672011118 0.8303290804227184 0.0207253762542668 T T T

0.1109717770124929 0.8265439150241740 0.0133202485801415 T T T

0.0657712073029093 0.8743878139407647 0.7990815422788105 T T T

0.1791510969008961 0.8289467821337591 0.6655688803672835 T T T

0.0754292606067521 0.9411971819096507 0.1486841487756109 T T T

0.1943157859056362 0.9701284603737265 0.2906885591395151 T T T

0.2164791680914161 0.9434597602550789 0.5160721485616721 T T T

0.3768258598094399 0.9355072203906708 0.5136283574576126 T T T

0.4330366839704806 0.9687625630264327 0.3015835951647655 T T T

0.3197235963795919 0.9359501288629213 0.1642815007054672 T T T

0.0812821208752062 0.1725554813445844 0.1664517828216905 T T T

0.1975788984683742 0.1289846393706683 0.3015925521453306 T T T

0.2311695721226729 0.1696862321788728 0.5191661183020128 T T T

0.3865760620763406 0.1739624607068047 0.5088956698762228 T T T

0.4348488853823640 0.1271342902389599 0.2958655990441953 T T T

0.3185361387765717 0.1724526620066881 0.1666550129819732 T T T

0.5788590499138543 0.5556297166285253 0.3560327143872797 T T T

0.6915136176652430 0.5271983732148281 0.2017595547749438 T T T

0.7156189244028255 0.5683410275976346 0.9862544077930963 T T T

0.8747213170109563 0.5729029089942886 0.9871517599810216 T T T

0.8101443184364794 0.5510712773964044 0.3455987201350447 T T T

0.5728575625822391 0.3291462453157553 0.3320011820844636 T T T

0.6947595282501647 0.3729862585791177 0.1946140584949426 T T T

0.7317335377189130 0.3278307919367314 0.9803571104368641 T T T

0.8865010967515463 0.3257126138355232 0.9924415316255191 T T T

0.9421938822055784 0.3735082442992823 0.1912449086536993 T T T

0.9200998681680563 0.4454316711635307 0.8609023344493167 T T T

0.8006232044372494 0.4733389824073734 0.7202092559645162 T T T

0.7763884319855692 0.4368176828688773 0.4963252383366229 T T T

0.6202804606757878 0.4281272825871317 0.4897304395092776 T T T

0.5703437627105306 0.4693838618770274 0.7015546931070510 T T T

0.6764245891220499 0.4478489489309324 0.8573329647659331 T T T

0.9207690196999230 0.6784079555295703 0.8298111533411037 T T T

0.7690745915292783 0.6690440797653198 0.4660420469130296 T T T

Structure files (CONTCAR) involved in this work:

0.6139637545356308	0.6735363421051662	0.4884151200094073	T	T	T
0.5605636083794808	0.6276522627969130	0.6981796482878576	T	T	T
0.6731656488540310	0.6743380596318918	0.8262160429941640	T	T	T
0.5775573691164193	0.9454808841463146	0.3581516688764039	T	T	T
0.6980642806710103	0.9745546691792076	0.2151727778965012	T	T	T
0.7190947756196231	0.9388115228066692	0.9930954010463864	T	T	T
0.8789244413744908	0.9347707566652658	0.9946649752967879	T	T	T
0.9306823620073403	0.9714422421941266	0.2051245198707794	T	T	T
0.8218596558180968	0.9463091138615594	0.3546174407142274	T	T	T
0.5778482220027371	0.1741011683538391	0.3293712132152886	T	T	T
0.6976348669858691	0.1328716876951509	0.1937692849330542	T	T	T
0.7325494649934874	0.1716469122660102	0.9721937802399607	T	T	T
0.8872006681771474	0.1734489541623077	0.9831531616075423	T	T	T
0.9350268637168936	0.1297646713666078	0.1982769587245857	T	T	T
0.8196166965668954	0.1747408939427691	0.3324734586017022	T	T	T
0.9229897785079029	0.0543889569674298	0.8556896049551536	T	T	T
0.8016090444041747	0.0262698260988192	0.7104725890875231	T	T	T
0.7808251887571470	0.0653893467655920	0.4921549631728933	T	T	T
0.6206011225969483	0.0698881070439946	0.4899291412627360	T	T	T
0.5674577352752276	0.0327104827219103	0.6989157424173736	T	T	T
0.6779697539253513	0.0543218689775667	0.8493785526758125	T	T	T
0.9229654143397792	0.8305658017644550	0.8376417203531399	T	T	T
0.8029195349158813	0.8687871318594660	0.6957166794598283	T	T	T
0.7694152913057271	0.8269913771093893	0.4780641695973149	T	T	T
0.6144862370638272	0.8271271291316470	0.4901575577077718	T	T	T
0.5634284811596001	0.8753735931113739	0.6981946297120863	T	T	T
0.6784729714996185	0.8330169685166399	0.8331668418095249	T	T	T
0.4236286783405066	0.4420578926511448	0.6446702544523610	T	T	T
0.3053787439564127	0.4695087996403269	0.7884015819335414	T	T	T
0.2794996119921874	0.4455308592638066	0.0146293081235916	T	T	T
0.1216374609999798	0.4376291021598540	0.0148633419759613	T	T	T
0.0638067000699340	0.4699618699101044	0.8017639799372754	T	T	T
0.1774128662844494	0.4365351429940116	0.6629711465676060	T	T	T
0.4154697478060307	0.6735478377121895	0.6669960484340133	T	T	T
0.3007157081448158	0.6279118319347000	0.8010162147745725	T	T	T
0.2670336449024177	0.6690284424532140	0.0201848167587295	T	T	T
0.1114715885908133	0.6729576537720227	0.0090033556597487	T	T	T
0.0631968516230318	0.6285382673993499	0.7943829358128751	T	T	T
0.1797014986258464	0.6718564703588478	0.6643993318905975	T	T	T
0.0781153232198825	0.5592837753070877	0.1489267363615295	T	T	T
0.1964650460558105	0.5292960303264489	0.2899214954557572	T	T	T
0.2148368810718978	0.5563792903546341	0.5156670702361535	T	T	T
0.3738761077319661	0.5658221604949065	0.5136948154324295	T	T	T
0.4308325786549433	0.5311853999837710	0.3043849591501758	T	T	T
0.3215663993768238	0.5632818041525887	0.1628286824132975	T	T	T
0.0863877581358372	0.3248477964282164	0.1611253401490083	T	T	T
0.1982372395147867	0.3711058230898898	0.3006723906917881	T	T	T
0.2299809065307872	0.3310035646102673	0.5192763414877244	T	T	T
0.3847674816690139	0.3279679752991484	0.5059130748434925	T	T	T
0.4304659541005930	0.3740959261042820	0.2930514607853213	T	T	T
0.3166195190063676	0.3300793493799062	0.1628200241653111	T	T	T
0.9219109140840478	0.5292003306788400	0.1967827779960549	T	T	T
0.8233630305198010	0.3360271497778605	0.3293482217948649	T	T	T

Structure files (CONTCAR) involved in this work:

0.7997232700130550	0.6360964645739052	0.6941916278014740	T	T	T
0.0113001008935738	0.5564958771745251	0.2285892566631921	T	T	T
0.3582060935039043	0.0705354813998744	0.7216350862242553	T	T	T
0.3160731628289582	0.0548841244789100	0.9069890481093641	T	T	T
0.2016499220788724	0.0482286207311699	0.0071973077721138	T	T	T
0.0920336440441267	0.0703238522765089	0.8999489372005492	T	T	T
0.1032269535288190	0.0641924178930283	0.7029759316623607	T	T	T
0.2289690128257743	0.0517224035045562	0.7596668121802558	T	T	T
0.3595952598887123	0.8280387833817567	0.7522922367951164	T	T	T
0.3008723235688417	0.8610297702405384	0.9208114788577647	T	T	T
0.1883451238700417	0.8506485115314698	0.0237353625563365	T	T	T
0.0880771239661828	0.8325357227262969	0.8978213292439069	T	T	T
0.1023861475294735	0.8409840787887131	0.7021442106268746	T	T	T
0.2285309047408684	0.8510025660347166	0.7567100815347947	T	T	T
0.3156314290717838	0.9515399777547370	0.7773545387339552	T	T	T
0.0887214650396977	0.9523888101038710	0.8100811463664122	T	T	T
0.4322024743848211	0.1278915309410461	0.5818072517897521	T	T	T
0.4118464646093478	0.9966497605597161	0.5739513171239219	T	T	T
0.3929970231959537	0.8645148748762227	0.5680067551729350	T	T	T
0.1957030848805665	0.1380777667647247	0.6171423393361974	T	T	T
0.1896496747289559	0.0060942881774526	0.5817527904878986	T	T	T
0.1943131781914871	0.8723857418027547	0.5656160495497309	T	T	T
0.9874596690831191	0.0395285104428469	0.7853816095861348	T	T	T
0.9852383253796846	0.8707787096899769	0.7859603619944038	T	T	T
0.1397349102190553	0.9321121432716091	0.2213549602449045	T	T	T
0.1830718357482083	0.9481558575354506	0.4059191856461646	T	T	T
0.2970102847975254	0.9480736018228361	0.5086083745241193	T	T	T
0.4071129381379561	0.9313542105626843	0.4019604308330370	T	T	T
0.3959847017085861	0.9364412645449414	0.2049014311795175	T	T	T
0.2695509158426977	0.9489488187418386	0.2581013903681424	T	T	T
0.1393210900100940	0.1737328237886038	0.2510130625249579	T	T	T
0.1941425769337698	0.1396251385290322	0.4211934433715311	T	T	T
0.3094619001236604	0.1481990218897668	0.5156186442515586	T	T	T
0.4126892079836257	0.1686686746100581	0.3948240667660015	T	T	T
0.3955959184433481	0.1585017984809419	0.1997693592422274	T	T	T
0.2704894621029984	0.1526492844141371	0.2607769077078287	T	T	T
0.1844755017830222	0.0505564878256329	0.2745787188524280	T	T	T
0.4152012162418734	0.0484479313773139	0.3094487028603491	T	T	T
0.0645103786943140	0.8719859552076747	0.0859394916701903	T	T	T
0.0853143140965284	0.0017394931237455	0.0690314906113319	T	T	T
0.1074725469628017	0.1328939097975859	0.0684839549173474	T	T	T
0.3047258608718084	0.8624265151899283	0.1165136707798267	T	T	T
0.3109867352565907	0.9946535885693903	0.0814056154097065	T	T	T
0.2998406772231272	0.1282743117048707	0.0687428041506881	T	T	T
0.5125847112432363	0.9565729542476819	0.2874079059052784	T	T	T
0.5149111214617126	0.1342818354776195	0.2791435901763006	T	T	T
0.6385272425511458	0.5632530039820699	0.2757657895323963	T	T	T
0.6994691462787787	0.5751162305289562	0.1047485738572165	T	T	T
0.7952440190624307	0.5606125227313759	0.9654727695647873	T	T	T
0.8911209679002168	0.5797553854231156	0.1043562368400158	T	T	T
0.8867582202627003	0.5356063600059288	0.3161160281244116	T	T	T
0.7632246109659412	0.5228834837721028	0.2583102671006675	T	T	T
0.6387783770075026	0.3363246090478528	0.2641068257233135	T	T	T

Structure files (CONTCAR) involved in this work:

0.6937411599256560	0.3350957543010773	0.0865563330347962	T	T	T
0.8093649678896351	0.3517367288085805	0.9912628532242835	T	T	T
0.9136298066984674	0.3214416500999689	0.1071538771256106	T	T	T
0.9078007642600054	0.3578760646051345	0.2999920316618585	T	T	T
0.7670355876764894	0.3697435656773527	0.2457713001418161	T	T	T
0.6698487921223709	0.4507641394941727	0.1756470142868014	T	T	T
0.9290233943189937	0.4488572238776330	0.1554919410097135	T	T	T
0.5697971253475850	0.6265549877774482	0.4144121359996232	T	T	T
0.5950320481140754	0.4973065332627486	0.4376816241301727	T	T	T
0.5826148278007720	0.3639111011097466	0.4415433759756964	T	T	T
0.7978190678715494	0.6307926278337274	0.3670522378302422	T	T	T
0.7922052669968980	0.5143875424743678	0.4549974854136711	T	T	T
0.8284476486834458	0.3868245845999385	0.4406398865862888	T	T	T
0.0223672770705235	0.3632824301404672	0.2064626083998290	T	T	T
0.8548873747592743	0.4351585133969494	0.7894852510004866	T	T	T
0.7912273351104545	0.4335894981087089	0.6146994717203071	T	T	T
0.7001047955467339	0.4184544611498831	0.4694792737129693	T	T	T
0.6059204063924269	0.4303532018392420	0.6086304648968399	T	T	T
0.6029890480503102	0.4444399537449633	0.8060814267081304	T	T	T
0.7285688334064974	0.4757249461128340	0.7737197247440163	T	T	T
0.8603826397994501	0.6818199417463886	0.7523931443879338	T	T	T
0.8154512624155835	0.6436144535236129	0.5609375229962980	T	T	T
0.6917286104413937	0.6480988747052983	0.4877051900917595	T	T	T
0.5841800845820712	0.6694048562320839	0.6002302213161111	T	T	T
0.5947272233833564	0.6605818787047955	0.7966765098225403	T	T	T
0.7199127901775213	0.6506096532408767	0.7346203678849166	T	T	T
0.8255412219824342	0.5496837207759028	0.6940756392507236	T	T	T
0.5818414443630086	0.5493803582910503	0.6852392451490241	T	T	T
0.9313380031549610	0.3769941638953607	0.9256102746378362	T	T	T
0.9134712024642629	0.5093697862013052	0.9351269543165579	T	T	T
0.9001192079378832	0.6414219219948375	0.9334835057657785	T	T	T
0.6959389741317910	0.3732145335526451	0.8950213103392015	T	T	T
0.6765098157538905	0.5008552675256709	0.9492352402473299	T	T	T
0.6882583087885407	0.6345302368898322	0.9299664881677572	T	T	T
0.4914434678364007	0.4514319592869246	0.7086398923207028	T	T	T
0.4796488427351601	0.6322062761977190	0.7085018879557117	T	T	T
0.6433458664780979	0.9403262557395957	0.2883382338295387	T	T	T
0.6983496006511893	0.9339910036184856	0.1099788730694149	T	T	T
0.7994409099303782	0.9474928284948955	0.9803442843526005	T	T	T
0.8982867037593674	0.9300639985985519	0.1121079639246874	T	T	T
0.8971929684766612	0.9478300219891574	0.3098016838534444	T	T	T
0.7714628468632583	0.9686596484113671	0.2655587092532931	T	T	T
0.6397025615774861	0.1742018380979329	0.2517996578450620	T	T	T
0.6966892142840435	0.1574185675790127	0.0785477452497790	T	T	T
0.8101650922056303	0.1472771655275425	0.9786402736929612	T	T	T
0.9137695591813418	0.1691200449303096	0.0971464841164742	T	T	T
0.8961759562762804	0.1599811385007916	0.2944803228474772	T	T	T
0.7699756530648528	0.1470813645313669	0.2438794184455431	T	T	T
0.6797601457423484	0.0531523710108737	0.1985562002143526	T	T	T
0.9176058568132730	0.0506637356954167	0.1849191559734684	T	T	T
0.5692847178296889	0.8754473676420567	0.4197176818132952	T	T	T
0.5818973146770933	0.0072233557235933	0.4375421488185979	T	T	T
0.5996355079909415	0.1393371598235345	0.4344800581359121	T	T	T

Structure files (CONTCAR) involved in this work:

0.8068717363565797	0.8702900989044504	0.3924705162624756	T	T	T
0.8158786314283656	0.9976990491209388	0.4482874256227240	T	T	T
0.8064038388288197	0.1318092398928467	0.4345250657874980	T	T	T
0.0099778680539911	0.9556807170032572	0.2161255610725502	T	T	T
0.0151537293886361	0.1386643694193017	0.2151551966471478	T	T	T
0.8568482970248156	0.0563588845012128	0.7864412542191820	T	T	T
0.8012043726774387	0.0714375954140725	0.6094283226738291	T	T	T
0.7003028290172517	0.0572497861953239	0.4801275417722288	T	T	T
0.5983604999530761	0.0759014256130365	0.6063472789693141	T	T	T
0.6029528545497181	0.0530537309809040	0.8035644786699674	T	T	T
0.7283974423611859	0.0290267784955130	0.7620677860593971	T	T	T
0.8599949790563886	0.8334113193944872	0.7623634547765917	T	T	T
0.8055092005081279	0.8347346747332544	0.5857430887926582	T	T	T
0.6921008607390747	0.8517956923741801	0.4862027236936402	T	T	T
0.5879355132169855	0.8295590540211045	0.6045818983398271	T	T	T
0.6028680972968528	0.8530385674183456	0.7988673544229791	T	T	T
0.7297215826535109	0.8570560238286602	0.7452432788732847	T	T	T
0.8186408414708707	0.9484587864555067	0.6847195841099426	T	T	T
0.5786439387466025	0.9536484835527633	0.6729067739840537	T	T	T
0.9325309786437744	0.1269199291779490	0.9099409947673858	T	T	T
0.9185149258064895	0.9967322212385237	0.9418473932388819	T	T	T
0.9018741493466560	0.8645160336517141	0.9436150463097474	T	T	T
0.6950725943963203	0.1303983392761238	0.8840015477755886	T	T	T
0.6823202575861990	0.0042014258260895	0.9451082410849089	T	T	T
0.6955777291993648	0.8702987506977428	0.9379841218389774	T	T	T
0.4885474185447016	0.0484967603363958	0.7146809279121511	T	T	T
0.4837836237629543	0.8645053946584117	0.7158029495658776	T	T	T
0.3609574789983654	0.4314322111714852	0.7206683844968991	T	T	T
0.3123855203895158	0.4459354870546337	0.9038978354467627	T	T	T
0.1994360848455048	0.4609317122150465	0.0100436771533230	T	T	T
0.0897583042869773	0.4353710184981027	0.9046501337953199	T	T	T
0.1020886443272767	0.4357432973342579	0.7074721474243972	T	T	T
0.2301513925110026	0.4507580957069042	0.7526628176090762	T	T	T
0.3583964693890124	0.6748238687248140	0.7533201468008333	T	T	T
0.3011719668311330	0.6378897653221536	0.9207956356776461	T	T	T
0.1883962949798684	0.6479069033835025	0.0208498516283249	T	T	T
0.0879236077429479	0.6682568245761777	0.8940722622721019	T	T	T
0.1026570493794948	0.6589738146951414	0.6979349839179285	T	T	T
0.2279515181020436	0.6488558595401136	0.7565152488594917	T	T	T
0.3170077253371422	0.5499124299572135	0.7748436300488035	T	T	T
0.0818097408875920	0.5495300609323034	0.8066517909188901	T	T	T
0.4318014442451504	0.3762418057176382	0.5736293582354283	T	T	T
0.4135240145353020	0.5075861740029052	0.5739405993990171	T	T	T
0.3847429261432456	0.6381361127732404	0.5672836351252915	T	T	T
0.1920800197948289	0.3630912876837270	0.6150120755704287	T	T	T
0.1822284964997831	0.4951156821964701	0.5785907491330616	T	T	T
0.1961407653242470	0.6286509561190607	0.5641678568837901	T	T	T
0.9845984485601685	0.4567754329038865	0.7885792485150638	T	T	T
0.9838541784400260	0.6382849758840075	0.7780943069170771	T	T	T
0.1433596717501068	0.5692009551934706	0.2185020580386892	T	T	T
0.1831454348917092	0.5540381543534036	0.4034596951274828	T	T	T
0.2950274548240926	0.5465093808707706	0.5105596101303850	T	T	T
0.4029995372857983	0.5714038234243691	0.4012954388814806	T	T	T

Structure files (CONTCAR) involved in this work:

0.3975888174329274	0.5638752764741481	0.2044933020031355	T	T	T
0.2718740143967489	0.5477409855131637	0.2570189226067960	T	T	T
0.1432916484202709	0.3237398556142950	0.2475859402176024	T	T	T
0.1938335954300330	0.3606069808167531	0.4200060453845582	T	T	T
0.3078894198529976	0.3538327573864094	0.5181521045614437	T	T	T
0.4064117873368044	0.3301905541383603	0.3891277046581240	T	T	T
0.3936796069362122	0.3470561959270647	0.1920202713885983	T	T	T
0.2719883480930246	0.3513204793156474	0.2601613836237215	T	T	T
0.1817432271328084	0.4496215650336686	0.2752963928600731	T	T	T
0.4103889090279040	0.4522165603121557	0.3133705705378451	T	T	T
0.0654886404684066	0.6243396563249848	0.0796216675044329	T	T	T
0.0795529700084493	0.4911329330381832	0.0845003554803144	T	T	T
0.1155379371373579	0.3632587288128590	0.0629272384470525	T	T	T
0.3038069876502936	0.6365803350413844	0.1168238957678224	T	T	T
0.3141388253996803	0.5048982416003075	0.0791903017385196	T	T	T
0.2930542979636370	0.3725284093181676	0.0651474370962484	T	T	T
0.5109748328502883	0.5384142166656544	0.2955462924296415	T	T	T
0.5102263559858308	0.3657739456802115	0.2759795363321453	T	T	T
0.4362498489018152	0.7501640068860873	0.6402701798089361	T	T	T
0.1910080202601963	0.7504208214939977	0.6375163086256098	T	T	T
0.2756305897953796	0.7495426386500725	0.0234801513527176	T	T	T
0.1030427980866588	0.7489981258264528	0.0495055541856924	T	T	T
0.0664873347461023	0.2489684612252302	0.1305193505299883	T	T	T
0.3079415166501011	0.2509783895432318	0.1373928125137143	T	T	T
0.2231046513780265	0.2503975631396771	0.5233388999738730	T	T	T
0.3917368529567161	0.2514156914156953	0.5458593919617644	T	T	T
0.5555737555702075	0.2508024692112658	0.3523174578520039	T	T	T
0.8094683490141696	0.2528086078361529	0.3549713025226864	T	T	T
0.7279082052090050	0.2504408371539393	0.9430460220399596	T	T	T
0.8921897563321869	0.2507542194210785	0.9447079864126179	T	T	T
0.9458612195364153	0.7539469575927424	0.8592195149883263	T	T	T
0.6837978566468300	0.7533409229401936	0.8518076825942407	T	T	T
0.7746706183505724	0.7486308976842634	0.4455844433488184	T	T	T
0.6090469637515623	0.7505126529202549	0.4491252918678184	T	T	T
0.9362267232618225	0.4928328422362410	0.5319594638732478	T	T	T
0.9264532050331020	0.4246847419155083	0.4341551478388250	T	T	T
0.8734122216985216	0.5574940367557576	0.5564841289043113	T	T	T
0.0437616622064909	0.4234779671496146	0.5097211514082635	T	T	T
0.0487100553722366	0.4317946975943185	0.3724575459887962	T	T	T
0.0279333904510821	0.3500488222131486	0.4270623757866561	T	T	T
0.0092553811554763	0.5611566110285376	0.3855231340498183	T	T	T
0.9773467784135557	0.6343276132547814	0.3221880719046415	T	T	T
0.0659623666528224	0.6193186751051815	0.3264108632497529	T	T	T
0.0282922172718599	0.4047478001469966	0.4366376838935000	T	T	T
0.0165706873214184	0.5959894644960673	0.3229406323610237	T	T	T

Figure 4(a) Route(a)-Zn ②

Si Al O Zn H C

1.0000000000000000		
20.0219999999999985	0.0000000000000000	0.0000000000000000
0.0000000000000000	19.8990000000000009	0.0000000000000000
0.0000000000000000	0.0000000000000000	13.3829999999999991
93	3	193
2	6	2

Structure files (CONTCAR) involved in this work:

Selective dynamics

Direct

0.4233100000000007	0.0616399999999970	0.6477999999999966	T	T	T
0.3049299999999988	0.0319300000000027	0.7900100000000023	T	T	T
0.2831499999999991	0.0572799999999987	0.0157099999999986	T	T	T
0.1233900000000006	0.0642500000000013	0.0120099999999965	T	T	T
0.0680899999999980	0.0321599999999975	0.8005799999999965	T	T	T
0.1796799999999976	0.0655900000000003	0.6634400000000014	T	T	T
0.4183099999999982	0.8291699999999977	0.6653299999999973	T	T	T
0.3014799999999980	0.8730199999999968	0.7996100000000013	T	T	T
0.2680199999999999	0.8327799999999996	0.0188300000000012	T	T	T
0.1130199999999988	0.8278699999999972	0.0097000000000023	T	T	T
0.0666000000000011	0.8753799999999998	0.7959499999999977	T	T	T
0.1801999999999992	0.8287499999999994	0.6639499999999998	T	T	T
0.0772100000000009	0.9412599999999998	0.1476600000000019	T	T	T
0.1953499999999977	0.9707000000000008	0.2902199999999979	T	T	T
0.2170599999999965	0.9446500000000029	0.5156599999999969	T	T	T
0.3768400000000014	0.9386200000000002	0.5119800000000012	T	T	T
0.4343199999999996	0.9703900000000019	0.3001700000000014	T	T	T
0.3208899999999986	0.9371300000000033	0.1641699999999986	T	T	T
0.0822900000000004	0.1741200000000021	0.1653400000000005	T	T	T
0.1985099999999989	0.1296099999999996	0.2998100000000008	T	T	T
0.2313299999999998	0.1712399999999974	0.5180999999999969	T	T	T
0.3872199999999992	0.1754999999999995	0.5090000000000003	T	T	T
0.4358599999999981	0.1293799999999976	0.2947500000000005	T	T	T
0.3193600000000032	0.1732299999999967	0.1644199999999998	T	T	T
0.5755499999999998	0.5568799999999996	0.3524499999999975	T	T	T
0.6900699999999986	0.5281499999999966	0.1999899999999997	T	T	T
0.7111900000000020	0.5713599999999985	0.9836200000000019	T	T	T
0.8678700000000035	0.5753399999999971	0.9864000000000033	T	T	T
0.8098799999999997	0.5512000000000015	0.3489599999999982	T	T	T
0.5728500000000025	0.3320900000000009	0.3351400000000027	T	T	T
0.6963000000000008	0.3738600000000005	0.1974799999999988	T	T	T
0.7294800000000023	0.3271299999999968	0.9856600000000029	T	T	T
0.8843200000000024	0.3269200000000012	0.9968700000000013	T	T	T
0.9422199999999989	0.3777699999999982	0.1882000000000019	T	T	T
0.9176500000000019	0.4469199999999987	0.8644200000000026	T	T	T
0.7964500000000001	0.4722399999999993	0.7256000000000000	T	T	T
0.7751799999999989	0.4371500000000026	0.4994399999999999	T	T	T
0.6180200000000013	0.4323600000000027	0.4917900000000017	T	T	T
0.5664000000000016	0.4711100000000030	0.7059599999999975	T	T	T
0.6711499999999972	0.4470499999999973	0.8621199999999973	T	T	T
0.9197800000000029	0.6794799999999981	0.8338099999999997	T	T	T
0.7701500000000010	0.6707499999999982	0.4673099999999977	T	T	T
0.6142200000000031	0.6736599999999981	0.4843199999999968	T	T	T
0.5582599999999971	0.6301600000000036	0.6976299999999966	T	T	T
0.6678199999999990	0.6778499999999994	0.8287400000000034	T	T	T
0.5786999999999978	0.9466499999999982	0.3592900000000014	T	T	T
0.7001800000000031	0.9755800000000008	0.2188900000000018	T	T	T
0.7199799999999996	0.9394199999999984	0.9949299999999965	T	T	T
0.8803199999999975	0.9353699999999989	0.9964599999999990	T	T	T
0.9325699999999983	0.9708100000000002	0.2061700000000002	T	T	T
0.8249500000000012	0.9480599999999981	0.3583799999999968	T	T	T

Structure files (CONTCAR) involved in this work:

0.5790500000000023	0.1765499999999989	0.3309399999999982	T	T	T
0.6993900000000011	0.1346500000000006	0.1964899999999972	T	T	T
0.7323200000000014	0.1716300000000004	0.9735700000000023	T	T	T
0.8870099999999965	0.1744199999999978	0.9843899999999977	T	T	T
0.9369700000000023	0.1289700000000025	0.1981299999999990	T	T	T
0.8228999999999971	0.1770899999999997	0.3320900000000009	T	T	T
0.9231399999999965	0.0557200000000009	0.8572399999999973	T	T	T
0.8023700000000034	0.0279400000000010	0.7090900000000033	T	T	T
0.7825199999999981	0.0693500000000000	0.4919900000000013	T	T	T
0.6223200000000020	0.0714899999999972	0.4900999999999982	T	T	T
0.5689800000000034	0.0332599999999985	0.6985400000000013	T	T	T
0.6791800000000023	0.0549699999999973	0.8492499999999978	T	T	T
0.9244399999999970	0.8325400000000016	0.8379699999999985	T	T	T
0.8017899999999969	0.8712099999999978	0.6993700000000018	T	T	T
0.7707899999999981	0.8278699999999972	0.4819600000000008	T	T	T
0.6157100000000000	0.8280000000000030	0.4908399999999986	T	T	T
0.5638999999999967	0.8761999999999972	0.6974900000000019	T	T	T
0.6768399999999986	0.8359299999999976	0.8364300000000000	T	T	T
0.4221100000000035	0.4444599999999994	0.6390200000000021	T	T	T
0.3025999999999982	0.4713199999999986	0.7800999999999974	T	T	T
0.2808100000000024	0.4441199999999981	0.0052999999999983	T	T	T
0.1223799999999997	0.4383399999999966	0.0111899999999991	T	T	T
0.0626400000000018	0.4706199999999967	0.8009600000000034	T	T	T
0.1733699999999985	0.4400899999999979	0.6553699999999978	T	T	T
0.4140099999999975	0.6759800000000027	0.6571399999999983	T	T	T
0.2991799999999998	0.6296899999999965	0.7931000000000026	T	T	T
0.2686199999999985	0.6716899999999981	0.0131999999999977	T	T	T
0.1139200000000002	0.6738500000000016	0.0028900000000007	T	T	T
0.0622299999999996	0.6297399999999982	0.7924999999999969	T	T	T
0.1764999999999972	0.6710500000000010	0.6590100000000021	T	T	T
0.0712100000000007	0.5612300000000019	0.1438899999999990	T	T	T
0.1936099999999996	0.5311400000000006	0.2793899999999994	T	T	T
0.2137099999999990	0.5575600000000023	0.5102800000000016	T	T	T
0.3719499999999982	0.5664900000000017	0.5096199999999982	T	T	T
0.4256200000000021	0.5295600000000036	0.2999500000000026	T	T	T
0.3215300000000028	0.5623599999999982	0.1493899999999968	T	T	T
0.0859999999999985	0.3267499999999970	0.1588700000000003	T	T	T
0.1978900000000010	0.3729999999999976	0.2963600000000000	T	T	T
0.2294600000000031	0.3324799999999968	0.5165300000000030	T	T	T
0.3847999999999985	0.3288099999999972	0.5038100000000014	T	T	T
0.4299699999999973	0.3726699999999994	0.2904499999999999	T	T	T
0.3169699999999978	0.3304899999999975	0.1585400000000021	T	T	T
0.9220699999999979	0.5323599999999971	0.1896899999999988	T	T	T
0.8262599999999978	0.3397900000000007	0.3303999999999974	T	T	T
0.7954999999999970	0.6376899999999992	0.7027599999999978	T	T	T
0.0039000000000016	0.5585999999999984	0.2080300000000008	T	T	T
0.3595299999999995	0.0706899999999990	0.7214900000000029	T	T	T
0.3164799999999985	0.0532899999999970	0.9054300000000026	T	T	T
0.2028200000000027	0.0493700000000032	0.0079100000000025	T	T	T
0.0933500000000009	0.0705400000000012	0.9003900000000016	T	T	T
0.1031800000000018	0.0661699999999996	0.7035100000000014	T	T	T
0.2296400000000034	0.0531700000000015	0.7576800000000006	T	T	T
0.3607700000000023	0.8285800000000023	0.7506600000000034	T	T	T

Structure files (CONTCAR) involved in this work:

0.3031500000000023	0.8630500000000012	0.9193599999999975	T	T	T
0.1897200000000012	0.8544899999999984	0.0188699999999997	T	T	T
0.0885699999999972	0.8337300000000027	0.8947700000000012	T	T	T
0.1034399999999991	0.8428600000000017	0.6986500000000007	T	T	T
0.2294199999999975	0.8484499999999997	0.7566399999999973	T	T	T
0.3144399999999976	0.9515200000000021	0.7724600000000024	T	T	T
0.0894199999999969	0.9533399999999972	0.8078399999999988	T	T	T
0.4328599999999980	0.1297500000000014	0.5823099999999997	T	T	T
0.4135599999999968	0.9987199999999987	0.5722099999999983	T	T	T
0.3913099999999972	0.8673599999999979	0.5662499999999966	T	T	T
0.1953400000000016	0.1385900000000007	0.6148600000000002	T	T	T
0.1877599999999973	0.0059200000000033	0.5819600000000023	T	T	T
0.1982900000000001	0.8725299999999976	0.5652400000000029	T	T	T
0.9878900000000002	0.0399099999999990	0.7881900000000002	T	T	T
0.9860499999999988	0.8710099999999983	0.7817700000000016	T	T	T
0.1417100000000033	0.9320000000000022	0.2200100000000020	T	T	T
0.1836100000000016	0.9485099999999989	0.4053800000000010	T	T	T
0.2973399999999984	0.9530900000000031	0.5076200000000028	T	T	T
0.4071899999999999	0.9338699999999989	0.4004800000000017	T	T	T
0.3974400000000031	0.9373500000000021	0.2039299999999997	T	T	T
0.2710200000000000	0.9503100000000018	0.2583899999999986	T	T	T
0.1407400000000010	0.1750899999999973	0.2492999999999981	T	T	T
0.1957000000000022	0.1408500000000004	0.4192899999999966	T	T	T
0.3098900000000029	0.1505999999999972	0.5163500000000028	T	T	T
0.4129399999999990	0.1692499999999981	0.3948200000000028	T	T	T
0.3965600000000009	0.1612500000000026	0.1989900000000020	T	T	T
0.2715400000000017	0.1519899999999978	0.2580400000000012	T	T	T
0.1845199999999991	0.0510799999999989	0.2741400000000027	T	T	T
0.4173100000000005	0.0503000000000000	0.3059599999999989	T	T	T
0.0664099999999976	0.8729000000000013	0.0829200000000014	T	T	T
0.0863299999999967	0.0036899999999989	0.0708800000000025	T	T	T
0.1088099999999983	0.1351599999999991	0.0667899999999975	T	T	T
0.3052800000000033	0.8640400000000028	0.1156900000000007	T	T	T
0.3123799999999974	0.9958900000000028	0.0815600000000032	T	T	T
0.3024600000000035	0.1289400000000001	0.0658799999999999	T	T	T
0.5139599999999973	0.9575999999999993	0.2881199999999993	T	T	T
0.5159700000000029	0.1379400000000004	0.2791100000000029	T	T	T
0.6313099999999991	0.5619000000000014	0.2656899999999993	T	T	T
0.7027399999999986	0.5758799999999979	0.1041299999999978	T	T	T
0.7895400000000024	0.5668900000000008	0.9509499999999989	T	T	T
0.8742400000000004	0.5776899999999969	0.1057699999999997	T	T	T
0.8849700000000027	0.5279700000000034	0.3159899999999993	T	T	T
0.7573700000000017	0.5266099999999980	0.2679100000000005	T	T	T
0.6404899999999998	0.3415499999999980	0.2717000000000027	T	T	T
0.6931999999999974	0.3309799999999967	0.0936999999999983	T	T	T
0.8068999999999988	0.3523300000000020	0.9945999999999984	T	T	T
0.9113699999999980	0.3215599999999981	0.1119500000000002	T	T	T
0.9106499999999969	0.3673500000000018	0.3020300000000020	T	T	T
0.7691999999999979	0.3718999999999966	0.2465199999999967	T	T	T
0.6732099999999974	0.4511099999999999	0.1707099999999997	T	T	T
0.9239299999999986	0.4504400000000004	0.1478999999999999	T	T	T
0.5696099999999973	0.6293300000000031	0.4075199999999981	T	T	T
0.5951200000000014	0.5013099999999966	0.4367700000000028	T	T	T

Structure files (CONTCAR) involved in this work:

0.5798599999999965	0.3681899999999985	0.4442900000000023	T	T	T
0.8055900000000022	0.6312399999999982	0.3736400000000017	T	T	T
0.7936899999999980	0.5160300000000007	0.4609000000000023	T	T	T
0.8272800000000018	0.3899199999999965	0.4408799999999999	T	T	T
0.0223299999999966	0.3672200000000032	0.2030400000000014	T	T	T
0.8533299999999997	0.4349399999999974	0.7910400000000024	T	T	T
0.7895800000000008	0.4343700000000013	0.6180700000000030	T	T	T
0.6981699999999975	0.4222499999999982	0.4735799999999983	T	T	T
0.6024799999999999	0.4357499999999987	0.6101699999999965	T	T	T
0.5984300000000005	0.4420799999999971	0.8088199999999972	T	T	T
0.7244299999999981	0.4714299999999980	0.7776199999999989	T	T	T
0.8581500000000020	0.6818099999999987	0.7579199999999986	T	T	T
0.8114500000000007	0.6461499999999987	0.5684600000000017	T	T	T
0.6923499999999976	0.6485800000000026	0.4796800000000019	T	T	T
0.5857200000000020	0.6654499999999999	0.5962600000000009	T	T	T
0.5898400000000024	0.6688199999999966	0.7936600000000027	T	T	T
0.7153100000000023	0.6505500000000026	0.7401300000000006	T	T	T
0.8193899999999985	0.5500600000000020	0.7018500000000003	T	T	T
0.5792500000000018	0.5513899999999978	0.6979699999999980	T	T	T
0.9288700000000034	0.3794200000000032	0.9310499999999990	T	T	T
0.9082500000000024	0.5122000000000000	0.9347100000000026	T	T	T
0.8994799999999969	0.6437299999999979	0.9388300000000029	T	T	T
0.6905799999999971	0.3738200000000020	0.9050500000000028	T	T	T
0.6711600000000004	0.5037299999999973	0.9490199999999973	T	T	T
0.6780800000000013	0.6374199999999988	0.9335599999999999	T	T	T
0.4872900000000016	0.4534299999999973	0.7094600000000000	T	T	T
0.4773199999999989	0.6352499999999992	0.7027500000000018	T	T	T
0.6445200000000000	0.9406999999999996	0.2897099999999995	T	T	T
0.7002600000000001	0.9372400000000027	0.1121300000000005	T	T	T
0.8004400000000018	0.9434699999999978	0.9794699999999992	T	T	T
0.8980999999999995	0.9299499999999981	0.1143199999999993	T	T	T
0.8997499999999974	0.9482199999999992	0.3118300000000005	T	T	T
0.7731899999999996	0.9666899999999998	0.2692899999999980	T	T	T
0.6415199999999999	0.1764700000000019	0.2541900000000012	T	T	T
0.6968099999999993	0.1564800000000020	0.0799999999999983	T	T	T
0.8100999999999985	0.1477399999999989	0.9796600000000026	T	T	T
0.9141699999999986	0.1686400000000035	0.0979000000000028	T	T	T
0.8986799999999988	0.1580099999999973	0.2956399999999988	T	T	T
0.7721200000000010	0.1510900000000035	0.2438199999999995	T	T	T
0.6831299999999985	0.0547899999999970	0.2060499999999976	T	T	T
0.9199600000000032	0.0499099999999970	0.1845599999999976	T	T	T
0.5701099999999997	0.8770299999999978	0.4220899999999972	T	T	T
0.5836600000000018	0.0088000000000008	0.4378099999999989	T	T	T
0.6000000000000014	0.1409299999999973	0.4358199999999997	T	T	T
0.8115400000000008	0.8733199999999997	0.4028199999999984	T	T	T
0.8196200000000005	0.0031299999999987	0.4472400000000007	T	T	T
0.8066400000000016	0.1369200000000035	0.4357100000000003	T	T	T
0.0116399999999999	0.9540999999999968	0.2157100000000014	T	T	T
0.0170499999999976	0.1382699999999986	0.2136599999999973	T	T	T
0.8577799999999982	0.0560600000000022	0.7862900000000010	T	T	T
0.8023700000000034	0.0747500000000016	0.6096199999999996	T	T	T
0.7021799999999985	0.0597599999999971	0.4787400000000019	T	T	T
0.6012500000000003	0.0766100000000023	0.6071600000000004	T	T	T

Structure files (CONTCAR) involved in this work:

0.6039600000000007	0.0522100000000023	0.8042599999999993	T	T	T
0.7292800000000028	0.0308500000000009	0.7609199999999987	T	T	T
0.8589399999999969	0.8376900000000020	0.7678599999999989	T	T	T
0.8024300000000011	0.8318399999999997	0.5931700000000006	T	T	T
0.6933099999999968	0.8524600000000007	0.4845899999999972	T	T	T
0.5909100000000009	0.8294500000000014	0.6062299999999965	T	T	T
0.6013200000000012	0.8545999999999978	0.8002600000000015	T	T	T
0.7290199999999984	0.8629099999999994	0.7517500000000013	T	T	T
0.8178800000000024	0.9501599999999968	0.6797100000000000	T	T	T
0.5796100000000024	0.9542399999999986	0.6713299999999975	T	T	T
0.9320900000000023	0.1292199999999966	0.9089299999999980	T	T	T
0.9172099999999972	0.9999499999999983	0.9459500000000034	T	T	T
0.9080099999999973	0.8670100000000005	0.9452100000000030	T	T	T
0.6949899999999971	0.1312199999999990	0.8844300000000018	T	T	T
0.6856900000000010	0.0054999999999978	0.9452700000000007	T	T	T
0.6916300000000035	0.8715400000000031	0.9431799999999981	T	T	T
0.4902099999999976	0.0499300000000034	0.7134700000000009	T	T	T
0.4840299999999971	0.8656700000000015	0.7114100000000008	T	T	T
0.3560900000000018	0.4338300000000004	0.7079999999999984	T	T	T
0.3096499999999978	0.4410900000000026	0.8920200000000023	T	T	T
0.2009400000000028	0.4587900000000005	0.0051500000000004	T	T	T
0.0914000000000001	0.4335700000000031	0.8994100000000032	T	T	T
0.0977900000000034	0.4389899999999969	0.7011299999999991	T	T	T
0.2262399999999971	0.4586600000000018	0.7430200000000013	T	T	T
0.3536199999999994	0.6767499999999984	0.7378000000000000	T	T	T
0.3028899999999979	0.6458700000000022	0.9108000000000018	T	T	T
0.1908900000000031	0.6482499999999973	0.0132400000000032	T	T	T
0.0910099999999971	0.6721300000000028	0.8865899999999982	T	T	T
0.0990600000000015	0.6573199999999986	0.6914200000000008	T	T	T
0.2247300000000010	0.6453199999999981	0.7496999999999971	T	T	T
0.3183900000000008	0.5513300000000001	0.7752699999999990	T	T	T
0.0793600000000012	0.5503700000000009	0.8068499999999972	T	T	T
0.4322099999999978	0.3786599999999964	0.5685300000000026	T	T	T
0.4162800000000004	0.5103200000000001	0.5673999999999992	T	T	T
0.3873499999999979	0.6404399999999981	0.5550799999999967	T	T	T
0.1904400000000024	0.3661799999999999	0.6105599999999995	T	T	T
0.1751300000000029	0.4965199999999967	0.5671299999999988	T	T	T
0.1921000000000035	0.6297199999999989	0.5567399999999978	T	T	T
0.9823400000000007	0.4576899999999995	0.7905299999999968	T	T	T
0.9821200000000019	0.6388000000000034	0.7806500000000014	T	T	T
0.1363500000000002	0.5705900000000028	0.2173700000000025	T	T	T
0.1908000000000030	0.5568200000000019	0.3944299999999998	T	T	T
0.2936100000000010	0.5464500000000001	0.5222800000000021	T	T	T
0.3917900000000003	0.5692700000000031	0.3928000000000011	T	T	T
0.3961400000000026	0.5607100000000003	0.1968900000000033	T	T	T
0.2678099999999972	0.5458300000000023	0.2370799999999988	T	T	T
0.1428300000000036	0.3246400000000023	0.2452800000000011	T	T	T
0.1949600000000018	0.3615500000000011	0.4157999999999973	T	T	T
0.3077699999999979	0.3540599999999969	0.5166400000000024	T	T	T
0.4059099999999987	0.3290199999999999	0.3867499999999993	T	T	T
0.3944800000000015	0.3442300000000031	0.1894500000000008	T	T	T
0.2715400000000017	0.3542699999999996	0.2537299999999973	T	T	T
0.1787899999999993	0.4507600000000025	0.2720600000000033	T	T	T

Structure files (CONTCAR) involved in this work:

0.4075399999999973	0.4501800000000031	0.3090499999999992	T	T	T
0.0667499999999990	0.6253299999999982	0.0684899999999971	T	T	T
0.0820599999999985	0.4934399999999997	0.0764100000000028	T	T	T
0.1151499999999999	0.3638300000000001	0.0598600000000005	T	T	T
0.3077400000000026	0.6371400000000023	0.1059899999999985	T	T	T
0.3175799999999995	0.5059800000000010	0.0619500000000031	T	T	T
0.2968400000000031	0.3727099999999979	0.0591799999999978	T	T	T
0.5056700000000021	0.5385599999999968	0.2994399999999970	T	T	T
0.5102600000000024	0.3662199999999984	0.2756200000000035	T	T	T
0.4358199999999997	0.7525899999999979	0.6326099999999997	T	T	T
0.1890000000000001	0.7499200000000030	0.6355399999999989	T	T	T
0.2754199999999969	0.7520999999999987	0.0227300000000028	T	T	T
0.1077700000000021	0.7501200000000026	0.0445199999999986	T	T	T
0.0650100000000009	0.2504500000000007	0.1311999999999998	T	T	T
0.3063700000000011	0.2513300000000029	0.1349599999999995	T	T	T
0.2219100000000012	0.2518900000000031	0.5230099999999993	T	T	T
0.3931200000000032	0.2529400000000024	0.5458599999999976	T	T	T
0.5576999999999970	0.2533600000000007	0.3554400000000015	T	T	T
0.8171600000000012	0.2558399999999992	0.3519300000000030	T	T	T
0.7269300000000030	0.2505600000000001	0.9449400000000026	T	T	T
0.8910399999999967	0.2523600000000030	0.9481200000000030	T	T	T
0.9454800000000034	0.7553199999999975	0.8588000000000022	T	T	T
0.6837500000000034	0.7560599999999980	0.8525899999999993	T	T	T
0.7768900000000016	0.7499600000000015	0.4460199999999972	T	T	T
0.6095899999999972	0.7515300000000025	0.4496299999999991	T	T	T
0.9221399999999988	0.4886800000000022	0.5384999999999991	T	T	T
0.9245200000000011	0.4444799999999987	0.4023200000000031	T	T	T
0.8619600000000034	0.5594499999999982	0.5664299999999969	T	T	T
0.0528300000000002	0.4553700000000021	0.4648400000000024	T	T	T
0.0389699999999991	0.4751699999999985	0.3310999999999993	T	T	T
0.9498400000000018	0.4716700000000031	0.5929100000000034	T	T	T
0.0244199999999992	0.5722000000000023	0.5137000000000000	T	T	T
0.9863799999999969	0.5874400000000009	0.3933200000000028	T	T	T
0.0725100000000012	0.5868899999999968	0.4037799999999976	T	T	T
0.0308500000000009	0.4892400000000023	0.4093700000000027	T	T	T
0.0271100000000004	0.5617500000000035	0.4333699999999965	T	T	T

Figure 4(a) Route(a)-Zn ③

Si Al O Zn H C

1.0000000000000000

20.0219999999999985 0.0000000000000000 0.0000000000000000

0.0000000000000000 19.8990000000000009 0.0000000000000000

0.0000000000000000 0.0000000000000000 13.3829999999999991

93 3 193 2 6 2

Selective dynamics

Direct

0.4234921859848466	0.0602981839036079	0.6485172903366696	T	T	T
0.3060798779652079	0.0322656607266418	0.7921932062470202	T	T	T
0.2831071599476155	0.0569562734471078	0.0170174721485705	T	T	T
0.1238715138934038	0.0624930025179708	0.0125436560210737	T	T	T
0.0688368204333313	0.0310170518721779	0.8010776005164129	T	T	T
0.1810606754991912	0.0646481660260797	0.6650569256669284	T	T	T
0.4192555017014392	0.8277039270679964	0.6677625269485215	T	T	T

Structure files (CONTCAR) involved in this work:

0.3018556604116298	0.8732798045965211	0.8005217753256693	T	T	T
0.2675521260110590	0.8318198214318339	0.0196800197000107	T	T	T
0.1124721339138482	0.8273468510779657	0.0111478557470488	T	T	T
0.0667747913745699	0.8745513334790305	0.7972449458043636	T	T	T
0.1804352791766428	0.8288080926948261	0.6649096957800152	T	T	T
0.0765640966711373	0.9405044425312041	0.1490804501855189	T	T	T
0.1953131481420718	0.9700296057106979	0.2906029122168757	T	T	T
0.2174222791071470	0.9435958871474721	0.5162094985091150	T	T	T
0.3776993589143149	0.9360671809841291	0.5134148985471058	T	T	T
0.4343237925153521	0.9693323583502897	0.3011574703670380	T	T	T
0.3210496394538114	0.9364623867305183	0.1646014537911910	T	T	T
0.0829672258643558	0.1727257917156490	0.1661282987424084	T	T	T
0.1983470348355530	0.1286026691729156	0.3017710197133914	T	T	T
0.2325292192635423	0.1692825040121173	0.5192455792497529	T	T	T
0.3879906125315742	0.1737111828159580	0.5086295071122179	T	T	T
0.4356559837593463	0.1279526861496817	0.2943874841140942	T	T	T
0.3186092909304815	0.1728889208180927	0.1662772002801338	T	T	T
0.5782143536463128	0.5558992319407871	0.3561304354999935	T	T	T
0.6929756699942320	0.5262126387341904	0.2043812464207132	T	T	T
0.7170101310937221	0.5689258910377401	0.9876535508409084	T	T	T
0.8755659397305668	0.5741605627270100	0.9852433784890967	T	T	T
0.8125929473581158	0.5512049739908663	0.3474299552322295	T	T	T
0.5750927596198675	0.3292989914434112	0.3334984231685579	T	T	T
0.6950152971634770	0.3727493853677054	0.1927894229049090	T	T	T
0.7324985288426620	0.3274989974727262	0.9808742743583695	T	T	T
0.8875133007687123	0.3251937214132837	0.9939293110408510	T	T	T
0.9437132566858448	0.3728229521048060	0.1919680021688084	T	T	T
0.9205418483078855	0.4454176868281364	0.8616801344399885	T	T	T
0.8012563299282807	0.4729430558428644	0.7204651501280069	T	T	T
0.7779802398456950	0.4357153862825196	0.4969819571782727	T	T	T
0.6194809449313285	0.4300176742426293	0.4921994658716283	T	T	T
0.5694971861199443	0.4689173998868743	0.7058691300271384	T	T	T
0.6780357460673320	0.4479391116643721	0.8577911569885420	T	T	T
0.9218726857845083	0.6790301154867012	0.8283269512203266	T	T	T
0.7684318760407566	0.6693769410887617	0.4672384585202788	T	T	T
0.6134205646643670	0.6733027358223285	0.4894318103859340	T	T	T
0.5603616202284134	0.6277891874036796	0.7008637067512616	T	T	T
0.6735019717125974	0.6738757216431368	0.8289520987441847	T	T	T
0.5786464406504778	0.9451178466809609	0.3587129510900687	T	T	T
0.6989095945199590	0.9736468808685348	0.2155736935212794	T	T	T
0.7201936560968080	0.9374953577544413	0.9936541771616404	T	T	T
0.8803080280305150	0.9338528699302105	0.9952199788214551	T	T	T
0.9317279604897596	0.9705140295794776	0.2053479082567004	T	T	T
0.8228483354841963	0.9468510926889380	0.3560963345993284	T	T	T
0.5787669986107612	0.1740131304889888	0.3300492572006583	T	T	T
0.6986753265381658	0.1312842911578770	0.1942928771722083	T	T	T
0.7330011369025882	0.1714900586261349	0.9728613338224146	T	T	T
0.8875731368853732	0.1731771531814165	0.9825868980307124	T	T	T
0.9363239282522817	0.1288196829810314	0.1969550971714509	T	T	T
0.8208999855545333	0.1731511284065523	0.3304133795595899	T	T	T
0.9238902673322924	0.0539438344569979	0.8562222530600798	T	T	T
0.8023034308387976	0.0267724967382830	0.7097810106209663	T	T	T
0.7820190553147518	0.0668140623291446	0.4922708266901165	T	T	T

Structure files (CONTCAR) involved in this work:

0.6216331653073747	0.0698181948903691	0.4905691502984474	T	T	T
0.5689549211723558	0.0321366458780950	0.6997252146002123	T	T	T
0.6790404659050177	0.0539217601897125	0.8505065348418550	T	T	T
0.9244760806808658	0.8316229243044411	0.8363319420503224	T	T	T
0.8025748205230313	0.8697020622802992	0.6963004168845864	T	T	T
0.7696435691071652	0.8268903305982410	0.4791705411736567	T	T	T
0.6147717544761490	0.8269923592178948	0.4906200400552005	T	T	T
0.5639532292265650	0.8749699558923887	0.6986474654926921	T	T	T
0.6785519576105026	0.8328720402122017	0.8339091760762735	T	T	T
0.4255004681770221	0.4418320626610385	0.6457702394629790	T	T	T
0.3052729720276278	0.4701918709046759	0.7869309495985575	T	T	T
0.2823181395309304	0.4452503992990503	0.0124738232252420	T	T	T
0.1238675219886976	0.4387472997396680	0.0167307973802816	T	T	T
0.0647662130710064	0.4694423557841563	0.8028051982365687	T	T	T
0.1773283494746860	0.4363890015257858	0.6622910476435971	T	T	T
0.4166764118315523	0.6741495228522496	0.6656852882910940	T	T	T
0.3016475020482108	0.6291850434191744	0.8016125190732236	T	T	T
0.2685324375315782	0.6703583977766565	0.0192851688449509	T	T	T
0.1136555695214777	0.6729788594051584	0.0084999132633955	T	T	T
0.0636657350374479	0.6285319862539871	0.7938227372247750	T	T	T
0.1813958281366840	0.6718042250971242	0.6663907913714612	T	T	T
0.0799394744871032	0.5610989136005951	0.1522265701481638	T	T	T
0.1982461229803820	0.5291299639924796	0.2909757462314758	T	T	T
0.2195112037725842	0.5551299371460142	0.5204404354616757	T	T	T
0.3774327805682819	0.5639666663315169	0.5160625934641370	T	T	T
0.4302272411857657	0.5306035319297275	0.3029464880018808	T	T	T
0.3231739443417962	0.5632828298761345	0.1574946729222526	T	T	T
0.0875884313683925	0.3251703954114915	0.1629965599585304	T	T	T
0.1995473945497525	0.3715291526283669	0.3014137260288031	T	T	T
0.2314796179327320	0.3306063585392103	0.5196623565404632	T	T	T
0.3865244592987196	0.3277292439972815	0.5069481596879868	T	T	T
0.4325520739027369	0.3732079265031039	0.2931337336897146	T	T	T
0.3182460286465926	0.3302261990478099	0.1639228085043599	T	T	T
0.9213344338806303	0.5290760209586917	0.1954324107389808	T	T	T
0.8221907361179488	0.3348112689178568	0.3263125536932437	T	T	T
0.7997470426499507	0.6355641133775625	0.6956453940961731	T	T	T
0.0102247318791547	0.5559325120619032	0.2249136947397030	T	T	T
0.3598485358764220	0.0710018336825555	0.7221876330981933	T	T	T
0.3174558600808216	0.0547350917520024	0.9072545545562619	T	T	T
0.2031049008853745	0.0464571284893136	0.0073951906250957	T	T	T
0.0933325998052146	0.0696537866571851	0.9012539093132524	T	T	T
0.1043759016939490	0.0647942827019085	0.7042137170095862	T	T	T
0.2303810550030966	0.0520990409452887	0.7599708449417638	T	T	T
0.3600784224830464	0.8280275202951241	0.7506516727003917	T	T	T
0.3027361456188216	0.8609993802152152	0.9198362846812254	T	T	T
0.1892349659746144	0.8536049931857854	0.0199121150044237	T	T	T
0.0878705226227616	0.8322779420308423	0.8962889594661893	T	T	T
0.1034529408582964	0.8408191666496431	0.7006162961210964	T	T	T
0.2292532698537097	0.8514519843086533	0.7564584506729617	T	T	T
0.3167775032404760	0.9518205438509391	0.7766104101149620	T	T	T
0.0906922171037582	0.9522063830380241	0.8091198317419982	T	T	T
0.4337674371677307	0.1275010681648396	0.5811065301727888	T	T	T
0.4129265738378468	0.9964853306785978	0.5748755358428203	T	T	T

Structure files (CONTCAR) involved in this work:

0.3937090090941316	0.8646644013343975	0.5666221529383241	T	T	T
0.1970053556144034	0.1377946234886925	0.6172120697735589	T	T	T
0.1901009379485709	0.0054883682615390	0.5830362109418271	T	T	T
0.1959403966129703	0.8719383878481367	0.5647533690138755	T	T	T
0.9887822326593855	0.0385114534786360	0.7871143745201836	T	T	T
0.9862206129709304	0.8718041718223897	0.7829937932437373	T	T	T
0.1409246230291030	0.9312327178505625	0.2217068840390572	T	T	T
0.1839821666162758	0.9487345861652007	0.4061152742546612	T	T	T
0.2979096363198358	0.9489054865615044	0.5086136947878883	T	T	T
0.4081190154981892	0.9326809769491722	0.4018755557934769	T	T	T
0.3973027446757109	0.9359000143355145	0.2052700695460549	T	T	T
0.2706850305947118	0.9491459068553239	0.2583122517701405	T	T	T
0.1397858958001390	0.1736367226619316	0.2525888797718546	T	T	T
0.1957240516604555	0.1385160804294006	0.4215756089896888	T	T	T
0.3108829488961115	0.1480724543823195	0.5160461450613317	T	T	T
0.4134613923036157	0.1686998129099326	0.3941491645990379	T	T	T
0.3958956465528611	0.1593915990119991	0.1987369264194289	T	T	T
0.2711445407322408	0.1523647194566446	0.2606624648402593	T	T	T
0.1851055502421558	0.0503320032432555	0.2735972046390767	T	T	T
0.4164947540402667	0.0490775612445744	0.3070594010280421	T	T	T
0.0658230305614607	0.8717786546536288	0.0848933082365765	T	T	T
0.0863166952751677	0.0020893047932954	0.0710635454210306	T	T	T
0.1108045167567604	0.1331111657602281	0.0689208761789138	T	T	T
0.3052223276796188	0.8635152890672720	0.1156709089550445	T	T	T
0.3134252342563387	0.9959196080514930	0.0827122194475580	T	T	T
0.2996344441573098	0.1290708358108583	0.0680573178605737	T	T	T
0.5139201925341687	0.9572848370683210	0.2878554710826150	T	T	T
0.5156185225141141	0.1359770332021197	0.2772512787696627	T	T	T
0.6385887305810788	0.5621183421509824	0.2764487841266173	T	T	T
0.7041283204619535	0.5737557199402582	0.1073958308627359	T	T	T
0.7961662627285677	0.5634639720916842	0.9611856888000039	T	T	T
0.8902194451696553	0.5791907360939914	0.1027965838699435	T	T	T
0.8890895238410610	0.5402913044619173	0.3150508457342168	T	T	T
0.7632877764662693	0.5201279712636807	0.2649335046304038	T	T	T
0.6408074121245527	0.3360851958551199	0.2651655695796424	T	T	T
0.6914311704334584	0.3353280601416376	0.0844214468190606	T	T	T
0.8101078111008612	0.3504888806520647	0.9963985627817701	T	T	T
0.9174837562606091	0.3204754186492904	0.1065902073574242	T	T	T
0.9073023980081256	0.3552185396941900	0.2983429246909696	T	T	T
0.7683399885837915	0.3692848447818332	0.2398423924137678	T	T	T
0.6701393526093451	0.4506486416115180	0.1755670769046118	T	T	T
0.9296404016612057	0.4481485626718772	0.1561767337472174	T	T	T
0.5697727868633572	0.6271215155359784	0.4138051611629120	T	T	T
0.5918282619214792	0.4978153645756049	0.4390648993122980	T	T	T
0.5855388073486937	0.3640897564818395	0.4428152688100674	T	T	T
0.7965074499246844	0.6300969898878706	0.3690140458073768	T	T	T
0.8004953080949472	0.5129352147314833	0.4580979675918189	T	T	T
0.8239034768472308	0.3816672392571278	0.4400695893385958	T	T	T
0.0238456053152501	0.3630766417786178	0.2107567599192155	T	T	T
0.8552349800479749	0.4351111570976313	0.7907260790371201	T	T	T
0.7951409801165028	0.4326054925277887	0.6150763593697677	T	T	T
0.6997501378163962	0.4257365984696643	0.4740730953493416	T	T	T
0.6032129591389350	0.4308523346488564	0.6105724604486894	T	T	T

Structure files (CONTCAR) involved in this work:

0.6039853171962589	0.4437240520684121	0.8089210795074987	T	T	T
0.7286109386899076	0.4757591672882659	0.7717510849891797	T	T	T
0.8604281390860379	0.6818776393285965	0.7528630769423906	T	T	T
0.8145201883540401	0.6446847021875253	0.5627019050241435	T	T	T
0.6912293664150935	0.6482746068062024	0.4894515231424793	T	T	T
0.5834617151766410	0.6679584360026630	0.6010877912981933	T	T	T
0.5951311829008509	0.6616264450887253	0.7981595928276426	T	T	T
0.7203124294314438	0.6474362670906779	0.7391305144759186	T	T	T
0.8267814128757741	0.5492357404485806	0.6945558238595063	T	T	T
0.5804489488933297	0.5490626537931632	0.6906036825131213	T	T	T
0.9313099790100029	0.3774065262914625	0.9268401211238039	T	T	T
0.9145350310976159	0.5105231785056989	0.9334534595641744	T	T	T
0.9029268964031910	0.6425976409652026	0.9332681013900943	T	T	T
0.6994761326326790	0.3735282999192948	0.8938498203234523	T	T	T
0.6789876413057880	0.5009861722039445	0.9497119696653544	T	T	T
0.6866655471620200	0.6352467861816620	0.9346211572908560	T	T	T
0.4909191292635347	0.4496009150348999	0.7158035624386428	T	T	T
0.4796645263078730	0.6336844556926918	0.7126834569444345	T	T	T
0.6442590998383425	0.9392368553609711	0.2886643912332776	T	T	T
0.7001452027461962	0.9328216911030793	0.1107258872361397	T	T	T
0.8006269807597370	0.9439668102205437	0.9793023895364809	T	T	T
0.8987394556862116	0.9288887337596622	0.1129704174324090	T	T	T
0.8979963474682003	0.9481069728432535	0.3104440645192440	T	T	T
0.7719895536187112	0.9683433271281461	0.2671439118515961	T	T	T
0.6419212362706816	0.1728104032312462	0.2547051854711359	T	T	T
0.6978354284992445	0.1578843582150856	0.0799776318179492	T	T	T
0.8105891419160554	0.1468306048639690	0.9775663470114588	T	T	T
0.9137905653653690	0.1684384755860538	0.0966598930889504	T	T	T
0.8977694971272163	0.1582275349348421	0.2939237168139747	T	T	T
0.7717841137798920	0.1422058894754997	0.2435371687084909	T	T	T
0.6795353844612886	0.0517910014208784	0.1968710888582865	T	T	T
0.9195839889219887	0.0496040782316801	0.1832420829854820	T	T	T
0.5694093278349645	0.8750896013944124	0.4200641146525745	T	T	T
0.5839689193858838	0.0062856672183615	0.4388755441397973	T	T	T
0.5979077569087173	0.1385612967221893	0.4357608925003070	T	T	T
0.8083991850350868	0.8711439647850031	0.3959826019233817	T	T	T
0.8171010916643581	0.9990330127495786	0.4487352360747077	T	T	T
0.8084297354793700	0.1330115752267848	0.4351474947353255	T	T	T
0.0108661032039453	0.9538651403083844	0.2165136917345781	T	T	T
0.0164657284184809	0.1381439873571150	0.2123539821490861	T	T	T
0.8584010040730682	0.0552223663753870	0.7856954122082651	T	T	T
0.8017107869689108	0.0729608630091236	0.6098159882240798	T	T	T
0.7015349610424895	0.0594396301862626	0.4786544292813559	T	T	T
0.6007791229010675	0.0751274206466153	0.6076776716645139	T	T	T
0.6039250399974422	0.0516574926886337	0.8051236420499223	T	T	T
0.7295695092035589	0.0298901053962449	0.7626371724274462	T	T	T
0.8600047574144687	0.8359334939739387	0.7641952283250717	T	T	T
0.8044834094523561	0.8328690089524978	0.5881833997708316	T	T	T
0.6923154289306712	0.8519390294952776	0.4859328618186778	T	T	T
0.5886502357403187	0.8291731003497398	0.6052070668831869	T	T	T
0.6026770595082787	0.8516548249193809	0.7994589612870834	T	T	T
0.7296690174291022	0.8594002336194088	0.7474309083730430	T	T	T
0.8179650027378775	0.9490953822516458	0.6808553367469857	T	T	T

Structure files (CONTCAR) involved in this work:

0.5799592292403710	0.9530834249357298	0.6736669497842570	T	T	T
0.9330758095229696	0.1269890985506754	0.9090678178741999	T	T	T
0.9184730369436340	0.9971988055787678	0.9435979376685669	T	T	T
0.9059091807910182	0.8645299028663299	0.9440136048912849	T	T	T
0.6946458900925789	0.1302203045657646	0.8856122934060835	T	T	T
0.6848234564582202	0.0037585381330198	0.9460168581405610	T	T	T
0.6942683027281541	0.8695132479072329	0.9395942125051575	T	T	T
0.4901196179473116	0.0485268765082942	0.7146343495272905	T	T	T
0.4841194844319691	0.8649807931191287	0.7151939082481384	T	T	T
0.3596657260858273	0.4334259131092095	0.7158481424392432	T	T	T
0.3127796860766305	0.4426519375043560	0.9003553592722905	T	T	T
0.2020923578846234	0.4602667461753785	0.0110295258611090	T	T	T
0.0911220578756986	0.4371685017803919	0.9067176389201961	T	T	T
0.1021159500038161	0.4345576556775350	0.7080526091872505	T	T	T
0.2295228479921636	0.4533729311787816	0.7515469405365669	T	T	T
0.3570699678582708	0.6756340282075963	0.7477646182904160	T	T	T
0.3055152828002517	0.6419096421764425	0.9205748835510050	T	T	T
0.1904333227083299	0.6466541632611761	0.0170490890957900	T	T	T
0.0870382608777782	0.6669227296547792	0.8951643188500347	T	T	T
0.1039156894884540	0.6591713669961708	0.6983223528726704	T	T	T
0.2275943494581148	0.6496120849867868	0.7613960919054221	T	T	T
0.3176201372591800	0.5507285618590357	0.7786461090070983	T	T	T
0.0815176213472241	0.5492218697762502	0.8039154563344544	T	T	T
0.4333878531437853	0.3756068970016786	0.5756270568858461	T	T	T
0.4215643902475310	0.5076721486154646	0.5737190802347432	T	T	T
0.3897819953745784	0.6376247884632417	0.5644758585839406	T	T	T
0.1938456596520843	0.3630024812794218	0.6156697354410914	T	T	T
0.1803483659402597	0.4947167772794458	0.5770905755831716	T	T	T
0.2006861325765047	0.6274527397243411	0.5685557425273657	T	T	T
0.9853196671320905	0.4556648446049392	0.7883912189657063	T	T	T
0.9843939187747809	0.6384337826003575	0.7752586223857572	T	T	T
0.1406148786390495	0.5711190220728899	0.2303268326170377	T	T	T
0.1945193334534681	0.5546003856159732	0.4051498687902618	T	T	T
0.2993038145716095	0.5421244681831361	0.5260766316382401	T	T	T
0.3993499428892643	0.5684173482395439	0.4000092630163274	T	T	T
0.3980750299762721	0.5640960093801395	0.2030150128024863	T	T	T
0.2714596154684628	0.5446967864404814	0.2472000843453787	T	T	T
0.1460162831177686	0.3232902479365246	0.2470137588395411	T	T	T
0.1952994112856350	0.3601893561206592	0.4205567317180149	T	T	T
0.3094790326873744	0.3532853140478859	0.5183966668060309	T	T	T
0.4089558891937236	0.3306390712539118	0.3906601665340036	T	T	T
0.3959139828227002	0.3438482130067069	0.1934467056794697	T	T	T
0.2738173279973449	0.3535464454223137	0.2604961063419520	T	T	T
0.1809834969523516	0.4498953267341577	0.2779529083152286	T	T	T
0.4111191859542875	0.4512994764179944	0.3094230741380412	T	T	T
0.0684892096672313	0.6263124906698446	0.0830768539747132	T	T	T
0.0842140875401780	0.4938028742329192	0.0863400356634912	T	T	T
0.1153967661192360	0.3647509420597452	0.0647432610364864	T	T	T
0.3052199324994179	0.6376458450498147	0.1156732096398415	T	T	T
0.3185978730110522	0.5068739156211003	0.0703090225542130	T	T	T
0.2968198058958949	0.3736455219462775	0.0662169801987266	T	T	T
0.5101632160613859	0.5398115552851334	0.2955715266310462	T	T	T
0.5125024314446252	0.3659791306078835	0.2773219330116713	T	T	T

Structure files (CONTCAR) involved in this work:

0.4374232729207804	0.7506657804724930	0.6386538472609605	T	T	T
0.1926532336633116	0.7501392561123680	0.6380079439315572	T	T	T
0.2741178087950821	0.7509476822129082	0.0250985357119255	T	T	T
0.1075056948629650	0.7495714907916277	0.0472237055030630	T	T	T
0.0682952965782941	0.2493278446309172	0.1306938891560590	T	T	T
0.3069983988981579	0.2514900088067542	0.1381205993976033	T	T	T
0.2243720163629437	0.2500140314764722	0.5234966602859304	T	T	T
0.3934619046288855	0.2510253077975980	0.5461398967175657	T	T	T
0.5578371693301468	0.2509944649647891	0.3536112998918622	T	T	T
0.8083511627471240	0.2511970447050929	0.3476148514147688	T	T	T
0.7286104198152016	0.2502336026887025	0.9431667524868327	T	T	T
0.8926234096866641	0.2506296102085260	0.9446345502654855	T	T	T
0.9474437318603977	0.7546947735617375	0.8552101961633974	T	T	T
0.6858402479783866	0.7531350178890259	0.8508267909856190	T	T	T
0.7744108392216604	0.7487957377800131	0.4448785291056793	T	T	T
0.6087996170081288	0.7502986432832784	0.4504826763441712	T	T	T
0.9395558608561598	0.4916570542146517	0.5243765005018748	T	T	T
0.9336921484700489	0.4073899809867742	0.4348150775843728	T	T	T
0.8737232097271097	0.5580120766546691	0.5580025332343553	T	T	T
0.0294494851243462	0.5886939205265668	0.5461897614623762	T	T	T
0.0772109511480270	0.5705867265869632	0.4315416936599382	T	T	T
0.9699252064834284	0.4812824163175740	0.5797908718532415	T	T	T
-0.0018658821906946	0.7005766978388631	0.4809067815620182	T	T	T
0.0141089000096370	0.5740092112485340	0.2932353652792580	T	T	T
0.0459176177786685	0.6842515790478286	0.3645456529964040	T	T	T
0.0452243156232562	0.6055133374857050	0.4723481238881723	T	T	T
0.0287022852060690	0.6659746082148691	0.4371199877552057	T	T	T

Figure 4(a) Route(b-i)-Zn ① as same as Route(a)-Zn ①**Figure 4(a) Route(b-i)-Zn ②**

Si Al O Zn H C

1.0000000000000000

20.0219999999999985 0.0000000000000000 0.0000000000000000

0.0000000000000000 19.8990000000000009 0.0000000000000000

0.0000000000000000 0.0000000000000000 13.3829999999999991

93 3 193 2 6 2

Selective dynamics

Direct

0.4226499999999973	0.0601399999999970	0.6481700000000004	T	T	T
0.3055299999999974	0.0322099999999992	0.7924999999999969	T	T	T
0.2821599999999975	0.0557900000000018	0.0170499999999976	T	T	T
0.1232400000000027	0.0613600000000005	0.0117100000000008	T	T	T
0.0683399999999992	0.0312100000000015	0.8008799999999994	T	T	T
0.1807099999999977	0.0649599999999992	0.6653400000000005	T	T	T
0.4183299999999974	0.8273200000000003	0.6683900000000023	T	T	T
0.3008000000000024	0.8732400000000027	0.8003500000000017	T	T	T
0.2667900000000003	0.8303599999999989	0.0198099999999997	T	T	T
0.1111199999999997	0.8264700000000005	0.0135700000000014	T	T	T
0.0665600000000026	0.8748000000000005	0.7990100000000027	T	T	T
0.1790700000000029	0.8290199999999999	0.6641400000000033	T	T	T
0.0752600000000001	0.9405100000000033	0.1489300000000000	T	T	T
0.1948500000000024	0.9698899999999995	0.2899000000000029	T	T	T
0.2164700000000011	0.9438999999999993	0.5159799999999990	T	T	T

Structure files (CONTCAR) involved in this work:

0.3768099999999990	0.9355199999999968	0.5136099999999999	T	T	T
0.4332300000000018	0.9688400000000001	0.3013899999999978	T	T	T
0.3203499999999977	0.9349399999999974	0.1642300000000034	T	T	T
0.0821899999999971	0.1716100000000012	0.1666299999999978	T	T	T
0.1978399999999993	0.1284100000000024	0.3017400000000023	T	T	T
0.2315899999999971	0.1688800000000015	0.5187600000000003	T	T	T
0.3871699999999976	0.1736999999999966	0.5084400000000002	T	T	T
0.4344299999999990	0.1272599999999997	0.2945399999999978	T	T	T
0.3177400000000006	0.1726900000000029	0.1659099999999967	T	T	T
0.5780000000000030	0.5556399999999968	0.3551000000000002	T	T	T
0.6899599999999992	0.5277799999999999	0.2028200000000027	T	T	T
0.7164399999999986	0.5682899999999975	0.9857000000000014	T	T	T
0.8750599999999977	0.5735600000000005	0.9864099999999993	T	T	T
0.8108399999999989	0.5510999999999981	0.3462600000000009	T	T	T
0.5730199999999996	0.3292599999999979	0.3320999999999970	T	T	T
0.6931099999999972	0.3740700000000032	0.1936400000000020	T	T	T
0.7326600000000028	0.3283600000000035	0.9798199999999966	T	T	T
0.8876700000000000	0.3251700000000000	0.9891300000000030	T	T	T
0.9432899999999975	0.3714000000000013	0.1884900000000016	T	T	T
0.9205499999999986	0.4465700000000012	0.8605000000000018	T	T	T
0.8004200000000026	0.4743599999999972	0.7203400000000002	T	T	T
0.7801699999999983	0.4367700000000028	0.4966700000000017	T	T	T
0.6227700000000027	0.4286400000000015	0.4893000000000001	T	T	T
0.5701600000000013	0.4692500000000024	0.7017099999999985	T	T	T
0.6766199999999998	0.4475199999999973	0.8558599999999998	T	T	T
0.9207200000000029	0.6791699999999992	0.8301400000000001	T	T	T
0.7678200000000004	0.6703400000000030	0.4651500000000013	T	T	T
0.6128300000000024	0.6731699999999989	0.4881600000000006	T	T	T
0.5601500000000001	0.6277699999999982	0.6990300000000005	T	T	T
0.6711900000000028	0.6747399999999999	0.8290099999999967	T	T	T
0.5777599999999978	0.9454300000000018	0.3584099999999992	T	T	T
0.6983000000000033	0.9745100000000022	0.2158900000000017	T	T	T
0.7191199999999967	0.9387200000000036	0.9936700000000016	T	T	T
0.8790899999999979	0.9345900000000000	0.9950600000000023	T	T	T
0.9303900000000027	0.9720500000000030	0.2055599999999984	T	T	T
0.8223199999999977	0.9473100000000017	0.3560099999999977	T	T	T
0.5772400000000033	0.1742199999999983	0.3293400000000020	T	T	T
0.6976399999999998	0.1327199999999991	0.1943699999999993	T	T	T
0.7321799999999996	0.1718899999999977	0.9723299999999995	T	T	T
0.8867499999999993	0.1732599999999991	0.9806000000000026	T	T	T
0.9344699999999975	0.1306200000000004	0.1968499999999977	T	T	T
0.8194999999999979	0.1760000000000019	0.3317400000000035	T	T	T
0.9233600000000024	0.0536699999999968	0.8549700000000016	T	T	T
0.8013100000000009	0.0264400000000009	0.7091500000000011	T	T	T
0.7813900000000018	0.0673800000000000	0.4916800000000023	T	T	T
0.6210200000000015	0.0702100000000030	0.4897700000000000	T	T	T
0.5682499999999990	0.0323399999999978	0.6987799999999993	T	T	T
0.6781199999999998	0.0545899999999975	0.8501499999999993	T	T	T
0.9236799999999974	0.8317400000000035	0.8375399999999971	T	T	T
0.8019699999999972	0.8689999999999998	0.6960699999999989	T	T	T
0.7686599999999970	0.8272600000000025	0.4787800000000004	T	T	T
0.6136499999999998	0.8268500000000003	0.4897599999999969	T	T	T
0.5631199999999978	0.8751600000000010	0.6977800000000016	T	T	T

Structure files (CONTCAR) involved in this work:

0.6774699999999996	0.8332300000000004	0.8345300000000009	T	T	T
0.42349000000000010	0.4418199999999999	0.6447399999999988	T	T	T
0.30445000000000028	0.46934000000000025	0.7869699999999966	T	T	T
0.27920000000000030	0.44581000000000016	0.0140999999999991	T	T	T
0.12113999999999969	0.43769000000000035	0.01525000000000018	T	T	T
0.06396000000000016	0.4701499999999967	0.80131000000000009	T	T	T
0.17638999999999978	0.43574000000000027	0.6608999999999980	T	T	T
0.41503000000000016	0.67349000000000010	0.66602000000000032	T	T	T
0.30017000000000014	0.62778000000000013	0.79984000000000032	T	T	T
0.26680999999999995	0.66892000000000000	0.01868999999999994	T	T	T
0.11149000000000034	0.67262000000000020	0.00804000000000012	T	T	T
0.06257999999999970	0.62890000000000016	0.7934199999999976	T	T	T
0.17913000000000007	0.6719399999999993	0.66353000000000015	T	T	T
0.07750999999999966	0.55924000000000026	0.14856000000000034	T	T	T
0.19617000000000022	0.52886000000000017	0.2886299999999977	T	T	T
0.21399000000000026	0.5558199999999971	0.5153899999999965	T	T	T
0.37299000000000015	0.56526000000000021	0.5144099999999980	T	T	T
0.42902999999999974	0.53041000000000034	0.30438000000000019	T	T	T
0.32144000000000026	0.56358000000000017	0.1613699999999980	T	T	T
0.08718999999999997	0.32376000000000000	0.16044000000000012	T	T	T
0.19908000000000021	0.37086000000000004	0.29898000000000002	T	T	T
0.22970999999999972	0.3301799999999986	0.5179299999999998	T	T	T
0.38470999999999983	0.32753000000000030	0.5061299999999989	T	T	T
0.42987999999999972	0.37369000000000034	0.29294000000000015	T	T	T
0.31730999999999991	0.32988000000000028	0.16163000000000024	T	T	T
0.92215000000000020	0.5270999999999972	0.19487000000000017	T	T	T
0.82242999999999971	0.3363999999999976	0.32612000000000031	T	T	T
0.79751000000000026	0.6380699999999990	0.6970499999999973	T	T	T
0.01026000000000024	0.5572099999999978	0.22668000000000018	T	T	T
0.35923999999999998	0.0708399999999969	0.7222399999999993	T	T	T
0.31723999999999982	0.05440000000000011	0.9076599999999999	T	T	T
0.20233999999999995	0.04495000000000000	0.00545000000000033	T	T	T
0.09228999999999984	0.07043000000000018	0.90093000000000025	T	T	T
0.10394999999999975	0.0648199999999974	0.7040099999999967	T	T	T
0.22988000000000014	0.0524199999999979	0.76046000000000019	T	T	T
0.35954999999999987	0.82795000000000013	0.75189000000000031	T	T	T
0.30008999999999973	0.8611999999999966	0.91964000000000011	T	T	T
0.18829000000000021	0.8511999999999986	0.0244199999999992	T	T	T
0.08823999999999990	0.8328599999999966	0.89802000000000025	T	T	T
0.10253000000000016	0.8408999999999978	0.7018899999999988	T	T	T
0.22874000000000019	0.85139000000000021	0.75466000000000012	T	T	T
0.31602999999999978	0.95174000000000009	0.77662000000000012	T	T	T
0.09047999999999994	0.9525099999999966	0.8099199999999982	T	T	T
0.43294999999999982	0.1273399999999967	0.5807599999999979	T	T	T
0.41190999999999989	0.9961899999999986	0.5747599999999977	T	T	T
0.39269000000000018	0.86419000000000007	0.5672199999999989	T	T	T
0.19644000000000026	0.13819000000000016	0.6175899999999999	T	T	T
0.19004999999999994	0.00585000000000024	0.58335000000000029	T	T	T
0.19377999999999967	0.8723999999999990	0.5639099999999999	T	T	T
0.98830999999999985	0.03824000000000018	0.78605000000000030	T	T	T
0.98593000000000033	0.8719699999999975	0.7858799999999988	T	T	T
0.13936999999999995	0.93189000000000028	0.2221299999999999	T	T	T
0.18323999999999978	0.95000000000000028	0.4058899999999994	T	T	T

Structure files (CONTCAR) involved in this work:

0.2970299999999995	0.9481200000000030	0.5085100000000011	T	T	T
0.4073899999999995	0.9318999999999988	0.4021400000000028	T	T	T
0.3964900000000000	0.9352799999999988	0.2053900000000013	T	T	T
0.2696400000000025	0.9468000000000032	0.2577799999999968	T	T	T
0.1379900000000021	0.1726600000000005	0.2545900000000003	T	T	T
0.1952199999999991	0.1364599999999996	0.4218600000000023	T	T	T
0.3100900000000024	0.1482000000000028	0.5162600000000026	T	T	T
0.4125000000000014	0.1684800000000024	0.3939400000000006	T	T	T
0.3948600000000013	0.1584500000000020	0.1986300000000014	T	T	T
0.2699500000000015	0.1545599999999965	0.2610200000000020	T	T	T
0.1867500000000035	0.0502299999999991	0.2709800000000016	T	T	T
0.4149600000000007	0.0484799999999979	0.3077899999999971	T	T	T
0.0643400000000014	0.8707899999999995	0.0873100000000022	T	T	T
0.0854900000000001	0.0000700000000009	0.0677900000000022	T	T	T
0.1108100000000007	0.1307299999999998	0.0712600000000023	T	T	T
0.3056399999999968	0.8617800000000031	0.1150700000000029	T	T	T
0.3121700000000018	0.9944199999999981	0.0824599999999975	T	T	T
0.2979100000000017	0.1276599999999988	0.0693100000000015	T	T	T
0.5129200000000012	0.9574199999999990	0.2877900000000011	T	T	T
0.5144499999999965	0.1349700000000027	0.2775699999999972	T	T	T
0.6349400000000003	0.5662000000000020	0.2708500000000029	T	T	T
0.7030900000000031	0.5737400000000008	0.1050200000000032	T	T	T
0.7957999999999998	0.5620100000000008	0.9609299999999976	T	T	T
0.8894900000000021	0.5783600000000035	0.1041299999999978	T	T	T
0.8858600000000010	0.5352299999999985	0.3124600000000015	T	T	T
0.7589100000000002	0.5223900000000015	0.2662300000000002	T	T	T
0.6373400000000018	0.3352999999999966	0.2606899999999968	T	T	T
0.6936000000000035	0.3374999999999986	0.0846999999999980	T	T	T
0.8104700000000022	0.3514199999999974	0.9917900000000017	T	T	T
0.9177200000000028	0.3200300000000027	0.1011999999999986	T	T	T
0.9054300000000026	0.3534399999999991	0.2920900000000017	T	T	T
0.7646999999999977	0.3718999999999966	0.2465800000000016	T	T	T
0.6671199999999970	0.4517099999999985	0.1766599999999983	T	T	T
0.9310800000000015	0.4471899999999991	0.1525900000000036	T	T	T
0.5679500000000033	0.6256199999999978	0.4159000000000006	T	T	T
0.5989599999999982	0.4972199999999987	0.4341599999999985	T	T	T
0.5861400000000003	0.3639000000000010	0.4409800000000033	T	T	T
0.7996699999999990	0.6308700000000016	0.3694800000000029	T	T	T
0.7968299999999999	0.5150500000000022	0.4582300000000004	T	T	T
0.8318799999999982	0.3872500000000016	0.4389899999999969	T	T	T
0.0231300000000019	0.3607900000000015	0.2075400000000016	T	T	T
0.8543499999999966	0.4376000000000033	0.7911900000000003	T	T	T
0.7971599999999981	0.4338800000000020	0.6145599999999973	T	T	T
0.7032700000000034	0.4193700000000007	0.4730100000000022	T	T	T
0.6058799999999991	0.4317700000000002	0.6074500000000000	T	T	T
0.6028200000000012	0.4434200000000033	0.8059399999999997	T	T	T
0.7271500000000017	0.4750000000000014	0.7694100000000006	T	T	T
0.8592500000000030	0.6825499999999991	0.7544899999999970	T	T	T
0.8122299999999996	0.6473099999999974	0.5636300000000034	T	T	T
0.6906800000000004	0.6480000000000032	0.4841399999999965	T	T	T
0.5851699999999980	0.6689500000000024	0.6012300000000010	T	T	T
0.5929500000000019	0.6612599999999986	0.7983199999999968	T	T	T
0.7177900000000008	0.6506899999999973	0.7374300000000034	T	T	T

Structure files (CONTCAR) involved in this work:

0.8237200000000016	0.5514399999999995	0.6949699999999979	T	T	T
0.5815399999999968	0.5494600000000034	0.6877300000000020	T	T	T
0.9316600000000008	0.3771199999999979	0.9219500000000025	T	T	T
0.9150199999999984	0.5105300000000028	0.9346299999999985	T	T	T
0.9013700000000000	0.6426099999999977	0.9348000000000027	T	T	T
0.6979899999999972	0.3733599999999981	0.8928999999999974	T	T	T
0.6777200000000008	0.5008600000000030	0.9473899999999986	T	T	T
0.6865200000000016	0.6346800000000030	0.9325600000000023	T	T	T
0.4913799999999995	0.4508799999999979	0.7087300000000027	T	T	T
0.4791999999999987	0.6321200000000005	0.7073499999999981	T	T	T
0.6434399999999982	0.9399200000000008	0.2884799999999998	T	T	T
0.6991399999999999	0.9339799999999983	0.1107500000000030	T	T	T
0.7995000000000019	0.9454500000000010	0.9791900000000027	T	T	T
0.8976200000000034	0.9306699999999992	0.1127899999999968	T	T	T
0.8974199999999968	0.9478300000000033	0.3103600000000029	T	T	T
0.7714500000000015	0.9685699999999997	0.2669899999999998	T	T	T
0.6397499999999994	0.1738399999999984	0.2528999999999968	T	T	T
0.6971500000000006	0.1578999999999979	0.0793999999999997	T	T	T
0.8096999999999994	0.1469200000000015	0.9762699999999995	T	T	T
0.9130400000000023	0.1687500000000028	0.0947000000000031	T	T	T
0.8960500000000025	0.1626400000000032	0.2922900000000013	T	T	T
0.7700600000000009	0.1461899999999972	0.2444300000000013	T	T	T
0.6796900000000008	0.0529700000000020	0.1985699999999966	T	T	T
0.9167300000000012	0.0512900000000016	0.1864399999999975	T	T	T
0.5685500000000019	0.8751699999999971	0.4192600000000013	T	T	T
0.5831400000000002	0.0065900000000028	0.4385699999999986	T	T	T
0.5975999999999999	0.1390400000000014	0.4348099999999988	T	T	T
0.8075400000000030	0.8718500000000020	0.3964199999999991	T	T	T
0.8168300000000031	0.9998300000000029	0.4481800000000007	T	T	T
0.8079999999999998	0.1336700000000022	0.4349100000000021	T	T	T
0.0096899999999991	0.9560099999999991	0.2155800000000028	T	T	T
0.0147499999999994	0.1385300000000029	0.2122900000000030	T	T	T
0.8579399999999993	0.0544799999999981	0.7843599999999995	T	T	T
0.8005799999999965	0.0729299999999995	0.6094599999999986	T	T	T
0.7009199999999964	0.0597500000000011	0.4776099999999985	T	T	T
0.6001199999999969	0.0754900000000021	0.6068899999999999	T	T	T
0.6032099999999971	0.0518900000000002	0.8041100000000014	T	T	T
0.7289299999999983	0.0300000000000011	0.7630199999999974	T	T	T
0.8602199999999982	0.8361000000000018	0.7632899999999978	T	T	T
0.8034499999999980	0.8319899999999976	0.5879499999999993	T	T	T
0.6912200000000013	0.8517799999999980	0.4857000000000014	T	T	T
0.5875300000000010	0.8290799999999976	0.6043799999999990	T	T	T
0.6020699999999977	0.8525800000000032	0.7986799999999974	T	T	T
0.7294800000000023	0.8574199999999976	0.7478499999999997	T	T	T
0.8161300000000011	0.9485900000000029	0.6799899999999965	T	T	T
0.5789499999999990	0.9532499999999970	0.6723199999999991	T	T	T
0.9322900000000018	0.1267199999999988	0.9076700000000031	T	T	T
0.9180199999999985	0.9969999999999999	0.9424300000000017	T	T	T
0.9036400000000029	0.8645599999999973	0.9447299999999998	T	T	T
0.6935300000000026	0.1310500000000019	0.8847999999999985	T	T	T
0.6834300000000013	0.0048600000000008	0.9462199999999967	T	T	T
0.6934499999999986	0.8707100000000025	0.9393999999999991	T	T	T
0.4894299999999987	0.0485499999999988	0.7139700000000033	T	T	T

Structure files (CONTCAR) involved in this work:

0.4834299999999985	0.8646499999999975	0.7150400000000019	T	T	T
0.3607099999999974	0.4312499999999986	0.7204800000000020	T	T	T
0.3106099999999969	0.4458199999999977	0.9024599999999978	T	T	T
0.1990100000000012	0.4610199999999978	0.0114400000000003	T	T	T
0.0893999999999977	0.4363099999999989	0.9045800000000028	T	T	T
0.1014399999999966	0.4352200000000011	0.7070799999999977	T	T	T
0.2295599999999993	0.4506399999999999	0.7497800000000012	T	T	T
0.3578499999999991	0.6746499999999997	0.7520799999999994	T	T	T
0.3011699999999990	0.6377799999999993	0.9195399999999978	T	T	T
0.1883300000000006	0.6471999999999980	0.0188599999999965	T	T	T
0.0870699999999971	0.6682100000000020	0.8933800000000005	T	T	T
0.1018800000000013	0.6596400000000031	0.6970699999999965	T	T	T
0.2273199999999989	0.6489800000000017	0.7557299999999998	T	T	T
0.3161399999999972	0.5497599999999991	0.7734900000000025	T	T	T
0.0814799999999991	0.5498499999999993	0.8042400000000001	T	T	T
0.4317100000000025	0.3762200000000036	0.5733299999999986	T	T	T
0.4137899999999988	0.5076699999999974	0.5744100000000003	T	T	T
0.3843900000000033	0.6380699999999990	0.5662799999999990	T	T	T
0.1913100000000014	0.3623300000000000	0.6133000000000024	T	T	T
0.1797100000000000	0.4946100000000015	0.5766500000000008	T	T	T
0.1949200000000033	0.6281400000000019	0.5636399999999995	T	T	T
0.9843400000000031	0.4580500000000001	0.7860099999999974	T	T	T
0.9830200000000033	0.6383200000000002	0.7769600000000025	T	T	T
0.1426099999999977	0.5690200000000019	0.2183700000000002	T	T	T
0.1839500000000029	0.5538600000000002	0.4023499999999984	T	T	T
0.2942099999999996	0.5454999999999970	0.5141300000000015	T	T	T
0.4004899999999978	0.5702300000000022	0.4011199999999988	T	T	T
0.3972399999999965	0.5642700000000005	0.2042599999999979	T	T	T
0.2713299999999990	0.5476900000000029	0.2547399999999982	T	T	T
0.1455600000000032	0.3226099999999974	0.2446800000000025	T	T	T
0.1950199999999995	0.3604300000000009	0.4182599999999965	T	T	T
0.3077600000000018	0.3526499999999970	0.5196100000000001	T	T	T
0.4057200000000023	0.3300399999999968	0.3891500000000008	T	T	T
0.3947199999999995	0.3453500000000034	0.1913499999999999	T	T	T
0.2732900000000029	0.3516300000000001	0.2592199999999991	T	T	T
0.1821600000000032	0.4492300000000000	0.2736000000000018	T	T	T
0.4079499999999996	0.4515600000000006	0.3111299999999986	T	T	T
0.0655100000000033	0.6242400000000004	0.0787100000000009	T	T	T
0.0787699999999987	0.4910599999999974	0.0843300000000013	T	T	T
0.1146600000000007	0.3631000000000029	0.0617299999999972	T	T	T
0.3038000000000025	0.6370000000000005	0.1155100000000004	T	T	T
0.3146800000000027	0.5055600000000027	0.0769599999999997	T	T	T
0.2940699999999978	0.3730699999999985	0.0644899999999993	T	T	T
0.5093200000000024	0.5365200000000030	0.2984599999999986	T	T	T
0.5100199999999973	0.3669700000000020	0.2788600000000017	T	T	T
0.4360199999999992	0.7500799999999970	0.6395899999999983	T	T	T
0.1907599999999974	0.7503999999999991	0.6362299999999976	T	T	T
0.2747499999999974	0.7494999999999976	0.0215499999999977	T	T	T
0.1038599999999974	0.7486699999999971	0.0485699999999980	T	T	T
0.0689700000000002	0.2476600000000033	0.1281999999999996	T	T	T
0.3078100000000035	0.2510100000000008	0.1349400000000003	T	T	T
0.2225699999999975	0.2495400000000032	0.5203399999999974	T	T	T
0.3929499999999990	0.2510300000000001	0.5457899999999967	T	T	T

Structure files (CONTCAR) involved in this work:

0.555349999999971	0.2510400000000033	0.3527600000000035	T	T	T
0.806429999999989	0.253709999999981	0.3533400000000029	T	T	T
0.727899999999982	0.250799999999981	0.9438000000000031	T	T	T
0.891629999999993	0.250289999999997	0.940559999999978	T	T	T
0.9463700000000017	0.754789999999998	0.8571900000000028	T	T	T
0.6828300000000027	0.753599999999987	0.854059999999969	T	T	T
0.7734700000000032	0.749549999999993	0.4424500000000009	T	T	T
0.607709999999973	0.7501600000000010	0.449039999999966	T	T	T
0.9373700000000014	0.5066800000000029	0.5190100000000015	T	T	T
0.933019999999991	0.4084300000000027	0.4373900000000006	T	T	T
0.868319999999971	0.562899999999991	0.558819999999972	T	T	T
0.9686400000000006	0.496139999999969	0.5727600000000024	T	T	T
0.061889999999982	0.4298000000000002	0.476649999999994	T	T	T
0.049559999999996	0.3437500000000000	0.431429999999989	T	T	T
0.9997800000000012	0.569339999999968	0.3813000000000031	T	T	T
0.9777800000000028	0.6420200000000023	0.307259999999994	T	T	T
0.0642500000000013	0.6201300000000032	0.3249300000000019	T	T	T
0.0262400000000014	0.391519999999999	0.451839999999971	T	T	T
0.013399999999972	0.600709999999994	0.317129999999988	T	T	T

Figure 4(a) Route(b-i)-Zn ③

Si Al O Zn H C

1.000000000000000

20.021999999999985 0.000000000000000 0.000000000000000

0.000000000000000 19.899000000000009 0.000000000000000

0.000000000000000 0.000000000000000 13.382999999999991

93 3 193 2 6 2

Selective dynamics

Direct

0.4228840452422206	0.0620393275568075	0.6459899928323448	T	T	T
0.3043477200335022	0.0304209287499697	0.7881772461352745	T	T	T
0.2823375374419343	0.0555445997402927	0.0135867224228079	T	T	T
0.1228850619609535	0.0623051284879766	0.0113958214859529	T	T	T
0.0672642371445372	0.0323260294196130	0.7998597389684271	T	T	T
0.1789350118185235	0.0660134728412405	0.6628698330342734	T	T	T
0.4175637325310126	0.8299094813931330	0.6674297344697339	T	T	T
0.3006268558539308	0.8715165419630192	0.8000159505780849	T	T	T
0.2656273896033974	0.8340413621837512	0.0201012478445648	T	T	T
0.1118188673714126	0.8281867255118278	0.0093403284243888	T	T	T
0.0660319787052170	0.8756278252601618	0.7947798795751509	T	T	T
0.1798572167706167	0.8278589706721996	0.6628802584755418	T	T	T
0.0753669898671789	0.9400773113469623	0.1476517520994717	T	T	T
0.1931802446538968	0.9703567311346162	0.2900712066459813	T	T	T
0.2160839024547959	0.9450791686348795	0.5154433513589449	T	T	T
0.3754963046465749	0.9388034875055951	0.5123338662994901	T	T	T
0.4331003570427178	0.9692157162834603	0.3016979325860734	T	T	T
0.3195510574590034	0.9373811485882676	0.1651530208586399	T	T	T
0.0821309565397651	0.1737221584052673	0.1642846660591344	T	T	T
0.1971956788796278	0.1288023149049891	0.2984661149165341	T	T	T
0.2307624118741882	0.1712138098120655	0.5167925351794133	T	T	T
0.3867016156587709	0.1763271536291076	0.5076154735378556	T	T	T
0.4347140347127053	0.1278382759652527	0.2945925997932899	T	T	T
0.3186721224543720	0.1706818790781105	0.1617793335086205	T	T	T

Structure files (CONTCAR) involved in this work:

0.5745134913333675	0.5578506456933697	0.3528617131233093	T	T	T
0.6900263846306379	0.5282372873484097	0.2011837855918024	T	T	T
0.7117976868385650	0.5695828429798884	0.9838971422346324	T	T	T
0.8692689648583720	0.5747026578893909	0.9836730033809278	T	T	T
0.8112906506303201	0.5515434148970749	0.3449316310922808	T	T	T
0.5736445048899641	0.3309368627589504	0.3325696757423539	T	T	T
0.6953288914878187	0.3741193935477138	0.1947921332962473	T	T	T
0.7286385575009982	0.3283187211151514	0.9816275256648526	T	T	T
0.8836115102417442	0.3278943624262090	0.9935454561870370	T	T	T
0.9414532802657405	0.3756508161478718	0.1879393457125608	T	T	T
0.9182174925110383	0.4475856395518497	0.8592530123979428	T	T	T
0.7958893342661266	0.4738007983539709	0.7220843490844161	T	T	T
0.7742589966855565	0.4377415764953856	0.4958940300658506	T	T	T
0.6165587739662481	0.4322598810251032	0.4894280112562647	T	T	T
0.565573577745169	0.4717449199505137	0.7025250479096738	T	T	T
0.6707333040569330	0.4478741976258360	0.8585276431782763	T	T	T
0.9172056479127061	0.6812116646515459	0.8303566576321237	T	T	T
0.7678819092734773	0.6704203227338541	0.4644429202421086	T	T	T
0.6124515347091257	0.6744610430017685	0.4858437371431325	T	T	T
0.5577301435899459	0.6307281567680219	0.6986638283093368	T	T	T
0.6691781478073896	0.6771207843644376	0.8276031892029224	T	T	T
0.5777741114250058	0.9465603940163120	0.3583400154413910	T	T	T
0.6986325682335741	0.9750376775138758	0.2170436801198146	T	T	T
0.7192146098504328	0.9393337709308176	0.9935055739090093	T	T	T
0.8793423079842774	0.9371164357547993	0.9947089837704612	T	T	T
0.9305765227572853	0.9719736304765395	0.2054344852149814	T	T	T
0.8230085312360366	0.9478550621921847	0.3575006285117072	T	T	T
0.5778793601022900	0.1756565179611973	0.3295802205021674	T	T	T
0.6977542408788752	0.1332446314584462	0.1943284082591414	T	T	T
0.7314174426903578	0.1723100585739256	0.9720865427630748	T	T	T
0.8862299290809148	0.1754411207438166	0.9804708272626355	T	T	T
0.9357571124494606	0.1305445980344358	0.1955740871187309	T	T	T
0.8208089152984701	0.1764102922724052	0.3295922798882778	T	T	T
0.9221913186633915	0.0565336244861848	0.8548206933018092	T	T	T
0.8007543349439722	0.0278830052578146	0.7077388869349563	T	T	T
0.7819763113525428	0.0689069003676447	0.4907689761415399	T	T	T
0.6218145059999736	0.0716844404751861	0.4888284547997439	T	T	T
0.5687210520662032	0.0334907711627968	0.6975945173262186	T	T	T
0.6779899169590468	0.0550755586328564	0.8492248392641447	T	T	T
0.9236343406116979	0.8339191222730367	0.8362967349075793	T	T	T
0.8006080625734689	0.8712303277010819	0.6969648156481955	T	T	T
0.7689493841606785	0.8276913511539580	0.4803774977323742	T	T	T
0.6140898712860692	0.8283471711213003	0.4907481098334838	T	T	T
0.5629226078691379	0.8766339151633215	0.6975186811269336	T	T	T
0.6762767869700295	0.8353530438029330	0.8349148273611278	T	T	T
0.4214086767851726	0.4469460662696184	0.6334840364997404	T	T	T
0.3015161890480646	0.4711842550314843	0.7793101111480837	T	T	T
0.2822166484630915	0.4397755077535234	-0.0000624930702689	T	T	T
0.1229746479641317	0.4376951080666946	0.0038075870896871	T	T	T
0.0629237233349034	0.4717049698972284	0.7933521583866194	T	T	T
0.1750773698525133	0.4418677425369625	0.6489757306547445	T	T	T
0.4169770649654294	0.6760735743884558	0.6488587001070378	T	T	T
0.2959154726030284	0.6302079581665575	0.7822912498747508	T	T	T

Structure files (CONTCAR) involved in this work:

0.2686635519545891	0.6747030568169283	0.0021145594142032	T	T	T
0.1148247859007010	0.6735163566298852	-0.0002652138440268	T	T	T
0.0597104892685734	0.6311281135854486	0.7893080046395761	T	T	T
0.1722149788400448	0.6704045514414376	0.6507975304776892	T	T	T
0.0737818017476947	0.5598957661178645	0.1406710847938437	T	T	T
0.1994527558339466	0.5312643394035417	0.2717833448269664	T	T	T
0.2173929542106623	0.5614227413215417	0.5053104291444807	T	T	T
0.3759224443690224	0.5705995267659485	0.5018316275355392	T	T	T
0.4258543054669243	0.5302820293914905	0.2906587312274593	T	T	T
0.3252686705673558	0.5618904743283990	0.1338313225361053	T	T	T
0.0854579994074822	0.3266429285621928	0.1529594891758430	T	T	T
0.2007231529408544	0.3718876380529043	0.2908570703020325	T	T	T
0.2286618079520247	0.3323661803110459	0.5113521357397800	T	T	T
0.3845047905225509	0.3298955670162583	0.4993144511802468	T	T	T
0.4318467067378178	0.3725501422366078	0.2849328870114405	T	T	T
0.3191412267334084	0.3275275782369129	0.1562130663969758	T	T	T
0.9232799108050785	0.5312467474032312	0.1894294043511657	T	T	T
0.8235350337173457	0.3382750187914607	0.3278212676965404	T	T	T
0.7952926781569044	0.6387774307210532	0.6973910617243335	T	T	T
0.0062888382645260	0.5551468056484971	0.2041704012050694	T	T	T
0.3591471944791690	0.0692602287583389	0.7201751324287686	T	T	T
0.3163344404026678	0.0505595624584294	0.9039347673528041	T	T	T
0.2021331583166005	0.0466808026115619	0.0049081236587474	T	T	T
0.0916304531437085	0.0701851254109173	0.9006697368375102	T	T	T
0.1026596445980908	0.0673183915879671	0.7038305493633048	T	T	T
0.2293669665437552	0.0531529998660512	0.7564409936953035	T	T	T
0.3610095841757153	0.8267958330025237	0.7542682255982660	T	T	T
0.3013253505932719	0.8628960571505735	0.9200522034674880	T	T	T
0.1877002082118472	0.8573182847947700	0.0188139030631707	T	T	T
0.0868731279890766	0.8345468792481883	0.8946944214517379	T	T	T
0.1033620572507110	0.8424049034316227	0.6984303889361881	T	T	T
0.2293721276624779	0.8453089975449071	0.7561850938117826	T	T	T
0.3126455882804101	0.9498244985638670	0.7699797651776457	T	T	T
0.0891240985843875	0.9535758387764169	0.8058174401199927	T	T	T
0.4320153017028231	0.1308841015441183	0.5819025693944085	T	T	T
0.4132952646661970	0.9996850013515147	0.5693165162753208	T	T	T
0.3879981282957276	0.8684567895368909	0.5702434238390981	T	T	T
0.1946877394240898	0.1388756556116054	0.6137591224139481	T	T	T
0.1861298733596508	0.0060486067829100	0.5816987142735399	T	T	T
0.1985614896036421	0.8727996541478009	0.5655665453126874	T	T	T
0.9870715229889606	0.0395511027652120	0.7866692227229829	T	T	T
0.9855706882578107	0.8713847241461877	0.7793971692530589	T	T	T
0.1394738065625581	0.9308883971217996	0.2209325032714551	T	T	T
0.1820219494729514	0.9485845363929073	0.4055512039932165	T	T	T
0.2962481591049823	0.9545950156193901	0.5064086125701489	T	T	T
0.4064977344184779	0.9313829802610770	0.4014081792362496	T	T	T
0.3959357676757432	0.9369182030018633	0.2052536195285995	T	T	T
0.2692022083169043	0.9509924200556642	0.2586144895595071	T	T	T
0.1393467180959044	0.1755284363797907	0.2503449514358494	T	T	T
0.1961724075821387	0.1394665660532952	0.4181179172910146	T	T	T
0.3094834466581376	0.1515403507807791	0.5165037804123530	T	T	T
0.4117071860559196	0.1694661126277435	0.3930921210204426	T	T	T
0.3954505261315773	0.1574632291213188	0.1972928424808349	T	T	T

Structure files (CONTCAR) involved in this work:

0.2700366440385344	0.1500978950161329	0.2547420887171497	T	T	T
0.1815422664430388	0.0505720810734915	0.2727075952301363	T	T	T
0.4161078003428899	0.0490479695447434	0.3096297123402342	T	T	T
0.0643224920733925	0.8710149755187184	0.0844351484833532	T	T	T
0.0857655834034408	0.0013426990986985	0.0691315322758845	T	T	T
0.1099653768880296	0.1326984676325161	0.0684691991702440	T	T	T
0.3034635057268754	0.8645949097595539	0.1167326243229738	T	T	T
0.3120488457776688	0.9957772032697559	0.0819466682118448	T	T	T
0.3010429084722758	0.1277453502025535	0.0622966688190468	T	T	T
0.5126896770810101	0.9572000725255413	0.2878553638567001	T	T	T
0.5147731023843559	0.1366651289582106	0.2784575456612790	T	T	T
0.6341519460949456	0.5629225342715333	0.2717859866065147	T	T	T
0.7001393967303249	0.5753996060847665	0.1038251629314820	T	T	T
0.7904298709497007	0.5615266694897812	0.9550369992742321	T	T	T
0.8797272938821536	0.5778384855854707	0.1021260528942046	T	T	T
0.8873559342409928	0.5308619747009674	0.3154087397483357	T	T	T
0.7601454513582375	0.5250463570409044	0.2626031952350322	T	T	T
0.6415945121799299	0.3387204071435818	0.2693801832738612	T	T	T
0.6911830755259843	0.3342506093537246	0.0885026325410501	T	T	T
0.8061346720464865	0.3531508040795129	0.9917674418147258	T	T	T
0.9110220128711135	0.3213005825829359	0.1083281873611808	T	T	T
0.9095234591068057	0.3627334432373424	0.3014950087393458	T	T	T
0.7689898490338000	0.3718752116258717	0.2415591815530536	T	T	T
0.6702682084999245	0.4515239311889868	0.1739467397184396	T	T	T
0.9226368537083944	0.4487618523188114	0.1504160633453701	T	T	T
0.5677857763451422	0.6294084777814287	0.4101132306748560	T	T	T
0.5896550387004545	0.5002322500667926	0.4360816313044450	T	T	T
0.5807836007308212	0.3667397375310105	0.4419212290332900	T	T	T
0.8011773107966145	0.6312721152562857	0.3689940219086295	T	T	T
0.7950851746697606	0.5156088247783048	0.4567279874605491	T	T	T
0.8252244635691911	0.3878767346572899	0.4392988270710064	T	T	T
0.0217361380229072	0.3647551863750502	0.2018515107052885	T	T	T
0.8531763510192077	0.4364093810470775	0.7868804350334541	T	T	T
0.7883509074673373	0.4355746272628978	0.6147467394151938	T	T	T
0.6969173424496383	0.4254658409900024	0.4692317674472108	T	T	T
0.6019337926674195	0.4348774380490600	0.6081650461600051	T	T	T
0.5976523488147426	0.4436059961990191	0.8059431311285211	T	T	T
0.7239654741129489	0.4737453750609373	0.7746822957367622	T	T	T
0.8567824536695087	0.6847436706075378	0.7523898253406534	T	T	T
0.8114454603658005	0.6456800211751623	0.5633179844094542	T	T	T
0.6903597758960647	0.6486027468576572	0.4820695477683823	T	T	T
0.5835132638325186	0.6682716878518372	0.5979688098945674	T	T	T
0.5907492712691634	0.6665577668003179	0.7958685489605423	T	T	T
0.7152825235966065	0.6514720900190974	0.7362721970897369	T	T	T
0.8196391862503138	0.5512405315320452	0.6979190146199226	T	T	T
0.5783723932614376	0.5519371252539198	0.6928607475180040	T	T	T
0.9279717782522764	0.3805654914605081	0.9275857111641829	T	T	T
0.9113138624870395	0.5139412963229469	0.9281426149526463	T	T	T
0.8949130527491594	0.6448093395901007	0.9338815600634855	T	T	T
0.6908833758655265	0.3739643697297086	0.8984026247320306	T	T	T
0.6706753159249342	0.5028973970180702	0.9478065965288850	T	T	T
0.6823606411495543	0.6364983963823128	0.9313865215805870	T	T	T
0.4861871458854116	0.4550625017536505	0.7050986762664063	T	T	T

Structure files (CONTCAR) involved in this work:

0.4767943403512047	0.6370149968573050	0.7072073657943602	T	T	T
0.6431336225204578	0.9398529428998467	0.2879144181309014	T	T	T
0.7004905322695878	0.9356578287186514	0.1110661968945376	T	T	T
0.7995045253319045	0.9443035153102824	0.9764519528951252	T	T	T
0.8960973690847484	0.9318376069850033	0.1128928927677267	T	T	T
0.8977028050862385	0.9483421372068297	0.3105693528263855	T	T	T
0.7712788606796098	0.9685754464332621	0.2693582960519662	T	T	T
0.6403821322284509	0.1750835301998934	0.2529617074263988	T	T	T
0.6962383784264390	0.1571871817860317	0.0787509592694777	T	T	T
0.8092992078951337	0.1486870854888262	0.9770560997356755	T	T	T
0.9141665954900137	0.1685638966900893	0.0933974294362038	T	T	T
0.8972336997978890	0.1622671695045637	0.2910958297914242	T	T	T
0.7706695822614091	0.1472394192891992	0.2427965477022563	T	T	T
0.6798414249462336	0.0536126679190329	0.2009939656821948	T	T	T
0.9180661562712704	0.0513641251824555	0.1861016751558453	T	T	T
0.5687051725259967	0.8773557158686979	0.4218354920150623	T	T	T
0.5833406904223726	0.0089653791297479	0.4363199005413371	T	T	T
0.5985638998365397	0.1410729579634331	0.4353170078209029	T	T	T
0.8088533711222679	0.8726334570265430	0.3995370903813687	T	T	T
0.8181172255604127	0.0013880550560678	0.4485407107604298	T	T	T
0.8083604016061315	0.1352268131493934	0.4334857087484534	T	T	T
0.0096163816361174	0.9548711672391902	0.2144263864741434	T	T	T
0.0158271151817039	0.1393569853952680	0.2117131780736058	T	T	T
0.8568910997874146	0.0554849307280871	0.7839979767770257	T	T	T
0.8004240055188804	0.0752238876783146	0.6087902938352361	T	T	T
0.7016193496636284	0.0608388818534714	0.4757263838108802	T	T	T
0.6015275278965798	0.0764200454795569	0.6062030112839351	T	T	T
0.6028806336711229	0.0526830157870978	0.8037961852134586	T	T	T
0.7282149266887648	0.0306974370269898	0.7612156706788232	T	T	T
0.858072222274765	0.8393198421064717	0.7664642078284795	T	T	T
0.8021220310296022	0.8317664122879207	0.5907282354094020	T	T	T
0.6917041226768277	0.8529458348409076	0.4855086836764048	T	T	T
0.5884281478801064	0.8296687540681080	0.6056539153175586	T	T	T
0.6004989220253976	0.8538564465563088	0.7995647458782945	T	T	T
0.7278702523269738	0.8619333284847620	0.7491187472067807	T	T	T
0.8156079548308408	0.9503091188314108	0.6769663850147150	T	T	T
0.5797975120309765	0.9544124533149629	0.6713734685251506	T	T	T
0.9309049153389864	0.1309204383211462	0.9035750177454918	T	T	T
0.9159436450575450	1.0024212172706468	0.9457515662595438	T	T	T
0.9081697915889089	0.8693392046587535	0.9431808233038819	T	T	T
0.6938101645353858	0.1314621190288922	0.8836970249303944	T	T	T
0.6840153878778122	0.0055912418948887	0.9454480254052252	T	T	T
0.6913105884326627	0.8715444800393015	0.9411029390550635	T	T	T
0.4899214768275109	0.0502930663080216	0.7111821985491824	T	T	T
0.4828734835534835	0.8678213506940365	0.7122598337104636	T	T	T
0.3546424582764586	0.4393115768542129	0.7012395953737073	T	T	T
0.3092995244151678	0.4331234114099065	0.8859043930475389	T	T	T
0.2024100791840349	0.4549309229520621	0.0015547371914066	T	T	T
0.0938948631499820	0.4348443491027512	0.8906289301896133	T	T	T
0.0983963330565619	0.4433215528623525	0.6913237568842631	T	T	T
0.2255319701413205	0.4593738517629948	0.7400635977201475	T	T	T
0.3486830663040969	0.6696230664737103	0.7125939762546790	T	T	T
0.2993197351752312	0.6640909341639967	0.8915517641216796	T	T	T

Structure files (CONTCAR) involved in this work:

0.1920603229285112	0.6471255398686088	0.0055083772388864	T	T	T
0.0891130122440393	0.6718155390895408	0.8846810101607109	T	T	T
0.0953963802149882	0.6597406029150192	0.6880091126465504	T	T	T
0.2211815014523159	0.6385380390846684	0.7360036575000659	T	T	T
0.3153557088777225	0.5512122770641767	0.7907129794971752	T	T	T
0.0766907054998432	0.5516894002926264	0.8015427180843646	T	T	T
0.4306509025997972	0.3799674550235890	0.5654928159323931	T	T	T
0.4169058086698402	0.5114761459467118	0.5589864353428008	T	T	T
0.4040937413592043	0.6429729662746745	0.5390443790391672	T	T	T
0.1903409507296102	0.3671801474971880	0.6052439208311430	T	T	T
0.1830909666909451	0.4968713463896614	0.5596857905316202	T	T	T
0.1833167124354469	0.6306153215546434	0.5455199658638360	T	T	T
0.9828743778802782	0.4557899819671235	0.7840414086987055	T	T	T
0.9796377038621730	0.6401888837211902	0.7784905300350745	T	T	T
0.1376409202970175	0.5682301880633543	0.2165970603380418	T	T	T
0.2029301983159257	0.5564622333452576	0.3868373755160482	T	T	T
0.2970014104502123	0.5620295981997967	0.5289462919326480	T	T	T
0.3871906561593662	0.5669229853594133	0.3824785813750896	T	T	T
0.3986094339350530	0.5612254462683661	0.1859479622556854	T	T	T
0.2697068987186882	0.5495622155640439	0.2200315917078177	T	T	T
0.1450072348811560	0.3268413464156047	0.2351858281766248	T	T	T
0.1934905475355879	0.3598065279952629	0.4099250316528320	T	T	T
0.3069467363250434	0.3542155529452233	0.5098411234444798	T	T	T
0.4072955767546427	0.3311491862646926	0.3831093114099565	T	T	T
0.3969341854588790	0.3411938713530688	0.1853369850618898	T	T	T
0.2746888296290376	0.3501206911040158	0.2531517771173407	T	T	T
0.1868129523996408	0.4505604963524645	0.2661679459012748	T	T	T
0.4093418252660799	0.4504909421267409	0.2973098208024304	T	T	T
0.0691611959254728	0.6257519086032026	0.0688669998056790	T	T	T
0.0847042191761744	0.4940989307019344	0.0693112727457497	T	T	T
0.1105186536069053	0.3635795586878477	0.0514112870722297	T	T	T
0.3140808935229160	0.6346144324285999	0.0825790482429119	T	T	T
0.3213453917923654	0.5023482862254243	0.0512144038335308	T	T	T
0.2976690892222872	0.3699550012169501	0.0579488377824675	T	T	T
0.5055658942495997	0.5422660105897761	0.2949322645724640	T	T	T
0.5122407400795723	0.3663099255651537	0.2719464318332082	T	T	T
0.4368749899242876	0.7541670060913107	0.6334717367701039	T	T	T
0.1878309151676404	0.7493245112918561	0.6318194354551666	T	T	T
0.2713494843484941	0.7535083117862460	0.0288262607616088	T	T	T
0.1095731826353847	0.7497945083440096	0.0416497139994516	T	T	T
0.0661899183049586	0.2496146718431754	0.1268551853586494	T	T	T
0.3076835821854395	0.2488313836590652	0.1317613845887830	T	T	T
0.2207357390516049	0.2518699616116490	0.5199885202171248	T	T	T
0.3930744860973426	0.2542218341842200	0.5421208372214227	T	T	T
0.5566717261520843	0.2526286919609995	0.3528513929375076	T	T	T
0.8104397771561158	0.2547579524919454	0.3495932080639805	T	T	T
0.7257817833628905	0.2511728401436021	0.9433929074623572	T	T	T
0.8900524753610940	0.2533989920666131	0.9443672001980666	T	T	T
0.9435604493217610	0.7564822565977488	0.8577710587643337	T	T	T
0.6834895502900503	0.7555957057060350	0.8520255320016423	T	T	T
0.7739270096593791	0.7498445661738238	0.4440047679166775	T	T	T
0.6083523696254034	0.7519507788089752	0.4490810153846112	T	T	T
0.9249119970437627	0.4884138336730272	0.5377267311261396	T	T	T

Structure files (CONTCAR) involved in this work:

0.9274558723798361	0.4348260774188177	0.4087875686344130	T	T	T
0.8624253476271763	0.5587100949406791	0.5615067390320158	T	T	T
0.9469062372169248	0.4708458004656147	0.5975424363187385	T	T	T
0.0478021106266521	0.4450714455793787	0.4890329727202830	T	T	T
0.0729853434574047	0.4500751733464292	0.3567716387947077	T	T	T
0.0120346336428813	0.5662473814681186	0.4833508961058294	T	T	T
1.0139288885127278	0.5611807046777497	0.3455928797895552	T	T	T
0.0860028911285969	0.5725925598285859	0.4081866775451681	T	T	T
0.0459373768107830	0.4731724921695402	0.4188916050123140	T	T	T
0.0375761386182856	0.5461559874235197	0.4177260291607225	T	T	T

Figure 4(a) Route(b-i)-Zn ④

Si Al O Zn H C

1.0000000000000000

20.0219999999999985 0.0000000000000000 0.0000000000000000

0.0000000000000000 19.8990000000000009 0.0000000000000000

0.0000000000000000 0.0000000000000000 13.3829999999999991

93 3 193 2 6 2

Selective dynamics

Direct

0.4236800437183868	0.0609667688449994	0.6474292138183307	T	T	T
0.3057192263581507	0.0327731264830428	0.7904034484631641	T	T	T
0.2833749239418963	0.0549649093368184	0.0163976329220478	T	T	T
0.1243366414365826	0.0616828115763838	0.0122764029001488	T	T	T
0.0686562585427950	0.0323750504638049	0.7999458292786825	T	T	T
0.1810930371410572	0.0674362663228960	0.6648075776787874	T	T	T
0.4187862300980352	0.8281318360289590	0.6688528932292097	T	T	T
0.2999871865808323	0.8742224575376168	0.7971397255376746	T	T	T
0.2674381678941331	0.8316547044299247	0.0165958258497592	T	T	T
0.1116179785759485	0.8274182057360864	0.0111711041348216	T	T	T
0.0664417298237890	0.8756244118363321	0.7960154989894751	T	T	T
0.1784578034583756	0.8290675011530289	0.6607766368977077	T	T	T
0.0759688335986975	0.9404741422383770	0.1495048815076964	T	T	T
0.1961524431563915	0.9699711650250110	0.2889270443027546	T	T	T
0.2167186076271190	0.9456747350792625	0.5160271184232713	T	T	T
0.3770489763753057	0.9364378216931447	0.5136924657454877	T	T	T
0.4338193865143336	0.9682764012079685	0.3012134485698837	T	T	T
0.3212665285887449	0.9339405561500875	0.1641689277245856	T	T	T
0.0833663990857149	0.1715924586947031	0.1660098881084430	T	T	T
0.2001740911462280	0.1281452592385121	0.2983455770416392	T	T	T
0.2324518524037983	0.1698373617164925	0.5153803717959253	T	T	T
0.3888380738582107	0.1746866666592796	0.5070065918359880	T	T	T
0.4355901326744319	0.1267015843700998	0.2928979792853001	T	T	T
0.3199834766381313	0.1728806031485249	0.1622937508311650	T	T	T
0.5776298510643180	0.5557529927259606	0.3548982829493471	T	T	T
0.6937253392810040	0.5252293590774761	0.2053308537139562	T	T	T
0.7152275038980306	0.5674240233516110	0.9882032329326199	T	T	T
0.8741905744113099	0.5729055170627196	0.9841665321437080	T	T	T
0.8131745185471160	0.5515904647792771	0.3458958158018833	T	T	T
0.5748244203367635	0.3281859085985518	0.3328893530200684	T	T	T
0.6948883876701528	0.3716759731351025	0.1931941388875106	T	T	T
0.7309204053597512	0.3269989695991423	0.9803280861239543	T	T	T
0.8859169276177155	0.3257917989109379	0.9935073672225097	T	T	T

Structure files (CONTCAR) involved in this work:

0.9426616072821663	0.3724278265191643	0.1939034220132283	T	T	T
0.9189573693850112	0.4446275411806258	0.8584715084563878	T	T	T
0.7986232003092119	0.4722636685214576	0.7202352940581394	T	T	T
0.7755732419868789	0.4358533111663290	0.4948458225681894	T	T	T
0.6171815524905836	0.4299895346665193	0.4904251546299163	T	T	T
0.5683811859245048	0.4690383738378875	0.7042678185750344	T	T	T
0.6755892066609790	0.4470453551163463	0.8583161763851992	T	T	T
0.9199562572188993	0.6788560603300526	0.8277662398122601	T	T	T
0.7672840532873627	0.6684937958446934	0.4676301562334014	T	T	T
0.6124310701596455	0.6730901130643299	0.4894785778756088	T	T	T
0.5587013049252270	0.6276974765101333	0.7002506922192908	T	T	T
0.6720108517917048	0.6728921714112056	0.8288461578767745	T	T	T
0.5786669472547662	0.9445236216017372	0.3589369478039465	T	T	T
0.6985389522645662	0.9723086362474379	0.2152265050769842	T	T	T
0.7204260809011347	0.9365259746397755	0.9934889008370283	T	T	T
0.8803230892879773	0.9340501224091536	0.9948426148881225	T	T	T
0.9309129207923637	0.9706101351820690	0.2054251297666265	T	T	T
0.8222737570930522	0.9460348331146772	0.3564186442126422	T	T	T
0.5782473746890795	0.1728880779946930	0.3303228602764340	T	T	T
0.6989276964039746	0.1296740273449526	0.1957628081239943	T	T	T
0.7325005941357561	0.1709851847259478	0.9742543480315723	T	T	T
0.8870330132197591	0.1733947319953959	0.9825514163029827	T	T	T
0.9362507535303407	0.1287148317165778	0.1963773110400489	T	T	T
0.8214150097083954	0.1720507873346627	0.3309687641712430	T	T	T
0.9237502066084088	0.0542383913486821	0.8559835393496898	T	T	T
0.8016692628383454	0.0262660169962859	0.7107249676962369	T	T	T
0.7824562871416900	0.0663868906340301	0.4925032156080327	T	T	T
0.6220152696538227	0.0699034363177828	0.4904442052936900	T	T	T
0.5692269061325465	0.0316675825962673	0.6995374048782553	T	T	T
0.6782420816296283	0.0531034568122919	0.8518008722977028	T	T	T
0.9241689713040347	0.8312625239348211	0.8369524679606745	T	T	T
0.8023108553531156	0.8688623364126895	0.6965424032589446	T	T	T
0.7695953842990196	0.8262822225795853	0.4794872648787698	T	T	T
0.6147190120939917	0.8266201735197233	0.4913747537668934	T	T	T
0.5639778377592646	0.8744968699430374	0.6992666084727289	T	T	T
0.6784080644865019	0.8316676988700920	0.8340339915697353	T	T	T
0.4235480907860631	0.4427030943247490	0.6441429001335417	T	T	T
0.3032227487271267	0.4694800862658430	0.7849796630053458	T	T	T
0.2803545817055875	0.4459778909320418	0.0117895376646162	T	T	T
0.1213940392685423	0.4373871685348256	0.0128703099909812	T	T	T
0.0629467535111535	0.4690054188597246	0.7984635323136527	T	T	T
0.1769734161318028	0.4343881059763847	0.6609052065415975	T	T	T
0.4154223293107903	0.6742651840629797	0.6635058952132576	T	T	T
0.2977055161199194	0.6283336105327885	0.7944386940430921	T	T	T
0.2679657793538984	0.6702922874467009	0.0127096516361938	T	T	T
0.1122631273665424	0.6732445841902028	0.0025722745477397	T	T	T
0.0616438818057627	0.6282435244544274	0.7886670576861474	T	T	T
0.1776566101764890	0.6722362995094726	0.6594608491990906	T	T	T
0.0794172037589011	0.5609040548548164	0.1465343592953925	T	T	T
0.1975947670783955	0.5304439126810385	0.2870148434053590	T	T	T
0.2176263407085606	0.5552311796580690	0.5158969095851930	T	T	T
0.3768812298830337	0.5658390604114982	0.5113983012341830	T	T	T
0.4317499458508464	0.5322478057332988	0.2981191385820570	T	T	T

Structure files (CONTCAR) involved in this work:

0.3213673668897132	0.5659922985252747	0.1583653354504530	T	T	T
0.0865240763895591	0.3244763470040392	0.1607429680450273	T	T	T
0.2012284116985023	0.3725566305832989	0.2945768780249029	T	T	T
0.2303879172560961	0.3309784851135802	0.5132644051748945	T	T	T
0.3864621532679665	0.3285909831385395	0.5035420965914513	T	T	T
0.4331087728023997	0.3742732063694464	0.2893699095340882	T	T	T
0.3199464650993534	0.3299112273678919	0.1582830506813138	T	T	T
0.9227891516558646	0.5302896009109013	0.1962860533724845	T	T	T
0.8214015986245220	0.3334787796904099	0.3268132199420642	T	T	T
0.7982814289712860	0.6353262326826951	0.6957823766406283	T	T	T
0.0110687239222843	0.5582994770417828	0.2211639550225374	T	T	T
0.3606161158337376	0.0714759647510159	0.7222705022602384	T	T	T
0.3181723605461561	0.0509524564425595	0.9069503191587583	T	T	T
0.2033761900502185	0.0449062671065813	0.0056039063751637	T	T	T
0.0929655513082377	0.0693344272482498	0.9016001160338943	T	T	T
0.1045325970488844	0.0677194455530099	0.7045560940628730	T	T	T
0.2308293588439758	0.0567079851931653	0.7598821102332844	T	T	T
0.3601117401638244	0.8288941777190322	0.7526023319610583	T	T	T
0.2987692947912338	0.8655256903956904	0.9171228348709001	T	T	T
0.1888182321646143	0.8514580853528054	0.0240963078371016	T	T	T
0.0892174875891971	0.8351505998016138	0.8957267039485751	T	T	T
0.1021285438677469	0.8411529909014951	0.6992071318241618	T	T	T
0.2287976298661788	0.8495344837076164	0.7515240187283022	T	T	T
0.3133704642490004	0.9524703533301724	0.7690646424717744	T	T	T
0.0902589001845014	0.9534342269824911	0.8048199839335557	T	T	T
0.4339421559578641	0.1282188499151360	0.5801368654448597	T	T	T
0.4125838225083672	0.9974153239243166	0.5734561951055287	T	T	T
0.3928725935779135	0.8654626223880041	0.5682292877202606	T	T	T
0.1962752822495645	0.1399577002044401	0.6140668581721546	T	T	T
0.1904135661148468	0.0067564488130934	0.5852824208052273	T	T	T
0.1934766339756069	0.8736207970761261	0.5617312058547568	T	T	T
0.9885903666848654	0.0399838207919689	0.7861733519824664	T	T	T
0.9858197568499014	0.8717394966176618	0.7839024942151489	T	T	T
0.1398133990342544	0.9315878191040206	0.2231723534670025	T	T	T
0.1838656406959053	0.9535217508027205	0.4058953158925749	T	T	T
0.2972954321872096	0.9493569534316053	0.5088479591986125	T	T	T
0.4072288488021490	0.9320633186087536	0.4020670100485888	T	T	T
0.3973922888014684	0.9339481488699559	0.2054607093828086	T	T	T
0.2702285688114893	0.9439285711624821	0.2579688542350737	T	T	T
0.1392726795510673	0.1723104465006834	0.2538679179039082	T	T	T
0.1986169334533330	0.1344279980288506	0.4187217073861720	T	T	T
0.3113255007597590	0.1509241289706136	0.5168158887128769	T	T	T
0.4130703703424348	0.1679130559571144	0.3921031922562311	T	T	T
0.3967442163703748	0.1581584052837424	0.1964577083323960	T	T	T
0.2714083944903121	0.1560339605620711	0.2570098818424119	T	T	T
0.1902596570132245	0.0501000421928866	0.2656042495192267	T	T	T
0.4155524715949424	0.0479926625525632	0.3055843672348336	T	T	T
0.0652733960016522	0.8715325018540085	0.0857800513836630	T	T	T
0.0863762537918356	0.0015570197271345	0.0708799107996958	T	T	T
0.1125308212993815	0.1322301600069371	0.0694257458361834	T	T	T
0.3069979962456753	0.8614621228888275	0.1123660375481360	T	T	T
0.3128344021495555	0.9947504708385166	0.0846411500843773	T	T	T
0.3002567412163216	0.1275581233979061	0.0658629762838049	T	T	T

Structure files (CONTCAR) involved in this work:

0.5135378688245018	0.9567403347127394	0.2890079666565850	T	T	T
0.5157851081133669	0.1339558566835217	0.2769825304255033	T	T	T
0.6415781614483923	0.5606251279075281	0.2815785818504437	T	T	T
0.7017803044721069	0.5729965969660186	0.1078429003221132	T	T	T
0.7944978562377440	0.5612389536437912	0.9628284602920988	T	T	T
0.8904561121683151	0.5776457271330676	0.1011414807683726	T	T	T
0.8904007849671973	0.5436310569735312	0.3157676641491745	T	T	T
0.7658716918020237	0.5196258667049726	0.2613644410380745	T	T	T
0.6411879076755252	0.3344157494960252	0.2658242262144225	T	T	T
0.6904981232526581	0.3349709799963422	0.0844007714243638	T	T	T
0.8084108528768246	0.3508884559396767	0.9941841472223389	T	T	T
0.9150210665476060	0.3219901073288265	0.1067168728662618	T	T	T
0.9066921246936894	0.3537641297698135	0.3003657430847059	T	T	T
0.7684968564237388	0.3680037691246776	0.2391219239000703	T	T	T
0.6700378413406882	0.4497360311889853	0.1777553347372134	T	T	T
0.9300059775014103	0.4484687828256324	0.1610642785405316	T	T	T
0.5693806799893326	0.6267728177934697	0.4133041394826615	T	T	T
0.5855415977689404	0.4962523257487206	0.4375973093458241	T	T	T
0.5849869689283148	0.3625368867775045	0.4426985099202707	T	T	T
0.7943511759100413	0.6297571851656009	0.3684239306790628	T	T	T
0.8008670555559523	0.5121569539348930	0.4557524367452870	T	T	T
0.8210833963719950	0.3800457097803232	0.4410273837264877	T	T	T
0.0227660334007676	0.3608647796453436	0.2108304886040691	T	T	T
0.8536429310316094	0.4333621275876270	0.7875253090644524	T	T	T
0.7903106974812745	0.4335458919982153	0.6137718800152373	T	T	T
0.6973254886788665	0.4288660401006119	0.4690734533660453	T	T	T
0.6028686456829623	0.4309529941246272	0.6094537369362163	T	T	T
0.6018845346355493	0.4436369207398531	0.8080047613642231	T	T	T
0.7267600839211060	0.4751863850190189	0.7734353979562866	T	T	T
0.8586181761529998	0.6826414603247618	0.7519809830989346	T	T	T
0.8135523674573246	0.6428625355595944	0.5624841636390883	T	T	T
0.6901757543388212	0.6478998787457990	0.4911969809272359	T	T	T
0.5814493473473638	0.6681409599635550	0.6005585575262847	T	T	T
0.5935638732695466	0.6611128831345848	0.7977990108614652	T	T	T
0.7186778594259524	0.6472301896112493	0.7383599064369080	T	T	T
0.8247089508104486	0.5487376447344195	0.6965822514600988	T	T	T
0.5794415725291946	0.5491791689894375	0.6891734465641596	T	T	T
0.9298491684542495	0.3774125909652061	0.9254128547006630	T	T	T
0.9129631531511688	0.5101877757001175	0.9292978783886318	T	T	T
0.8999833433917864	0.6419548366589073	0.9319111223445242	T	T	T
0.6965610447559916	0.3723045700155431	0.8935101577499613	T	T	T
0.6766449806743295	0.4995520130448365	0.9509196497875079	T	T	T
0.6853271569633080	0.6334571134287775	0.9337978177200046	T	T	T
0.4896127153329145	0.4504869147348166	0.7127045767113612	T	T	T
0.4778507889843442	0.6334151155506103	0.7117681030585140	T	T	T
0.6435790240837769	0.9376277450384447	0.2875950411482369	T	T	T
0.7008204487149609	0.9311595311923804	0.1106785915243982	T	T	T
0.8006945272148184	0.9445525735623559	0.9783175926232908	T	T	T
0.8981230293370108	0.9291521665574961	0.1127927257683296	T	T	T
0.8973574327700966	0.9478623118956827	0.3105220773448253	T	T	T
0.7712965008906228	0.9677145613888851	0.2678226060318666	T	T	T
0.6423900192786821	0.1709987868792147	0.2569985625046284	T	T	T
0.6985100733705473	0.1580187747447813	0.0823627861935267	T	T	T

Structure files (CONTCAR) involved in this work:

0.8101965873645718	0.1466136324830089	0.9777538794803997	T	T	T
0.9137367739670801	0.1685525719332674	0.0963289705961919	T	T	T
0.8983589585963005	0.1591019271441417	0.2932410450159975	T	T	T
0.7720062564437343	0.1390528798498410	0.2460001244051636	T	T	T
0.6789485948880059	0.0503336485924760	0.1955618023081372	T	T	T
0.9183842018026913	0.0496703807166599	0.1836043258402419	T	T	T
0.5692647102750655	0.8749721139756921	0.4213653815738931	T	T	T
0.5853428437254169	0.0059456243545127	0.4383573213520708	T	T	T
0.5962250040811105	0.1384982026292730	0.4372920971224710	T	T	T
0.8081460822794483	0.8700057534730895	0.3954100533952167	T	T	T
0.8161361099356031	0.9975961229119398	0.4498035421554839	T	T	T
0.8115012626873283	0.1318418242841614	0.4363028911902744	T	T	T
0.0100752838679096	0.9541401695036761	0.2163192437869801	T	T	T
0.0165854856921534	0.1367164170575222	0.2107487550987466	T	T	T
0.8580080093338081	0.0549277537039310	0.7859941108570921	T	T	T
0.8009924897583469	0.0720725266326167	0.6104429665400315	T	T	T
0.7019730007854571	0.0614711732398669	0.4767012029728814	T	T	T
0.6021194951507359	0.0742196609283321	0.6079550480573104	T	T	T
0.6033429728007593	0.0511082065303952	0.8055854666279216	T	T	T
0.7291196235962890	0.0297729221998498	0.7640187781788912	T	T	T
0.8597317173460103	0.8355381629617153	0.7648019086871478	T	T	T
0.8051121652419732	0.8328367255175931	0.5878855914568762	T	T	T
0.6923017020417125	0.8514649240348797	0.4866128802494153	T	T	T
0.5887515720515434	0.8284328222976444	0.6061086305873867	T	T	T
0.6026021244737134	0.8514580953776647	0.8003231329904745	T	T	T
0.7292568855427392	0.8569938861147308	0.7464267122844680	T	T	T
0.8169888877145887	0.9484751251103629	0.6824029941019482	T	T	T
0.5799994972883243	0.9525285261433917	0.6738752657494312	T	T	T
0.9325364137244300	0.1273018988551946	0.9089210903298918	T	T	T
0.9190979029663592	0.9970012900267089	0.9429238168104043	T	T	T
0.9057147958866461	0.8643362405976801	0.9445615251973560	T	T	T
0.6935128873497388	0.1291059078551715	0.8883621954005826	T	T	T
0.6835905263408127	0.0021771394026545	0.9464511618362168	T	T	T
0.6956174666004407	0.8682397232298967	0.9392101517938020	T	T	T
0.4904620246684844	0.0486792720573503	0.7128917115409769	T	T	T
0.4841156916797911	0.8648203300578626	0.7157565812255174	T	T	T
0.3589337943260766	0.4324404135243574	0.7163500830530111	T	T	T
0.3132170662605618	0.4490174414720960	0.9011544988970011	T	T	T
0.1998274588096732	0.4576878932598556	0.0065006544855327	T	T	T
0.0884982539516153	0.4369494253696140	0.9029043930807154	T	T	T
0.1010654540926952	0.4339852227259415	0.7043646151128279	T	T	T
0.2284776570338643	0.4458669953750123	0.7532111931247574	T	T	T
0.3542805503168942	0.6746492672677421	0.7431087899955126	T	T	T
0.3021887432599122	0.6381032833872828	0.9141178111652577	T	T	T
0.1894375430440044	0.6487827771564557	0.0133628016251749	T	T	T
0.0874810508071571	0.6674024385427495	0.8882138497687361	T	T	T
0.1002795871128853	0.6586313284112286	0.6912809182776867	T	T	T
0.2242467515716827	0.6510525947798529	0.7545853232876378	T	T	T
0.3109857426313178	0.5499886777330695	0.7669697386284761	T	T	T
0.0795041919939188	0.5488557414274085	0.7989048228187587	T	T	T
0.4322620471967032	0.3776254480383552	0.5719193722396182	T	T	T
0.4169648905032021	0.5090238474588070	0.5739912339206266	T	T	T
0.3899736139027045	0.6392388494624428	0.5603096889420839	T	T	T

Structure files (CONTCAR) involved in this work:

0.1916013143308032	0.3620952070681300	0.6092427093379180	T	T	T
0.1841087215561109	0.4952321476785431	0.5805084703987732	T	T	T
0.1969736488373717	0.6280283957529410	0.5612375676927693	T	T	T
0.9834036941598608	0.4546204695624602	0.7838669339104178	T	T	T
0.9820301785064171	0.6379023113453451	0.7742491132104615	T	T	T
0.1415061944089103	0.5715805473181410	0.2222768827266054	T	T	T
0.1872728435696090	0.5499280764776172	0.4033034170153605	T	T	T
0.2979005567009202	0.5466512948237036	0.5133155867798223	T	T	T
0.4034681487016892	0.5690816901448025	0.3976087003159552	T	T	T
0.3973030926261938	0.5661350939291673	0.2001109953253362	T	T	T
0.2715579239398763	0.5532583805535402	0.2530869846120323	T	T	T
0.1464158573277664	0.3246577563671038	0.2425325646286655	T	T	T
0.1969616172732248	0.3643132199444133	0.4144372555889357	T	T	T
0.3088355798907189	0.3517779256462819	0.5166611668805273	T	T	T
0.4077197690557722	0.3325367244550785	0.3867657465334614	T	T	T
0.3971636107436876	0.3451952651294358	0.1888962102012171	T	T	T
0.2749481830564688	0.3511726374764249	0.2552701705053451	T	T	T
0.1857108775051987	0.4508929406936254	0.2660767192702155	T	T	T
0.4130180765961015	0.4528493685066657	0.3040354673202494	T	T	T
0.0676347483270145	0.6247560424455687	0.0747333585186999	T	T	T
0.0825225702728468	0.4923899481977434	0.0833042108240052	T	T	T
0.1117635283967395	0.3633870573453890	0.0603808402128674	T	T	T
0.3048593792405115	0.6388804898482522	0.1099335729759967	T	T	T
0.3123785787505807	0.5063353961237300	0.0772178822263640	T	T	T
0.2972132513725672	0.3733877316620809	0.0611234611006592	T	T	T
0.5115960975302509	0.5425453853167860	0.2876922664731227	T	T	T
0.5131328391935955	0.3657012383120422	0.2757846918397373	T	T	T
0.4364964648970562	0.7511025155084390	0.6393364399180287	T	T	T
0.1885273379317336	0.7505861522088340	0.6304949908000630	T	T	T
0.2763093522556377	0.7508676249908078	0.0137551008777765	T	T	T
0.1036238335724226	0.7491575362069576	0.0432208793080969	T	T	T
0.0686605291602024	0.2479884144265446	0.1302064918527603	T	T	T
0.3109433702545883	0.2511747650557648	0.1305049132965050	T	T	T
0.2213290903835444	0.2503777705521412	0.5121069552564339	T	T	T
0.3965238595603945	0.2521947346531497	0.5425021799493723	T	T	T
0.5565827747549134	0.2499673954906831	0.3517748502485806	T	T	T
0.8070112772089738	0.2498397118224086	0.3475290248168132	T	T	T
0.7275428089565581	0.2495215377490287	0.9434870571124581	T	T	T
0.8915482199474364	0.2509559215773950	0.9451185942174768	T	T	T
0.9465714087905045	0.7541036310870950	0.8556709375722807	T	T	T
0.6845340874786694	0.7519449443528122	0.8519234997895943	T	T	T
0.7740383236655416	0.7479600827866735	0.4463153232648170	T	T	T
0.6085022330720312	0.7501187250488465	0.4504068240705491	T	T	T
0.9368471779955023	0.4878990691770002	0.5343281244128419	T	T	T
0.9325075571728361	0.4033244469933792	0.4417651333212921	T	T	T
0.8709421257717272	0.5556633650901917	0.5601960600130981	T	T	T
0.9612095475453178	0.4752313051461665	0.5952135266043646	T	T	T
-0.0141226666383906	0.5835438373965255	0.4616918331307684	T	T	T
0.0750666257967605	0.5677477663586660	0.4363963805947593	T	T	T
-0.0009598846729195	0.7014678885978372	0.4007096201581173	T	T	T
0.0168482522575713	0.5832441817149761	0.2859785153099128	T	T	T
0.0888367442058213	0.6845304424163683	0.3744061133318207	T	T	T
0.0332606389755839	0.6028773010403221	0.4338332257715322	T	T	T

Structure files (CONTCAR) involved in this work:

0.0406101140711404 0.6659022995462590 0.4007623016908738 T T T

Figure 4(a) Route(b-ii)-Zn ① as same as Route(a)-Zn ①**Figure 4(a) Route(b-ii)-Zn ②**

Si Al O Zn H C

1.0000000000000000

20.0219999999999985 0.0000000000000000 0.0000000000000000

0.0000000000000000 19.8990000000000009 0.0000000000000000

0.0000000000000000 0.0000000000000000 13.3829999999999991

93 3 193 2 6 2

Selective dynamics

Direct

0.4221703160734269 0.0602280796646796 0.6482828235018778 T T T

0.3048429578618740 0.0319975010462721 0.7922671240107377 T T T

0.2819691633065966 0.0564279624667406 0.0169253832447207 T T T

0.1225792692502936 0.0622015814358209 0.0114850536415256 T T T

0.0677097711791388 0.0313823816107129 0.8002654958327660 T T T

0.1802067203140636 0.0647177826321175 0.6646497847064416 T T T

0.4184940851270258 0.8274309751470993 0.6688904792907897 T T T

0.3008212927123305 0.8730118786949019 0.8011650976966868 T T T

0.2669399697612808 0.8303467719571483 0.0204686682969439 T T T

0.1109306132181895 0.8265774811690954 0.0129598579239192 T T T

0.0659153830304979 0.8747216902352392 0.7986002517934114 T T T

0.1791282716721615 0.8289132980614362 0.6651361490506053 T T T

0.0754782958033817 0.9408290464024455 0.1487024408993690 T T T

0.1945205844147246 0.9699858679208656 0.2904245112862594 T T T

0.2164743064083894 0.9435223540784345 0.5159992483509931 T T T

0.3768335609360099 0.9355717164797615 0.5135670440621153 T T T

0.4331627531986616 0.9686698401649704 0.3014620039269856 T T T

0.3199633540663861 0.9356790523263609 0.1643163670641654 T T T

0.0816659731678050 0.1720655885789327 0.1666117223964955 T T T

0.1976999509433803 0.1286958892892221 0.3018470524220334 T T T

0.2314940029243025 0.1694180338454297 0.5191768949489215 T T T

0.3868817219615357 0.1738483277213756 0.5088573720646576 T T T

0.4348773378638493 0.1270446693073366 0.2955941514552319 T T T

0.3183749888448623 0.1723229114838306 0.1666704415025755 T T T

0.5785018138634577 0.5555562476890942 0.3566512023473331 T T T

0.6910201540450669 0.5272943500381632 0.2029749790398618 T T T

0.7155488087935010 0.5685499674015901 0.9866047570380989 T T T

0.8745700857622757 0.5733574918420646 0.9862321299257958 T T T

0.8108796769795247 0.5514721103629420 0.3460900318310240 T T T

0.5727136509029652 0.3292133853901600 0.3324028034929388 T T T

0.6935115931815091 0.3733386305152100 0.1941772166896842 T T T

0.7317032489523980 0.3278894433580349 0.9801473006610167 T T T

0.8866292406525796 0.3254711351496390 0.9891153322755326 T T T

0.9424129034182550 0.3717817213868091 0.1889910597988016 T T T

0.9201596819234206 0.4464116120829681 0.8597580260849471 T T T

0.7998734464829815 0.4744913398830554 0.7198458751737145 T T T

0.7787195708603158 0.4367007142168954 0.4959452583699141 T T T

0.6214077916264865 0.4283740159611072 0.4904570402968377 T T T

0.5698510015973931 0.4692992003628896 0.7021920606059110 T T T

0.6760278087351280 0.4477099778518021 0.8568683779129692 T T T

0.9207026187496091 0.6789544518918006 0.8297269265425977 T T T

Structure files (CONTCAR) involved in this work:

0.7672643491551099	0.6706013605273626	0.4653343861079811	T	T	T
0.6126893032131771	0.6736255357682133	0.4886044890668194	T	T	T
0.5600983791213059	0.6276476715342921	0.6990275416081305	T	T	T
0.6712817447311444	0.6748183878550105	0.8287950167438630	T	T	T
0.5776440399676114	0.9457284913716489	0.3580834344785100	T	T	T
0.6982025239774226	0.9746857335035333	0.2152033275123503	T	T	T
0.7192851937330093	0.9388159673552734	0.9933196592849541	T	T	T
0.8791819730270934	0.9347632185469931	0.9948432232818899	T	T	T
0.9308359145375621	0.9718608903743196	0.2050631332088247	T	T	T
0.8221262516924777	0.9470384453324017	0.3548271656515733	T	T	T
0.5777490424627412	0.1742362418943661	0.3295742550296242	T	T	T
0.6974888733842549	0.1328529527190007	0.1936135497258672	T	T	T
0.7323350190546272	0.1716825957583565	0.9721600853155438	T	T	T
0.8868916830891148	0.1735312938665321	0.9824127774805095	T	T	T
0.9348143001329090	0.1302788465130793	0.1977338871902978	T	T	T
0.8191616651486773	0.1749161943962835	0.3320774850493682	T	T	T
0.9231133044058186	0.0542622456425731	0.8555790012876104	T	T	T
0.8016314079924899	0.0261965005614312	0.7100126543238043	T	T	T
0.7808513995646806	0.0659081914212820	0.4921969669262666	T	T	T
0.6206416252023098	0.0700967466972606	0.4899893894097470	T	T	T
0.5675900383315801	0.0326855899964718	0.6988798084690258	T	T	T
0.6781496060590738	0.0542194624614272	0.8493903916275234	T	T	T
0.9232442709088396	0.8311433508729965	0.8373319181897624	T	T	T
0.8026231304381339	0.8687963690261969	0.6955844051197226	T	T	T
0.7689125990167317	0.8276596177423293	0.4779228175871144	T	T	T
0.6140373607155355	0.8273466547577748	0.4902028396741822	T	T	T
0.5632642258187490	0.8755238488590946	0.6981469913471032	T	T	T
0.6780998233168000	0.8334129357570910	0.8335728520672139	T	T	T
0.4232698203290647	0.4418815557828073	0.6454394142052603	T	T	T
0.3048952848826774	0.4694495561594060	0.7886752793318087	T	T	T
0.2794517744941785	0.4455254117773585	0.0153458030796541	T	T	T
0.1217190641562971	0.4370919925392227	0.0154579223860868	T	T	T
0.0640534027785575	0.4699993108297689	0.8019137766845540	T	T	T
0.1772678296321354	0.4362819763487516	0.6626867456641019	T	T	T
0.4151418444108787	0.6736009537747519	0.6666782458362100	T	T	T
0.3004388432976213	0.6278846281230320	0.8007459101992342	T	T	T
0.2671765772410055	0.6690382193903940	0.0197668784520849	T	T	T
0.1118287926422566	0.6730844570551148	0.0073189416999097	T	T	T
0.0628889199685068	0.6285742172904056	0.7935317097066198	T	T	T
0.1794884897912274	0.6716926550402473	0.6640626253823969	T	T	T
0.0797111901680001	0.5593241020471503	0.1469310596244776	T	T	T
0.1967436016851773	0.5286266095386758	0.2898880164782149	T	T	T
0.2148294800810548	0.5560989270969519	0.5156442664815198	T	T	T
0.3737870750185300	0.5655481516475999	0.5141339183427805	T	T	T
0.4305545944978819	0.5310206351471177	0.3045029135359728	T	T	T
0.3217638048035288	0.5633052259106933	0.1627875259020836	T	T	T
0.0865822846446617	0.3241001162561869	0.1611779459021848	T	T	T
0.1983214290613699	0.3706133499122314	0.3006002888601089	T	T	T
0.2300575361892804	0.3307520869694922	0.5192915185259953	T	T	T
0.3847998819898650	0.3278845060368862	0.5064629495471223	T	T	T
0.4300957894062887	0.3741127653145604	0.2932930448877986	T	T	T
0.3166943485880049	0.3297838734180895	0.1630146026763137	T	T	T
0.9206741710761667	0.5280678082308917	0.1953504632217779	T	T	T

Structure files (CONTCAR) involved in this work:

0.8225688991319756	0.3353816785740757	0.3272405409921652	T	T	T
0.7974116143803516	0.6382259932613278	0.6969240240892942	T	T	T
0.0111111979040700	0.5596643775527984	0.2268282245854505	T	T	T
0.3583935264725003	0.0705603103329854	0.7217182121481902	T	T	T
0.3164195904147671	0.0548094907655376	0.9071472382621727	T	T	T
0.2019272720295571	0.0468235275012762	0.0066561402558726	T	T	T
0.0922453815095022	0.0703236392349509	0.9001915356569853	T	T	T
0.1034033272923484	0.0645854001160233	0.7031276528339767	T	T	T
0.2291378573259544	0.0517275654448523	0.7599133129915979	T	T	T
0.3595585271224559	0.8279795661146828	0.7521548574572513	T	T	T
0.3007775869205991	0.8609374517569185	0.9204908637074078	T	T	T
0.1883005282487359	0.8506786793019298	0.0233217260802188	T	T	T
0.0878442495225176	0.8328722654497752	0.8975581218712246	T	T	T
0.1023812987595147	0.8410097397595511	0.7017788402697357	T	T	T
0.2285665947797570	0.8510064577327870	0.7561655390063399	T	T	T
0.3157158038376883	0.9515500568711983	0.7772714582087751	T	T	T
0.0892653080356840	0.9525751989634288	0.8095296334869436	T	T	T
0.4325558487601651	0.1278008570951494	0.5817755240122943	T	T	T
0.4118906811447410	0.9966443428938678	0.5739938337261592	T	T	T
0.3929591050749076	0.8645251043913504	0.5678422653970167	T	T	T
0.1961663179514906	0.1380368376439411	0.6174010628544185	T	T	T
0.1896327696826452	0.0059295826773091	0.5821564368554393	T	T	T
0.1942988602557760	0.8722763791071686	0.5651148495705697	T	T	T
0.9877134012964994	0.0393479074400422	0.7856074591033482	T	T	T
0.9853414009007104	0.8713755738774618	0.7852829415370228	T	T	T
0.1398604612410151	0.9318993875362727	0.2212950793405161	T	T	T
0.1831272842529873	0.9484900049164650	0.4058402039677823	T	T	T
0.2970199430748419	0.9481066017105995	0.5085704706150589	T	T	T
0.4072627755441292	0.9314366182532812	0.4019939397600204	T	T	T
0.3962013096335454	0.9359181290268518	0.2050310863631922	T	T	T
0.2697259820816909	0.9485270940394792	0.2580884524932707	T	T	T
0.1389973045478977	0.1732998892576403	0.2522940062336303	T	T	T
0.1945951220805147	0.1385928453588514	0.4216212164366385	T	T	T
0.3098305165382932	0.1480597897734717	0.5158034634726749	T	T	T
0.4128364310594645	0.1685113502625357	0.3946919768791773	T	T	T
0.3955097320508431	0.1583510728304074	0.1995465582747020	T	T	T
0.2704914397063574	0.1529027547591288	0.2611367320380650	T	T	T
0.1850149954892322	0.0503670946808284	0.2736742800554724	T	T	T
0.4152313487894998	0.0483413481084197	0.3089699060537664	T	T	T
0.0644989762990791	0.8714515536698060	0.0863291950984368	T	T	T
0.0853426118526470	0.0009414565439415	0.0683414368159260	T	T	T
0.1087102358340466	0.1318509026759900	0.0696331808550391	T	T	T
0.3047657005875886	0.8623048595177785	0.1162202495597918	T	T	T
0.3115772740747056	0.9945325630750519	0.0816153956362947	T	T	T
0.2992054079688540	0.1279599676656953	0.0691245757282991	T	T	T
0.5127477206918473	0.9567500735091199	0.2872078064928220	T	T	T
0.5149590783893575	0.1343398485103521	0.2789813558367946	T	T	T
0.6378031232685689	0.5641535910581196	0.2758059873506615	T	T	T
0.7005606634641979	0.5745120731404645	0.1055078906031019	T	T	T
0.7950626133095551	0.5613079995019826	0.9638709801321658	T	T	T
0.8905056880562340	0.5793628139181254	0.1034829890681100	T	T	T
0.8867601300959554	0.5378422324462843	0.3137226081925672	T	T	T
0.7619741200627717	0.5226360018094335	0.2616474850817909	T	T	T

Structure files (CONTCAR) involved in this work:

0.6375562901438052	0.3358305935342220	0.2623660548035862	T	T	T
0.6932484425584556	0.3357901744121600	0.0858535376125828	T	T	T
0.8093805201820937	0.3515452140161251	0.9912984372634533	T	T	T
0.9165895681471902	0.3211280899223571	0.1011356789294647	T	T	T
0.9050082978545863	0.3525889666650773	0.2919517043585587	T	T	T
0.7650666137429775	0.3706938984150436	0.2469732252774023	T	T	T
0.6685891593509018	0.4512432197331817	0.1760828327803766	T	T	T
0.9310020315460261	0.4481996585771592	0.1548526693778223	T	T	T
0.5682739688862875	0.6262344933998675	0.4155340578101077	T	T	T
0.5960422287542605	0.4973629498419502	0.4379456113572249	T	T	T
0.5845986575078598	0.3639533285327091	0.4415142089975440	T	T	T
0.7983454664603954	0.6310340414500754	0.3693313483834485	T	T	T
0.7953009136320405	0.5146913586235750	0.4566295478880407	T	T	T
0.8308007874663932	0.3865240877179406	0.4400936374160969	T	T	T
0.0225323194604450	0.3619613849042063	0.2064486616140778	T	T	T
0.8544891223537928	0.4375552105819881	0.7893230250846576	T	T	T
0.7952811675238004	0.4343457874453273	0.6139672058641574	T	T	T
0.7017265395088742	0.4196055703209566	0.4717912120827305	T	T	T
0.6055995429848954	0.4304781568463923	0.6090425284041335	T	T	T
0.6022539513566533	0.4441950851706927	0.8068604676840584	T	T	T
0.7271631977622470	0.4746994216826816	0.7709945983175395	T	T	T
0.8598793834991588	0.6824996098103496	0.7529133406156507	T	T	T
0.8121011743285587	0.6480048128571566	0.5635143813977809	T	T	T
0.6904179700082492	0.6481589607803481	0.4856099808868895	T	T	T
0.5845140908365936	0.6693603494444673	0.6013655712183961	T	T	T
0.5930904873515559	0.6607452770847341	0.7984735268784919	T	T	T
0.7177511159514542	0.6508672045687814	0.7371010054834054	T	T	T
0.8226528412141731	0.5515782445532958	0.6939959928622826	T	T	T
0.5814775925803686	0.5493752186877877	0.6863825370311482	T	T	T
0.9305828407362148	0.3770655023959958	0.9216464498083725	T	T	T
0.9139733549055913	0.5101763199094337	0.9343475714128571	T	T	T
0.9000659715450636	0.6422404341029880	0.9335759761523162	T	T	T
0.6962287073647736	0.3733681965451880	0.8945754205443828	T	T	T
0.6768338777851219	0.5012304977324075	0.9481243607632492	T	T	T
0.6869920032765168	0.6351674952267844	0.9324998915862489	T	T	T
0.4909884441404666	0.4514126160524268	0.7096350951468944	T	T	T
0.4792007600057390	0.6321086752199148	0.7081662765923339	T	T	T
0.6435446219597627	0.9404429962974598	0.2885196937710703	T	T	T
0.6986649449235059	0.9339071820057795	0.1102063124419638	T	T	T
0.7996444440151689	0.9469115481294039	0.9801398197470955	T	T	T
0.8983367154472798	0.9301938836595408	0.1123293792280865	T	T	T
0.8973882186126527	0.9483737443747315	0.3098858391428468	T	T	T
0.7715733675614789	0.9689719730727320	0.2657451836342326	T	T	T
0.6397770584338620	0.1741428597724375	0.2522842382150751	T	T	T
0.6963037738448228	0.1577789560497039	0.0785171611280880	T	T	T
0.8098712285453388	0.1471113940382599	0.9786776948170471	T	T	T
0.9135674563972186	0.1695674124031368	0.0964157201877871	T	T	T
0.8958134779351599	0.1605551768564119	0.2938510690033259	T	T	T
0.7700323216068083	0.1463890783684202	0.2433118747121607	T	T	T
0.6795569014484310	0.0531120665399888	0.1978952225987574	T	T	T
0.9176339143011287	0.0510203698943776	0.1844833356128500	T	T	T
0.5690250154980609	0.8757196064436802	0.4197109085124626	T	T	T
0.5819943232905663	0.0074330896174425	0.4375036335562845	T	T	T

Structure files (CONTCAR) involved in this work:

0.5994029530175828	0.1395446087155933	0.4348140667898815	T	T	T
0.8070867249304789	0.8712221779288046	0.3935671730458503	T	T	T
0.8162306386282854	0.9984249091151455	0.4483742480345979	T	T	T
0.8064145079860501	0.1321548885145426	0.4344404996227194	T	T	T
0.0100666307321871	0.9557179395327355	0.2160334070937540	T	T	T
0.0150021262046558	0.1386464408424320	0.2143714227382000	T	T	T
0.8571298864552684	0.0557363941794210	0.7859834899192769	T	T	T
0.8011002154444447	0.0719082455691662	0.6095455251291175	T	T	T
0.7003476709724865	0.0575140778288803	0.4800028129432811	T	T	T
0.5985844537002347	0.0759771175817508	0.6065199111893763	T	T	T
0.6031185169665648	0.0526555059369673	0.8036431730176733	T	T	T
0.7285822683180757	0.0288534742872087	0.7621364406632127	T	T	T
0.8599509648201603	0.8341309543158286	0.7626091329522026	T	T	T
0.8047444837405127	0.8335725181598612	0.5861848208419567	T	T	T
0.6915914396961491	0.8522623930924744	0.4862072965429706	T	T	T
0.5877757295995000	0.8295411742562087	0.6047397246354050	T	T	T
0.6025924520457409	0.8533642267539694	0.7989809822497717	T	T	T
0.7296152290820624	0.8571513172558238	0.7458567161035746	T	T	T
0.8181007189265084	0.9483904105526445	0.6829376714807426	T	T	T
0.5786665793506591	0.9536664710067841	0.6724418907496875	T	T	T
0.9323433315397678	0.1268250233737344	0.9095924732860595	T	T	T
0.9185532269980329	0.9968003237171235	0.9419789714812619	T	T	T
0.9026221050734800	0.8646202558011112	0.9437825683453527	T	T	T
0.6949452163348013	0.1303803523112728	0.8839129229407278	T	T	T
0.6827100809680539	0.0042785433984236	0.9453041911658464	T	T	T
0.6952706433349832	0.8704505550220819	0.9384012264201318	T	T	T
0.4886845851802118	0.0484067912267182	0.7147180317498464	T	T	T
0.4836482067189979	0.8646115534312094	0.7157206540151803	T	T	T
0.3604941024854183	0.4311679620580623	0.7212188391169774	T	T	T
0.3115964042244915	0.4458286961674547	0.9041494123100081	T	T	T
0.1993283917040796	0.4612702420777515	0.0119360179467961	T	T	T
0.0899274474356475	0.4358440067267344	0.9050692077146218	T	T	T
0.1020647614815423	0.4356590249212428	0.7076902280834563	T	T	T
0.2297120704279150	0.4509774558334381	0.7526501173321185	T	T	T
0.3579050960572351	0.6748840363334273	0.7527072841714345	T	T	T
0.3014911138937723	0.6380730730642992	0.9204723809870621	T	T	T
0.1885689637265993	0.6477274768976466	0.0193481755685785	T	T	T
0.0878601427658635	0.6687069634212014	0.8925933347894562	T	T	T
0.1021689107305312	0.6585990479822621	0.6966097374592467	T	T	T
0.2274766673260170	0.6487046487278936	0.7565752415580431	T	T	T
0.3167517239792171	0.5498344377821445	0.7750121252969424	T	T	T
0.0816444721030580	0.5496870524088059	0.8063532775914977	T	T	T
0.4318136050239563	0.3761337145360064	0.5743714219755635	T	T	T
0.4134146553071759	0.5075104296266119	0.5748244307754373	T	T	T
0.3845124854392204	0.6381246771462392	0.5670043619240909	T	T	T
0.1922937013875233	0.3628722638319675	0.6151639450956020	T	T	T
0.1818366656318781	0.4950628570443918	0.5785605121089652	T	T	T
0.1961501572440090	0.6284928755510614	0.5639098712892616	T	T	T
0.9847669695517526	0.4574039672365976	0.7875474582579852	T	T	T
0.9833915311781918	0.6382984541774690	0.7776135225309614	T	T	T
0.1437044793963902	0.5689687356615256	0.2184112436987701	T	T	T
0.1834963865238902	0.5538461258727745	0.4032024040862813	T	T	T
0.2949947731470647	0.5460688036943210	0.5112024883929499	T	T	T

Structure files (CONTCAR) involved in this work:

0.4029633671562562	0.5709411742045518	0.4017920909109951	T	T	T
0.3977036540322885	0.5645859177149479	0.2049008365560120	T	T	T
0.2720407750906976	0.5473824412172575	0.2567426734169833	T	T	T
0.1441172832109267	0.3229249467883766	0.2467170678865636	T	T	T
0.1945979647533568	0.3604020556072558	0.4198425746722002	T	T	T
0.3080062603378082	0.3536144050435494	0.5191936589669780	T	T	T
0.4062337898330604	0.3304495834757646	0.3896467092893270	T	T	T
0.3939134968887537	0.3463463813958959	0.1922094445937260	T	T	T
0.2723436783123519	0.3510510137324407	0.2604372337996155	T	T	T
0.1821009678771894	0.4491554339743731	0.2746043852273622	T	T	T
0.4093624982978597	0.4522161733553980	0.3122843275771699	T	T	T
0.0661895947927828	0.6237035446102398	0.0772860187489171	T	T	T
0.0792280396956426	0.4902710594276194	0.0854906948561386	T	T	T
0.1155708293762289	0.3627282521719024	0.0627041799180876	T	T	T
0.3034937954428178	0.6364512309976387	0.1166363056049593	T	T	T
0.3149151521069554	0.5048455960310406	0.0790994940657197	T	T	T
0.2930707954496847	0.3725260021243542	0.0656163285470599	T	T	T
0.5107957467762743	0.5374804186374127	0.2963984804326218	T	T	T
0.5100068863481024	0.3664466153633616	0.2776694439611654	T	T	T
0.4361721321986682	0.7501716108322847	0.6401099322369350	T	T	T
0.1907367670273101	0.7502796921587572	0.6374177884852077	T	T	T
0.2755235494238937	0.7495361710301549	0.0234567505591425	T	T	T
0.1032699868256911	0.7488415488586645	0.0484431123072102	T	T	T
0.0675537974516200	0.2481961122224309	0.1293001618026937	T	T	T
0.3079390791325449	0.2507763939975149	0.1369189931430179	T	T	T
0.2233717113372398	0.2501039013195879	0.5229409883956181	T	T	T
0.3922029677684968	0.2512593643736429	0.5459184448137464	T	T	T
0.5553275143189118	0.2509059409374775	0.3528085253799172	T	T	T
0.8069296162427296	0.2525901663531782	0.3548184513921657	T	T	T
0.7276202635918507	0.2504912774809157	0.9429589350499987	T	T	T
0.8911852904551276	0.2503464785018772	0.9415788836902854	T	T	T
0.9462018611728262	0.7544018687908817	0.8582260547221219	T	T	T
0.6828639373222509	0.7537605662815876	0.8530234592368925	T	T	T
0.7731337560082673	0.7497283342884765	0.4427245768242403	T	T	T
0.6080963761445468	0.7506351933407660	0.4494803495819836	T	T	T
0.9345029212611324	0.5050285984516423	0.5246738980220255	T	T	T
0.9323468797561322	0.4088638424598546	0.4416965593145815	T	T	T
0.8682324889984872	0.5649731206720118	0.5583659300484037	T	T	T
0.0508804554071700	0.4170664402670248	0.5124323060094247	T	T	T
0.0492578249682282	0.4295421708372024	0.3797298051970826	T	T	T
0.0441830049698712	0.3467417206265194	0.4288632503940353	T	T	T
0.9775758001839308	0.5235149693456139	0.5049173892600757	T	T	T
0.9694296892476064	0.6265714411649500	0.3317436646276576	T	T	T
0.0658345812504197	0.6173738951317674	0.3323399940952653	T	T	T
0.0295111886526714	0.3991186609308625	0.4417982393817084	T	T	T
0.0159699732304114	0.6040383454218873	0.3076665855594505	T	T	T

Figure 4(a) Route(b-ii)-Zn ③

Si Al O Zn H C

1.0000000000000000		
20.0219999999999985	0.0000000000000000	0.0000000000000000
0.0000000000000000	19.8990000000000009	0.0000000000000000
0.0000000000000000	0.0000000000000000	13.3829999999999991

Structure files (CONTCAR) involved in this work:

93	3	193	2	6	2
Selective dynamics					
Direct					
0.4227091908098011	0.0607798299312813	0.6488053828131328	T	T	T
0.3052732528278072	0.0320970774096265	0.7921412483934248	T	T	T
0.2822343370642091	0.0563995547083539	0.0172075310270207	T	T	T
0.1230520689797300	0.0617966102665275	0.0126134617185283	T	T	T
0.0679990145875820	0.0314891694859569	0.8010184307423727	T	T	T
0.1804000651589431	0.0650646944243645	0.6651824767164368	T	T	T
0.4189963496177550	0.8280456879471583	0.6687322328645221	T	T	T
0.3013095714709511	0.8730703314151702	0.8006697492972946	T	T	T
0.2670328472953416	0.8317019683844235	0.0201132512401556	T	T	T
0.1118689037956214	0.8270758363882472	0.0119159997768415	T	T	T
0.0661400130139884	0.8748232136076675	0.7977821498110091	T	T	T
0.1795896277050086	0.8285694543302471	0.6650576601668714	T	T	T
0.0757545900514443	0.9400866902466956	0.1494165312703191	T	T	T
0.1947549310623245	0.9698054454493863	0.2909671599150790	T	T	T
0.2166802203452551	0.9437268909078357	0.5166968467937709	T	T	T
0.3770200683590511	0.9364635108259248	0.5139385634303207	T	T	T
0.4338179634750772	0.9690217209709336	0.3017005474154402	T	T	T
0.3205135903181654	0.9360649714013751	0.1650971220984338	T	T	T
0.0821564950313209	0.1716737993348065	0.1671983511144522	T	T	T
0.1978683608697027	0.1283813638411031	0.3021897655514357	T	T	T
0.2319039677940298	0.1694867198347992	0.5192125453215363	T	T	T
0.3874949065150052	0.1741049215442760	0.5086745208940967	T	T	T
0.4352115270819673	0.1277000523372240	0.2947017350612928	T	T	T
0.3180185275847470	0.1724963307346091	0.1664603831362967	T	T	T
0.5766609733975806	0.5556165532225743	0.3575484948940167	T	T	T
0.6914938051744461	0.5259173085538045	0.2055559032187103	T	T	T
0.7153635781060914	0.5686551758173040	0.9894320004012721	T	T	T
0.8742377945206005	0.5736247278499718	0.9871867903977161	T	T	T
0.8116217890483909	0.5500847695978702	0.3476742089845050	T	T	T
0.5741280191119768	0.3291098528855053	0.3341524479407314	T	T	T
0.6941529120534795	0.3727455338684715	0.1940228756906071	T	T	T
0.7314124558176638	0.3274788615362714	0.98192441311178749	T	T	T
0.8865459271269578	0.3259522636670592	0.9958687365891343	T	T	T
0.9434465970978767	0.3728319247923942	0.1953607407390375	T	T	T
0.9194202691154023	0.4454925328038474	0.8621314844723360	T	T	T
0.7992479027659725	0.4725787146723477	0.7224247366593879	T	T	T
0.7759478252590984	0.4351857061991632	0.4981514443131742	T	T	T
0.6177152712269165	0.4296760631288875	0.4929610727257887	T	T	T
0.5681160632673190	0.4690771590352100	0.7059782953022432	T	T	T
0.6756806902595190	0.4479963705031293	0.8597666274451911	T	T	T
0.9202532324105942	0.6789602669759158	0.8304349482076856	T	T	T
0.7677479108759626	0.6684813743569585	0.4679423872985415	T	T	T
0.6126994335416267	0.6730604216185333	0.4901541872424865	T	T	T
0.5593925360118863	0.6278255414244993	0.7013355866121996	T	T	T
0.6723429485817346	0.6739417290239809	0.8298931105368408	T	T	T
0.5780373497996489	0.9448136494179649	0.3591388512113187	T	T	T
0.6979023206018412	0.9735833468103533	0.2156098895823467	T	T	T
0.7193679704755250	0.9381943594584630	0.9935414576733733	T	T	T
0.8793652629824203	0.9347384659356999	0.9950119176290246	T	T	T
0.9309053569693899	0.9702782348720980	0.2053262405938598	T	T	T

Structure files (CONTCAR) involved in this work:

0.8218276048918485	0.9461203956214509	0.3553300523830317	T	T	T
0.5782467417324909	0.1739766323684089	0.3296674760397654	T	T	T
0.6976541308264684	0.1312321350661845	0.1938080734768059	T	T	T
0.7326959985865135	0.1715371333864012	0.9729716010863495	T	T	T
0.8874536335382870	0.1736994994183841	0.9834797522492279	T	T	T
0.9358316017384998	0.1283905976153822	0.1976370034025282	T	T	T
0.8199232121120201	0.1727944085184077	0.3300481825239789	T	T	T
0.9231130716030113	0.0546011707030277	0.8559965419591600	T	T	T
0.8017084750691928	0.0262882636096008	0.7096873960142432	T	T	T
0.7811480368187794	0.0658333769453825	0.4918646270917032	T	T	T
0.6208135822598599	0.0696778756436347	0.4903710913340260	T	T	T
0.5681157467110605	0.0325904286732430	0.6996713984420672	T	T	T
0.6785000388359888	0.0541246064679441	0.8499645457123042	T	T	T
0.9236172911092920	0.8313547379823141	0.8366925159035055	T	T	T
0.8025349796143295	0.8689494217826341	0.6955587293327290	T	T	T
0.7693021459491274	0.8262671390683668	0.4785247623486932	T	T	T
0.6144822130610269	0.8267756047020071	0.4913279029540858	T	T	T
0.5637744015736933	0.8753783210099862	0.6991551016044111	T	T	T
0.6784937475435474	0.8328230926309433	0.8338535933255554	T	T	T
0.4235110706717021	0.4422500756893637	0.6450598305157423	T	T	T
0.3032900899936155	0.4699022698282099	0.7855967657645520	T	T	T
0.2797688557952573	0.4443775751846816	0.0118650300387687	T	T	T
0.1210664643524225	0.4375605768778112	0.0158638656658358	T	T	T
0.0637616647733682	0.4696323863049369	0.8016223592043785	T	T	T
0.1755583359006604	0.4374915364641201	0.6586084577513068	T	T	T
0.4160382316727756	0.6744401388209231	0.6637967050629692	T	T	T
0.3000740256062894	0.6287432869883830	0.7982051527728374	T	T	T
0.2681691832756717	0.6704183343007064	0.0169028906486545	T	T	T
0.1134850012645959	0.6731761781025808	0.0050507642734395	T	T	T
0.0622595776772243	0.6286045256216649	0.7926325077528974	T	T	T
0.1787607609568417	0.6711432596179900	0.6632685403407160	T	T	T
0.0789030112242203	0.5605826057218273	0.1476559122825614	T	T	T
0.1982841994027679	0.5286839192360706	0.2860753330144645	T	T	T
0.2168119558225976	0.5563577899811909	0.5155582803559411	T	T	T
0.3756598945542040	0.5649883970592482	0.5136626189437005	T	T	T
0.4292635487037845	0.5303850446824679	0.3008601528160906	T	T	T
0.3229297487090170	0.5626842972480199	0.1550230162162901	T	T	T
0.0862014065458263	0.3237515172069089	0.1627487385761106	T	T	T
0.1994144173969069	0.3710338768875318	0.2990936660903987	T	T	T
0.2301766586307209	0.3307651035199182	0.5179259469746492	T	T	T
0.3854007674282025	0.3280428568117412	0.5062624957379463	T	T	T
0.4319221440443981	0.3730006648807553	0.2920683951157858	T	T	T
0.3180432088998635	0.3298103810540697	0.1628576429883750	T	T	T
0.9236555540793414	0.5297122596503817	0.1974603524568682	T	T	T
0.8209696467229666	0.3346778936772747	0.3277780629045379	T	T	T
0.7984784674926864	0.6355784226543502	0.6970664532008569	T	T	T
0.0111942977402952	0.5615622351910418	0.2243813436855478	T	T	T
0.3589695827073484	0.0711430753241530	0.7223785945261469	T	T	T
0.3166917015394790	0.0539598719185692	0.9074959520881887	T	T	T
0.2022705584016740	0.0458627914586309	0.0071310076612811	T	T	T
0.0923034258392084	0.0698604458690483	0.9015685275261958	T	T	T
0.1037132227381465	0.0653605643509051	0.7043638602493911	T	T	T
0.2296941529429762	0.0523901061326336	0.7600905365098071	T	T	T

Structure files (CONTCAR) involved in this work:

0.3601193522632672	0.8278283877710361	0.7521887757069396	T	T	T
0.3015424971261831	0.8616254803526006	0.9201777985527749	T	T	T
0.1886599772291519	0.8530144645013348	0.0217962476110175	T	T	T
0.0877033338618880	0.8329775128743233	0.8969654410816714	T	T	T
0.1028393718471751	0.8411130108328454	0.7011911942850708	T	T	T
0.2290933216003322	0.8501886671410274	0.7563060788138835	T	T	T
0.3158490553527213	0.9516247261495502	0.7756893538198842	T	T	T
0.0896232733780583	0.9526247396766740	0.8090005463167713	T	T	T
0.4331035631340628	0.1281979369513394	0.5819367548133826	T	T	T
0.4121964329677602	0.9972586333229699	0.5745559886421087	T	T	T
0.3929099741944106	0.8654421157872162	0.5682818985662228	T	T	T
0.1965373446534792	0.1382563255649426	0.6175506709146918	T	T	T
0.1893676954897082	0.0057103584843652	0.5833470207816526	T	T	T
0.1952671857230287	0.8720029780338643	0.5652270677653742	T	T	T
0.9879683889390355	0.0391823397772878	0.7867733290391783	T	T	T
0.9856403128161547	0.8713567391246040	0.7839151908489154	T	T	T
0.1401100665704859	0.9312704609697143	0.2222206568925670	T	T	T
0.1832468088325615	0.9488471311816639	0.4065822788756767	T	T	T
0.2971861882837299	0.9490987383051452	0.5089576038267937	T	T	T
0.4075419259263706	0.9323600459823599	0.4024613073061562	T	T	T
0.3967909857840665	0.9357491539268206	0.2056869096204400	T	T	T
0.2700422776475732	0.9484389436905211	0.2588068015272593	T	T	T
0.1391488901011829	0.1733877592884471	0.2534100068863676	T	T	T
0.1950464005285013	0.1380660703720568	0.4219983097741842	T	T	T
0.3103405843739728	0.1485646929704932	0.5157522081989881	T	T	T
0.4133147909868721	0.1687619967391038	0.3943746063485171	T	T	T
0.3953072197081217	0.1588383245615866	0.1989644238949578	T	T	T
0.2705505015885663	0.1526954925152058	0.2612173457284845	T	T	T
0.1850670250378434	0.0501282824377363	0.2734566045797841	T	T	T
0.4162163890837962	0.0488093830136899	0.3079366609971173	T	T	T
0.0650433439891365	0.8708851344834845	0.0863034738256227	T	T	T
0.0855158666072844	0.0009095731111902	0.0701221004642315	T	T	T
0.1100733539123910	0.1318031334013941	0.0703532073713246	T	T	T
0.3050373166714867	0.8630849676673441	0.1160519362176541	T	T	T
0.3125189886027988	0.9954914025353617	0.0832483301128423	T	T	T
0.2987497820266163	0.1284440941948936	0.0685429019833411	T	T	T
0.5133433592678841	0.9566204892667838	0.2881265224977212	T	T	T
0.5151286184127696	0.1357172497078458	0.2772589585858422	T	T	T
0.6377676148572305	0.5613702262722486	0.2791325255693403	T	T	T
0.7016982735883402	0.5740936677384451	0.1090180199587468	T	T	T
0.7947005978147405	0.5617795402414257	0.9647631908359749	T	T	T
0.8901162858886863	0.5783307167357377	0.1044296024572363	T	T	T
0.8879561054887070	0.5389747090329027	0.3154856374091722	T	T	T
0.7620147357862468	0.5195540255246783	0.2653549300719336	T	T	T
0.6402213419162716	0.3362327691696944	0.2669340876917443	T	T	T
0.6909871365661836	0.3347411811736798	0.0861366798760414	T	T	T
0.8089694666973760	0.3508592691852346	0.9968445754139741	T	T	T
0.9153993086742622	0.3217856189003158	0.1092557318147818	T	T	T
0.9059903214025690	0.3561447837452617	0.3013221751902555	T	T	T
0.7673566999837462	0.3698285892394343	0.2416364764552928	T	T	T
0.6688200133304890	0.4504200806084652	0.1759304907443168	T	T	T
0.9332983939042424	0.4487378293223399	0.1596329341849982	T	T	T
0.5684786034414921	0.6269232827589909	0.4151908183931703	T	T	T

Structure files (CONTCAR) involved in this work:

0.5888457368031241	0.4973958033916451	0.4408771670214713	T	T	T
0.5839113241549946	0.3635488974797119	0.4438798490553463	T	T	T
0.7964276825291288	0.6291403115695375	0.3701044835508746	T	T	T
0.7997216380893052	0.5118413517251216	0.4585161297691654	T	T	T
0.8215024415515871	0.3797992746225045	0.4432865120745643	T	T	T
0.0231007287606021	0.3600596730942537	0.2147940215349825	T	T	T
0.8541543903826336	0.4345298172577680	0.7909763632990260	T	T	T
0.7914393342803944	0.4327347600355703	0.6168001483765344	T	T	T
0.6978504062809990	0.4263165113710051	0.4731790226501695	T	T	T
0.6022498476198769	0.4301787610893159	0.6116797068242379	T	T	T
0.6018978047510986	0.4439276304200044	0.8097226648758580	T	T	T
0.7270324335486852	0.4756157089541314	0.7747926405943472	T	T	T
0.8592113130469800	0.6818423548389633	0.7541597791848553	T	T	T
0.8134791392004649	0.6436736243827449	0.5638557219038043	T	T	T
0.6903980104236515	0.6475159784975127	0.4892075279614642	T	T	T
0.5832130208509392	0.6682715889648078	0.6021740663905515	T	T	T
0.5939306982658169	0.6611662723270010	0.7992969520371243	T	T	T
0.7189281040322728	0.6482554029694245	0.7393017908738654	T	T	T
0.8247464733443863	0.5490045085709595	0.6974032221424955	T	T	T
0.5796598296504528	0.5491453322040537	0.6902608813806420	T	T	T
0.9304771043091802	0.3781651004179276	0.9288166284548832	T	T	T
0.9133686848774920	0.5108390060555602	0.9332985366497304	T	T	T
0.9002548593192341	0.6426239814155474	0.9350794984119458	T	T	T
0.6971779749812010	0.3736305594145284	0.8960923543949548	T	T	T
0.6763090877955673	0.5012750706672142	0.9514278341429863	T	T	T
0.6863592556576400	0.6351553615056452	0.9352338996323950	T	T	T
0.4891918078766959	0.4508129276792794	0.7143769004026810	T	T	T
0.4785391823349403	0.6337755988880682	0.7121186078832890	T	T	T
0.6437147245924157	0.9389025367150592	0.2892747441407784	T	T	T
0.6986810599363485	0.9331094008929227	0.1103623477652800	T	T	T
0.7997456265960953	0.9460773225961221	0.9802862439248108	T	T	T
0.8984279788310183	0.9287870081168446	0.1124608019196074	T	T	T
0.8970468428097279	0.9475081707537836	0.3101627821682637	T	T	T
0.7712785913076098	0.9682380469125020	0.2662952061945505	T	T	T
0.6410536128802675	0.1733496698585914	0.2537319599794048	T	T	T
0.6965350238158966	0.1571456318683064	0.0791149832801904	T	T	T
0.8103874366409239	0.1475587743204170	0.9795026765133495	T	T	T
0.9145137303492714	0.1683341257739090	0.0970239643412005	T	T	T
0.8969185943684667	0.1580960129173877	0.2940134113672344	T	T	T
0.7708397287108906	0.1424327136036603	0.2426376175903583	T	T	T
0.6782478587178851	0.0517721890702693	0.1976953514377713	T	T	T
0.9183313274885390	0.0493549509912446	0.1837741135598824	T	T	T
0.5691233263515266	0.8749665982389038	0.4209374867884724	T	T	T
0.5827641866297172	0.0063025928146097	0.4388313130742365	T	T	T
0.5979835191133821	0.1385483691729043	0.4351163514818567	T	T	T
0.8072676591802572	0.8701007526346096	0.3940114759262994	T	T	T
0.8159123726426019	0.9977551380432045	0.4486500500169948	T	T	T
0.8072347850706363	0.1319542618973440	0.4342210282003380	T	T	T
0.0100857438188962	0.9539255641082265	0.2166406397290935	T	T	T
0.0159508532567280	0.1369466358457164	0.2142802947136948	T	T	T
0.8574888369195528	0.0554237052395168	0.7856366063300793	T	T	T
0.8012418788817677	0.0721282047221831	0.6093164331090124	T	T	T
0.7006075197007472	0.0583654125688831	0.4789342388040921	T	T	T

Structure files (CONTCAR) involved in this work:

0.5994874480882419	0.0755627743389396	0.6072376599696846	T	T	T
0.6033662535942851	0.0528426523886167	0.8045252298610643	T	T	T
0.7288543089192673	0.0291893191176929	0.7623371815125931	T	T	T
0.8599574513685529	0.8347130902132590	0.7628226866186084	T	T	T
0.8048945441276060	0.8329999051285448	0.5868226673907733	T	T	T
0.6920714973142196	0.8514023352393888	0.4862062915230702	T	T	T
0.5885493957890259	0.8293099183448706	0.6060115865314748	T	T	T
0.6027062104644403	0.8524099354795746	0.7999348420888046	T	T	T
0.7295934423840895	0.8577300195116060	0.7462542593348315	T	T	T
0.8178390263267847	0.9485300975741783	0.6817471732548622	T	T	T
0.5795167924504638	0.9535124456444773	0.6739245235237448	T	T	T
0.9321818387533524	0.1277704872530059	0.9085430715162583	T	T	T
0.9179686470598002	0.9979277834071816	0.9436452483429025	T	T	T
0.9036866044048034	0.8652351901398280	0.9430965325700087	T	T	T
0.6954483737484163	0.1301799241044858	0.8847528729450325	T	T	T
0.6830214527601447	0.0037856336316030	0.9454397153615463	T	T	T
0.6951963159299396	0.8698017963525794	0.9388871275034658	T	T	T
0.4892214508670655	0.0486299983853791	0.7150666861206845	T	T	T
0.4839712213712597	0.8652821408206377	0.7159474260802415	T	T	T
0.3582108145625623	0.4326337895235934	0.7160079915766794	T	T	T
0.3085990768203118	0.4414933306676058	0.8988188502032420	T	T	T
0.1994491041062175	0.4592321214782596	0.0138942672293191	T	T	T
0.0911150517121169	0.4359499319768940	0.9039815746866102	T	T	T
0.1004430528850756	0.4361877840570190	0.7050458422625576	T	T	T
0.2278400962468757	0.4547291538715155	0.7475968273390908	T	T	T
0.3548041597302737	0.6754652908755838	0.7432524571893785	T	T	T
0.3040246888596326	0.6429611808185567	0.9167634770866849	T	T	T
0.1901622950963417	0.6469739005610824	0.0143340740540908	T	T	T
0.0878927744588181	0.6689877910617371	0.8910389807155468	T	T	T
0.1012060999454188	0.6580218841131046	0.6948689408982093	T	T	T
0.2258003521205517	0.6470712226510651	0.7563192057865330	T	T	T
0.3173886221110786	0.5502123764426957	0.7784420625767692	T	T	T
0.0802431227664293	0.5494648257812882	0.8055040911371729	T	T	T
0.4320867885059065	0.3760770716683370	0.5749668198341402	T	T	T
0.4177160589233512	0.5077965348841562	0.5728115248846396	T	T	T
0.3906957578074411	0.6384432858013391	0.5612304257960308	T	T	T
0.1919862732772337	0.3638067798868794	0.6129103142430806	T	T	T
0.1789234606232289	0.4951555261010426	0.5723497283493179	T	T	T
0.1957387671462666	0.6284400044447283	0.5627650353929288	T	T	T
0.9841048594119211	0.4555884749702445	0.7881832316444984	T	T	T
0.9826926470123450	0.6380671508002100	0.7776428293578854	T	T	T
0.1433809311824037	0.5696923949608187	0.2192879984053667	T	T	T
0.1925351496383331	0.5554392397266688	0.3998113264706216	T	T	T
0.2968391476857861	0.5458783298539845	0.5232447270836389	T	T	T
0.3976881166833653	0.5680413479877997	0.3975714311446278	T	T	T
0.3981524218240367	0.5632700594649286	0.1996278764820222	T	T	T
0.2726148467310478	0.5442020010936458	0.2465213873114822	T	T	T
0.1467596266407802	0.3225101711343658	0.2433742530785133	T	T	T
0.1942313733786304	0.3595948697852148	0.4181865172094907	T	T	T
0.3082163915745806	0.3533376276830701	0.5174439428994613	T	T	T
0.4079897948959778	0.3309028502199678	0.3899559605927611	T	T	T
0.3958136184758939	0.3435710844727632	0.1918906062704675	T	T	T
0.2741831388184637	0.3533649294742826	0.2599127568920154	T	T	T

Structure files (CONTCAR) involved in this work:

0.1810243137350091	0.4493385970926759	0.2752368277866791	T	T	T
0.4103477655613735	0.4510804847741808	0.3073553541950425	T	T	T
0.0680539632489514	0.6250822561737959	0.0765147139764956	T	T	T
0.0795679728307730	0.4920371446672122	0.0842175465863205	T	T	T
0.1112659783633120	0.3635621539126861	0.0631082566185048	T	T	T
0.3050508157326102	0.6369000179697658	0.1125639506654507	T	T	T
0.3167758727658362	0.5062392077901445	0.0681297801554667	T	T	T
0.2956592168082410	0.3728730660439474	0.0652076144919878	T	T	T
0.5091977246782177	0.5400935455021191	0.2953747124820886	T	T	T
0.5119719413813437	0.3659503839291795	0.2771742713077514	T	T	T
0.4373320159911733	0.7511531200062754	0.6388308018089179	T	T	T
0.1904654095014976	0.7497983686560009	0.6374985496406280	T	T	T
0.2741354677837488	0.7509014850426355	0.0244119822026777	T	T	T
0.1066106359645393	0.7490636903577794	0.0466654287585609	T	T	T
0.0669447438534338	0.2478625116375700	0.1305994104271385	T	T	T
0.3067887414731776	0.2510031567597797	0.1375648586909862	T	T	T
0.2232322122543415	0.2501807103843505	0.5229593214099468	T	T	T
0.3927861948001841	0.2514692417005023	0.5459338241504537	T	T	T
0.5569413799790012	0.2507670977409217	0.3535820286277971	T	T	T
0.8077253924068217	0.2507926431079575	0.3479282443055273	T	T	T
0.7279052343863458	0.2503214100190194	0.9436749800156670	T	T	T
0.8924307777138336	0.2514042347350904	0.9466285046382681	T	T	T
0.9462420068543400	0.7545096383007671	0.8576357782360047	T	T	T
0.6845027210090294	0.7531598302832547	0.8524121362301378	T	T	T
0.7739589848424211	0.7478998664056742	0.4455237562711205	T	T	T
0.6083424896141510	0.7500899155771338	0.4511718579472746	T	T	T
0.9348860405191659	0.4854981951368165	0.5378578319841915	T	T	T
0.9316730345742136	0.4015678898877622	0.4449991018742415	T	T	T
0.8716051462203994	0.5562920350116189	0.5610958044087135	T	T	T
0.0288049834868611	0.6210611374059327	0.4633392054546219	T	T	T
0.0787743403852195	0.5589695204335283	0.4050738914455979	T	T	T
-0.0081004448439591	0.5445298355270515	0.4227238677711785	T	T	T
0.9618900696555712	0.4747032653937316	0.5970068675962165	T	T	T
0.9657428231252875	0.6398239830566399	0.3033636820165433	T	T	T
0.0528314412592673	0.6512095998786123	0.2817678808107180	T	T	T
0.0294028611093182	0.5825485210172637	0.4041559196428562	T	T	T
0.0145731028998253	0.6148784282167484	0.3050693113147042	T	T	T

Figure 4(a) Route(b-ii)-Zn ④

Si Al O Zn H C

1.0000000000000000		
20.0219999999999985	0.0000000000000000	0.0000000000000000
0.0000000000000000	19.8990000000000009	0.0000000000000000
0.0000000000000000	0.0000000000000000	13.3829999999999991
93	3	193
2	6	2

Selective dynamics

Direct

0.4247402562620565	0.0593715117031816	0.6496565531218057	T	T	T
0.3076107178229630	0.0305324333261743	0.7945029268366219	T	T	T
0.2844389483514430	0.0555330255925546	0.0186199900715033	T	T	T
0.1258229035941300	0.0609598301333821	0.0135797289267322	T	T	T
0.0705015226566736	0.0300575770293178	0.8031830760430307	T	T	T
0.1827800783045147	0.0637298169403631	0.6671765322640817	T	T	T

Structure files (CONTCAR) involved in this work:

0.4203786958730484	0.8270261960876569	0.6690206552518559	T	T	T
0.3037390884990527	0.8713153322166658	0.8038812129629985	T	T	T
0.2684383725492450	0.8303651736596936	0.0228990078025499	T	T	T
0.1133354894406955	0.8254627439747443	0.0145673795320578	T	T	T
0.0683108636236770	0.8734392057105099	0.8005486876892143	T	T	T
0.1821830587876169	0.8279745075827780	0.6675072197033322	T	T	T
0.0781208016109175	0.9398015860418217	0.1502380656486497	T	T	T
0.1963767634149815	0.9696664637098760	0.2928748343322101	T	T	T
0.2188578916844709	0.9431029161560630	0.5177002787740677	T	T	T
0.3787553196494481	0.9356186400228439	0.5142292420033938	T	T	T
0.4354614680894209	0.9680235809550731	0.3026966025788100	T	T	T
0.3221106205377092	0.9357616164869201	0.1668695509966232	T	T	T
0.0845088808408958	0.1717795586791824	0.1666752857228701	T	T	T
0.1982841249834927	0.1284563643405918	0.3049975833284118	T	T	T
0.2334564126611424	0.1689696015784220	0.5222977682450147	T	T	T
0.3887023345602614	0.1730009262873315	0.5107530122803606	T	T	T
0.4355180047433583	0.1264295189697969	0.2963439228197369	T	T	T
0.3183011274271842	0.1719450279610311	0.1682924352592522	T	T	T
0.5778341788295864	0.5558217392945423	0.3542310162980164	T	T	T
0.6909573812774403	0.5263099984324724	0.2038808323159652	T	T	T
0.7180537284400050	0.5677749640473878	0.9860024337653311	T	T	T
0.8750822770733935	0.5731024914104532	0.9901179732118098	T	T	T
0.8120822835063459	0.5495999084437995	0.3500183865366283	T	T	T
0.5754269938956067	0.3280370186813508	0.3297890367673912	T	T	T
0.6946733080296849	0.3716330471613102	0.1894299937060753	T	T	T
0.7334346217622763	0.3278050482417802	0.9756762264641414	T	T	T
0.8882598280444896	0.3242220171543282	0.9913168529357185	T	T	T
0.9445111055107014	0.3725403417146798	0.1851129503890708	T	T	T
0.9228771769215939	0.4463330729505706	0.8644822072936454	T	T	T
0.8054593392995405	0.4728078559523924	0.7184151985471334	T	T	T
0.7810885094768465	0.4378933820777888	0.4986253266789410	T	T	T
0.6232403547970830	0.4291394376653409	0.4878279906982044	T	T	T
0.5713482830733836	0.4689210869092544	0.6999192653008397	T	T	T
0.6804840958873918	0.4486344868865423	0.8525434841186674	T	T	T
0.9233150838113546	0.6771992291931922	0.8350489585105723	T	T	T
0.7717964712589255	0.6697616200050995	0.4654426648047841	T	T	T
0.6167206469751664	0.6729044308363235	0.4860179324191072	T	T	T
0.5634377167060701	0.6274392826141555	0.6966452748658412	T	T	T
0.6749702354952206	0.6720928972292890	0.8287495959569637	T	T	T
0.5803823031411350	0.9453627386115351	0.3586397988364471	T	T	T
0.7012721644291600	0.9735165669463377	0.2146494168033461	T	T	T
0.7215408089865902	0.9358045531446755	0.9938867383745492	T	T	T
0.8816674407318521	0.9332436468498438	0.9966391065844712	T	T	T
0.9335493014235852	0.9707115289097874	0.2060554780345969	T	T	T
0.8248227555400708	0.9469030466520831	0.3561065898260640	T	T	T
0.5784044556411858	0.1729086771316824	0.3300993291732806	T	T	T
0.7002710950916415	0.1322418393411271	0.1946673717964446	T	T	T
0.7337087040439031	0.1716539255992893	0.9724334909696185	T	T	T
0.8884254959107898	0.1727741173674512	0.9817451585721260	T	T	T
0.9369997514462843	0.1287974706671808	0.1961972134297442	T	T	T
0.8230514172895803	0.1742308257309924	0.3329059572643336	T	T	T
0.9254663977550115	0.0529955337174470	0.8570764605503606	T	T	T
0.8040388717827275	0.0256019541466655	0.7105874537992193	T	T	T

Structure files (CONTCAR) involved in this work:

0.7831931902255511	0.0669860676820652	0.4928899105239651	T	T	T
0.6226299557910315	0.0700780860098535	0.4910058660229983	T	T	T
0.5704733954151223	0.0309963877034393	0.6996303811286452	T	T	T
0.6802737568164862	0.0524270388637508	0.8512126739177005	T	T	T
0.9257962901006083	0.8303189354725105	0.8382383408221963	T	T	T
0.8048385788763162	0.8683557866673510	0.6965234644482651	T	T	T
0.7722421151594990	0.8266780241101089	0.4789104834272327	T	T	T
0.6173212985508919	0.8265444056341874	0.4897021853653700	T	T	T
0.5659034194813449	0.8739436613564704	0.6976688230927609	T	T	T
0.6804814870741877	0.8315347458892270	0.8330561355515403	T	T	T
0.4258223890892133	0.4418062369863197	0.6422604473561211	T	T	T
0.3062188749100917	0.4696215837832078	0.7839011410239932	T	T	T
0.2834533977864373	0.4429661332570803	0.0091188012978185	T	T	T
0.1253569216879428	0.4376621552141466	0.0148769630309885	T	T	T
0.0673538982982386	0.4695675179269593	0.8032163982381832	T	T	T
0.1771452908003635	0.4384028633471073	0.6572826726883372	T	T	T
0.4181861621890473	0.6735671123345693	0.6630614072214683	T	T	T
0.3032428843848283	0.6280467456705330	0.7994152217485788	T	T	T
0.2692556688721043	0.6692891757295476	0.0199966231146539	T	T	T
0.1145317558759252	0.6713227432744272	0.0118265730888005	T	T	T
0.0665331318341400	0.6284374432525341	0.7983476819505604	T	T	T
0.1807411754168225	0.6706968761477208	0.6636639314339391	T	T	T
0.0744743217425347	0.5581403482650574	0.1517350926557237	T	T	T
0.1962618038678345	0.5287875492419040	0.2848898520048845	T	T	T
0.2159332406645059	0.5566729928044873	0.5142297340437499	T	T	T
0.3743806374010775	0.5645223618230679	0.5145051731168017	T	T	T
0.4277710445750572	0.5282879279388107	0.3043572776487033	T	T	T
0.3237398108635440	0.5598208346575119	0.1542540173714186	T	T	T
0.0891086582757990	0.3240469062515775	0.1593877049644919	T	T	T
0.1992450973479591	0.3710121601368898	0.2998858393187553	T	T	T
0.2322804085713366	0.3301401271086012	0.5191819394457278	T	T	T
0.3871136735608617	0.3266431030850691	0.5060850839979885	T	T	T
0.4322068511381694	0.3714599675447746	0.2933066330439036	T	T	T
0.3185320032235163	0.3294762875973150	0.1622685735458388	T	T	T
0.9271144261406821	0.5279743876169793	0.1945377886207160	T	T	T
0.8231294526445591	0.3354689925485123	0.3244361804373539	T	T	T
0.8021051119010300	0.6341774784815032	0.6961916597459403	T	T	T
0.0090528250442696	0.5525479818590673	0.2210214864888771	T	T	T
0.3613379577530884	0.0688368784276650	0.7239501553454329	T	T	T
0.3193612624168863	0.0538686242866711	0.9091645567185151	T	T	T
0.2047128393639064	0.0434986602586243	0.0075151901392028	T	T	T
0.0947827880997719	0.0696235194208193	0.9027421472505293	T	T	T
0.1060135312660492	0.0631781129752679	0.7058921905720379	T	T	T
0.2319318796066910	0.0504247904993878	0.7620619088699090	T	T	T
0.3626951807884655	0.8267619279917261	0.7542431186515168	T	T	T
0.3043214273938783	0.8592358839294831	0.9231761436709004	T	T	T
0.1901272214423362	0.8520891148663873	0.0221774438165479	T	T	T
0.0886764380445874	0.8311513587290030	0.8996175292514533	T	T	T
0.1053966572607303	0.8405237324432504	0.7036283286823437	T	T	T
0.2314564481113340	0.8487919389092426	0.7593797668517906	T	T	T
0.3179186975835667	0.9500007533224082	0.7796874158348989	T	T	T
0.0917441464175863	0.9512181064209293	0.8129921938973483	T	T	T
0.4345912444155537	0.1273683909389210	0.5839613159533148	T	T	T

Structure files (CONTCAR) involved in this work:

0.4143685523782226	0.9963884746639674	0.5744177020267838	T	T	T
0.3931778339251377	0.8647047508091370	0.5695886965385278	T	T	T
0.1984458871494175	0.1373036215349263	0.6206204195713646	T	T	T
0.1918949013102184	0.0054261980270374	0.5838880550454408	T	T	T
0.1982756669985484	0.8718458556186939	0.5682392932708923	T	T	T
0.9904798557405903	0.0375607701648032	0.7884736410622487	T	T	T
0.9877881732702339	0.8700082869520119	0.7848687010483214	T	T	T
0.1427040286657157	0.9311137935803010	0.2225245040050423	T	T	T
0.1846962053540309	0.9471588385850737	0.4079204825861662	T	T	T
0.2992021320878077	0.9491976873908275	0.5079789161819266	T	T	T
0.4103193061524702	0.9305969737120093	0.4034765322050268	T	T	T
0.3984990685878074	0.9343702905649106	0.2070825098901635	T	T	T
0.2720761201392678	0.9498547016936733	0.2606064955157251	T	T	T
0.1393367008001845	0.1731796212135558	0.2559742620012278	T	T	T
0.1959768763393449	0.1388483331356921	0.4247340715595511	T	T	T
0.3116692647708337	0.1472354808988082	0.5179721389655507	T	T	T
0.4142964218417222	0.1673196947335580	0.3963886764510402	T	T	T
0.3954961629436352	0.1578838796741724	0.2010436359434598	T	T	T
0.2708404906131553	0.1523277679441237	0.2630688421381900	T	T	T
0.1852931728932783	0.0500258005660184	0.2776164430388589	T	T	T
0.4165852354913890	0.0475130555975890	0.3095049181990381	T	T	T
0.0668116721085652	0.8705627291460764	0.0878852399300388	T	T	T
0.0874408178102905	0.0005795110816022	0.0707519003913729	T	T	T
0.1144595532313874	0.1311218329880551	0.0719125710328339	T	T	T
0.3054055426931677	0.8628691037573113	0.1189748448992243	T	T	T
0.3155263825214082	0.9950245949780610	0.0845046556571535	T	T	T
0.2991309192770041	0.1277669620510599	0.0704767305424143	T	T	T
0.5152302430173380	0.9570811200639312	0.2886025137323320	T	T	T
0.5154971211043096	0.1340571855511153	0.2782564524171630	T	T	T
0.6330602731443523	0.5641964006205369	0.2668094944224672	T	T	T
0.7069281400804712	0.5712757109660807	0.1061713201494403	T	T	T
0.7968076079061830	0.5627571766389077	0.9575283014603421	T	T	T
0.8839921500964345	0.5765639188226220	0.1090039753672443	T	T	T
0.8862117950039790	0.5251193741816109	0.3159178850396217	T	T	T
0.7572382670612068	0.5218983585970801	0.2742205169979677	T	T	T
0.6398324764976744	0.3326613064520759	0.2579555168437414	T	T	T
0.6922999197705897	0.3375460612352328	0.0788234062325330	T	T	T
0.8111301260831580	0.3499590950657285	0.9918673753974588	T	T	T
0.9160007373114887	0.3176878740422262	0.1054865670291851	T	T	T
0.9086030181723390	0.3568148747708944	0.2947329727506305	T	T	T
0.7676393301522990	0.3665699460574046	0.2382985028374526	T	T	T
0.6700191334581900	0.4498606886451025	0.1774240503463366	T	T	T
0.9266348673060733	0.4465205410645319	0.1500515461415161	T	T	T
0.5706677929651240	0.6264842598111666	0.4140309996926510	T	T	T
0.5987294128757136	0.4976101392326884	0.4336231348607452	T	T	T
0.5895760114409712	0.3635293168386554	0.4376152042125251	T	T	T
0.8061033225853367	0.6301622148334448	0.3702544864417911	T	T	T
0.8012581491679115	0.5166360946143282	0.4648922753082648	T	T	T
0.8296367248887289	0.3905848760575996	0.4311593108316266	T	T	T
0.0241100117491835	0.3620878216538639	0.2039567999295233	T	T	T
0.8580836950719603	0.4363450069210975	0.7919815092956077	T	T	T
0.7985754245976677	0.4291207719044638	0.6155426856660056	T	T	T
0.7041078535554179	0.4232130157393130	0.4733181460192751	T	T	T

Structure files (CONTCAR) involved in this work:

0.6051106504237952	0.4299786449308775	0.6054337477487768	T	T	T
0.6067276656688850	0.4442886638620352	0.8026048374336961	T	T	T
0.7323316068250241	0.4779585550264581	0.7687265020750610	T	T	T
0.8634072546414371	0.6781606471898413	0.7562350684384721	T	T	T
0.8148505946710862	0.6478462131791162	0.5644862217477333	T	T	T
0.6943105082297423	0.6468444408938441	0.4793076020718010	T	T	T
0.5902117625813164	0.6685640494084730	0.5997104730535013	T	T	T
0.5969468358284640	0.6593794378082405	0.7963459307922091	T	T	T
0.7228591003630428	0.6439899051327451	0.7412005455345456	T	T	T
0.8320769318724617	0.5482241413453849	0.6870809551098138	T	T	T
0.5829651836132435	0.5487834923323824	0.6833056688971815	T	T	T
0.9332455905908350	0.3771357379429163	0.9274766969930309	T	T	T
0.9157356124035245	0.5104212822257546	0.9378548568483787	T	T	T
0.9034802034656828	0.6422111648952734	0.9405247232177391	T	T	T
0.7018188635793596	0.3737171012180179	0.8872465744758995	T	T	T
0.6797901144844255	0.5003212089737579	0.9463085126916357	T	T	T
0.6867672021731126	0.6347664645041604	0.9358585745490988	T	T	T
0.4925259959151340	0.4506969290145165	0.7096666366329177	T	T	T
0.4827498928613334	0.6334996791422152	0.7057756423504944	T	T	T
0.6459426392952965	0.9410511066088333	0.2884035966954500	T	T	T
0.7009927043637222	0.9313935084773014	0.1108670221721363	T	T	T
0.8019418618681531	0.9434687742147349	0.9811124082623308	T	T	T
0.9007356316673696	0.9283874809896894	0.1142067053016897	T	T	T
0.9002039457698117	0.9488757174528230	0.3117375737476768	T	T	T
0.7742920513449775	0.9669472501091735	0.2660562997365998	T	T	T
0.6414310747217146	0.1708522793461453	0.2546694523681469	T	T	T
0.6997219491110218	0.1601584173613354	0.0810244885342187	T	T	T
0.8112888100779987	0.1469972699792294	0.9762437199548250	T	T	T
0.9135987854145968	0.1685181700547613	0.0964203504237299	T	T	T
0.8990116947741086	0.1586189518915904	0.2936474707884416	T	T	T
0.7720952762803739	0.1463495458880397	0.2464408002016237	T	T	T
0.6845184755452298	0.0520593037350167	0.1942915155433805	T	T	T
0.9200786960648352	0.0495833012984927	0.1831516716564460	T	T	T
0.5723026142046449	0.8748766121940490	0.4191742301036884	T	T	T
0.5856437832504661	0.0061124996804506	0.4395046106001705	T	T	T
0.5978455283149031	0.1386594921246323	0.4366660408983428	T	T	T
0.8113253988041882	0.8712434396740356	0.3966497377155176	T	T	T
0.8175544980577995	0.9992780194000650	0.4482066618922728	T	T	T
0.8106745740259153	0.1333156203154936	0.4368590480842228	T	T	T
0.0126855006061515	0.9546839110520757	0.2177329209127677	T	T	T
0.0170740470909522	0.1377399810229727	0.2107568019512266	T	T	T
0.8602415442222586	0.0543603704509609	0.7859376242919790	T	T	T
0.8028347609407963	0.0717674945723620	0.6105169312047553	T	T	T
0.7026889181536612	0.0610776479641953	0.4784154605245636	T	T	T
0.6021878678706256	0.0747646047182075	0.6082757947785817	T	T	T
0.6054220714958449	0.0501099176986168	0.8051088637236311	T	T	T
0.7314481235157211	0.0288601159959408	0.7638698668636612	T	T	T
0.8617908263329871	0.8339773209495064	0.7647139223696379	T	T	T
0.8071649352894800	0.8316671027727462	0.5880675148683175	T	T	T
0.6949406677395491	0.8515149803067094	0.4861436650852490	T	T	T
0.5907681808116587	0.8281938495434130	0.6041216995339870	T	T	T
0.6047689633547161	0.8509878419417936	0.7986451331197445	T	T	T
0.7316306276839186	0.8580845725033880	0.7466147605113792	T	T	T

Structure files (CONTCAR) involved in this work:

0.8201740401998306	0.9478956420514161	0.6819278890857062	T	T	T
0.5819102636668335	0.9521089672732296	0.6726167141121988	T	T	T
0.9343356368268542	0.1260954130650410	0.9097784658343379	T	T	T
0.9196815270877671	0.9964860482029757	0.9446115743267358	T	T	T
0.9065827607864089	0.8638839027893198	0.9451026574838830	T	T	T
0.6949202290340425	0.1286838121160646	0.8875304279908323	T	T	T
0.6856543290129796	0.0016545870836530	0.9459520014028426	T	T	T
0.6968368539307801	0.8674753810728458	0.9392139498759445	T	T	T
0.4916461865220650	0.0470168381726362	0.7149709469210248	T	T	T
0.4861511288648495	0.8638442263792594	0.7145334468928716	T	T	T
0.3609172842247859	0.4321803739487320	0.7138016595624656	T	T	T
0.3114909039167101	0.4388870772501028	0.8956228784407565	T	T	T
0.2037624996885379	0.4588714985122629	0.0106522048897669	T	T	T
0.0954239320390133	0.4332787219789504	0.9025899456265644	T	T	T
0.1021067322651915	0.4368711825232472	0.7042831114829787	T	T	T
0.2305135177759727	0.4575519905228932	0.7439590401605432	T	T	T
0.3599263358706034	0.6740311519078410	0.7472401749977948	T	T	T
0.3035280910005494	0.6437571534840610	0.9173820772848981	T	T	T
0.1915287261658812	0.6458110504734645	0.0214215760359915	T	T	T
0.0925235844353690	0.6692505999549379	0.8952338324992707	T	T	T
0.1036925821058697	0.6584820639557520	0.6992161085163235	T	T	T
0.2300084506309993	0.6451456418205387	0.7528229341472996	T	T	T
0.3220058844199257	0.5496602855951359	0.7811727014823300	T	T	T
0.0849132506194406	0.5492031980899773	0.8082534036406167	T	T	T
0.4345995129699215	0.3755668652371884	0.5722174145894644	T	T	T
0.4185744000312919	0.5073588290084584	0.5703426834184209	T	T	T
0.3900604870857901	0.6378542323914611	0.5620492148149948	T	T	T
0.1940797301945286	0.3643331544508179	0.6133384264383080	T	T	T
0.1774165805030883	0.4949784930715684	0.5694091754008762	T	T	T
0.1938969474892715	0.6284739833419839	0.5616567121633224	T	T	T
0.9873610220825987	0.4574854401470547	0.7912399678056097	T	T	T
0.9865991327409946	0.6368714035007645	0.7838422316040594	T	T	T
0.1412496073342168	0.5691658792207924	0.2200782040279117	T	T	T
0.1934144940956255	0.5568103575150486	0.3984410191055051	T	T	T
0.2958244127267655	0.5455585814365785	0.5272943995426826	T	T	T
0.3941653886478552	0.5679486765658308	0.3975767573434172	T	T	T
0.3984039332204091	0.5595576152244471	0.2013970771113461	T	T	T
0.2710150181984007	0.5404264653215511	0.2419994000389609	T	T	T
0.1456029649080944	0.3223163406193975	0.2461671326687423	T	T	T
0.1963371865887946	0.3570648624956327	0.4185746488590688	T	T	T
0.3103107781180761	0.3528338537436619	0.5174999737442306	T	T	T
0.4093360575059795	0.3271502177425599	0.3895493702213867	T	T	T
0.3961334182544362	0.3429392565026203	0.1928403621611889	T	T	T
0.2733969381036782	0.3543852033682895	0.2570134230954168	T	T	T
0.1790313608680413	0.4488640885085420	0.2793834492065367	T	T	T
0.4098538012994806	0.4488175406508824	0.3134176696418891	T	T	T
0.0668963215778801	0.6232359356803254	0.0780667493638336	T	T	T
0.0841437392312186	0.4918138940188243	0.0807462149076614	T	T	T
0.1179176366393653	0.3627237830226592	0.0616795897252367	T	T	T
0.3083936593705823	0.6347970941783393	0.1127290475188389	T	T	T
0.3212670948176374	0.5045388886367207	0.0650164171796729	T	T	T
0.2988274501792846	0.3713138799070554	0.0624872993312118	T	T	T
0.5077174311358106	0.5376287875947032	0.3020842028382151	T	T	T

Structure files (CONTCAR) involved in this work:

0.5123372404818133	0.3656340859987326	0.2767799920144835	T	T	T
0.4383306268054404	0.7504483859469463	0.6372573459530109	T	T	T
0.1929268982503039	0.7494252744154895	0.6387713781670543	T	T	T
0.2756855758744618	0.7497673868979206	0.0294683820295436	T	T	T
0.1081273613844025	0.7480856526415702	0.0513203426517557	T	T	T
0.0699692834769284	0.2477860652031842	0.1285927905539188	T	T	T
0.3072896230225238	0.2503325590778858	0.1390942766038612	T	T	T
0.2256942973278297	0.2496488717299757	0.5277521977249686	T	T	T
0.3939077634286830	0.2504677664315978	0.5476747679900634	T	T	T
0.5572770363034372	0.2501530636963356	0.3518908290123673	T	T	T
0.8133981582191414	0.2527137299646635	0.3541432938179491	T	T	T
0.7288757427961818	0.2500308844803590	0.9401310722682287	T	T	T
0.8940757122669081	0.2498347808296354	0.9418375393625368	T	T	T
0.9479877187967135	0.7534963095171586	0.8591865141179400	T	T	T
0.6874289032139671	0.7515948798346468	0.8482496841650351	T	T	T
0.7772543001316553	0.7490429029782162	0.4418090143124694	T	T	T
0.6120318159274113	0.7501051978913579	0.4479430583188787	T	T	T
0.9318260679550165	0.4797766593035297	0.5257792062887897	T	T	T
0.9224067804192786	0.4326452623865812	0.3966133780745217	T	T	T
0.8829631647487147	0.5649760772201354	0.5557207949978910	T	T	T
-0.0350617602387321	0.6685698117578943	0.6022401077064234	T	T	T
0.0167158123335721	0.5942622427746527	0.5691401677915092	T	T	T
1.0001253422095666	0.4428128084006673	0.3697876034569250	T	T	T
0.9718676364516946	0.4689821787795043	0.5641548214413324	T	T	T
-0.0694621226380939	0.6790423739985002	0.4233747904742829	T	T	T
-0.0178384320832723	0.6044431708588177	0.3909048544791431	T	T	T
-0.0196173703302825	0.6321213256635260	0.5457704101310517	T	T	T
-0.0370140167859987	0.6382800236550796	0.4485451790820462	T	T	T

Figure 4(b) Route(a)-Cu ①

Si O Al Cu C H

1.0000000000000000

20.0219993591000005 0.0000000000000000 0.0000000000000000

0.0000000000000000 19.8990001678000006 0.0000000000000000

0.0000000000000000 0.0000000000000000 13.3830003737999998

93 195 3 3 2 7

Selective dynamics

Direct

0.4228167551894634	0.0545020086035881	0.6382603212405609	T	T	T
0.3024221388419872	0.0262866167870042	0.7821838410436620	T	T	T
0.2804628500591627	0.0636752180902226	0.0025246283431977	T	T	T
0.1209916290630737	0.0654459388298675	0.0033384210301446	T	T	T
0.0715310631062978	0.0294478517093998	0.7930131313848138	T	T	T
0.1787483937592559	0.0525741793575414	0.6419270728736717	T	T	T
0.4221075748246522	0.8265818105714996	0.6625205667818591	T	T	T
0.3029581621670490	0.8687088837761767	0.8021210168058026	T	T	T
0.2681407827660470	0.8284957335772265	0.0226968843731640	T	T	T
0.1135835080133060	0.8261849223072880	0.0128127762844632	T	T	T
0.0658905822605980	0.8738162320554018	0.8012579379447536	T	T	T
0.1791927271782487	0.8279595104920058	0.6671152727635405	T	T	T
0.0770237791447687	0.9448534662101742	0.1416302597994630	T	T	T
0.1982547897869203	0.9727428363253121	0.2867523851066728	T	T	T
0.2180840760613201	0.9330908643108800	0.5057095329255947	T	T	T

Structure files (CONTCAR) involved in this work:

0.3774425920934740	0.9304108302162098	0.5069251066137497	T	T	T
0.4288050494183517	0.9700053945078585	0.2977182232703774	T	T	T
0.3216965473720467	0.9477160069377233	0.1447750163460558	T	T	T
0.0778527743574523	0.1695097502766782	0.1612828609015964	T	T	T
0.1966170087851964	0.1293034161630437	0.3038157852870464	T	T	T
0.2323663827927870	0.1726707332192281	0.5197789600945182	T	T	T
0.3866905874693262	0.1732530365869229	0.5065616173249670	T	T	T
0.4341047253358170	0.1271995543104553	0.2964194197443175	T	T	T
0.3177848676699112	0.1684660700054101	0.1642379441950141	T	T	T
0.5746619518590484	0.5558750300176145	0.3552511613321190	T	T	T
0.6952227190564637	0.5303419915087098	0.2169985168258982	T	T	T
0.7144176086645121	0.5500902151676476	0.9851346910668578	T	T	T
0.8725320166132855	0.5684536058642116	0.9956430412825614	T	T	T
0.9290919459541729	0.5229401075259411	0.2019256868953096	T	T	T
0.8192477784544089	0.5605603673983355	0.3458082525949285	T	T	T
0.5798306257171573	0.3254477059123259	0.3303680571124484	T	T	T
0.7042877846192042	0.3718322798597107	0.2105611747612615	T	T	T
0.7310134027938031	0.3276371309221009	0.9910363601003530	T	T	T
0.8881608939641841	0.3278236527710725	0.9960277820113573	T	T	T
0.9366264810197739	0.3660853707740725	0.2064654885833369	T	T	T
0.8253910829921228	0.3282449461588057	0.3471265136818010	T	T	T
0.9239611694651240	0.4475955938338576	0.8635610777418299	T	T	T
0.8033828247211160	0.4665660843291423	0.7226916692790389	T	T	T
0.7801288366644533	0.4426745850499972	0.4971512003480434	T	T	T
0.6199165324785054	0.4300118646611406	0.4919156510613790	T	T	T
0.5627447362288752	0.4640251076992241	0.7021996946429664	T	T	T
0.6764228116515175	0.4284039741970839	0.8403861983802191	T	T	T
0.7953674926610333	0.6240767615779133	0.7145731532827541	T	T	T
0.6121617545952217	0.6698872414472213	0.4873942437585031	T	T	T
0.5605929387754932	0.6217914229890198	0.6990994423941168	T	T	T
0.6687499985504699	0.6666759939538509	0.8344529794904966	T	T	T
0.5750933737110713	0.9399934383879266	0.3509315171549406	T	T	T
0.6935589869058789	0.9711601238962654	0.2084102626059783	T	T	T
0.7192386133122785	0.9515029141518129	0.9849208893381448	T	T	T
0.8766739181108462	0.9450573714638268	0.9814397947311476	T	T	T
0.9327741614672875	0.9680280846963369	0.1929774074264355	T	T	T
0.8176358240475522	0.9302642547075541	0.3263377730405508	T	T	T
0.5802022742706774	0.1707313530957339	0.3199565822031533	T	T	T
0.7021131026703740	0.1275719172253673	0.2008902937179755	T	T	T
0.7348032766996287	0.1676137520130065	0.9812618148418085	T	T	T
0.8920115282814852	0.1765495369616949	0.9754007413992921	T	T	T
0.9333303823329148	0.1259211791283897	0.1943527997406186	T	T	T
0.8226887965149265	0.1738165010350538	0.3381967959259259	T	T	T
0.9257167057001345	0.0631604473015615	0.8401486689466775	T	T	T
0.8055798389644276	0.0306116692718193	0.7033074726219184	T	T	T
0.7838861355827133	0.0526812969407221	0.4758578313729488	T	T	T
0.6237718329239709	0.0652745178980319	0.4804299248053721	T	T	T
0.5676435146687903	0.0337945450896440	0.6906492537288721	T	T	T
0.6814957287439272	0.0666543118434107	0.8279664257792424	T	T	T
0.9181762731060767	0.8348943335033696	0.8250960965437142	T	T	T
0.8007790243817459	0.8738875258932288	0.6978889881143989	T	T	T
0.7672916350137075	0.8333714179308412	0.4834643461412728	T	T	T
0.6117741676986147	0.8255363248062668	0.4888596947713437	T	T	T

Structure files (CONTCAR) involved in this work:

0.5658909416224395	0.8757196806056775	0.7020630068790409	T	T	T
0.4189976744911884	0.4438869567152611	0.6465819927954012	T	T	T
0.2984049360751101	0.4729598479213549	0.7883757420803339	T	T	T
0.2799498352117326	0.4348005107954433	0.0100049762061873	T	T	T
0.1212595263149975	0.4318497790802634	0.0102431705773793	T	T	T
0.0699244595444513	0.4694427072156264	0.8003247000363447	T	T	T
0.1755279922463085	0.4460777890447579	0.6480521819254745	T	T	T
0.4179503200593808	0.6713937068212825	0.6605730879725515	T	T	T
0.3001815513365339	0.6298700273515611	0.8028546730274744	T	T	T
0.2684135544293863	0.6720786668024504	0.0238741667234684	T	T	T
0.1148210022829091	0.6720787478375917	0.0119057248476224	T	T	T
0.0625678932498032	0.6272975275002870	0.8013160725124771	T	T	T
0.1772089932775093	0.6690455361657337	0.6663360944051456	T	T	T
0.0739066391946951	0.5544186772125852	0.1416962164153760	T	T	T
0.1955964947971264	0.5265363785457380	0.2844307829324045	T	T	T
0.2148114893909839	0.5629132478061284	0.5071992567044026	T	T	T
0.3741860026355530	0.5654221454242278	0.5092370959915815	T	T	T
0.4282213102276130	0.5258832096773178	0.2995466820370939	T	T	T
0.3222524062936357	0.5536776340240669	0.1461609073219180	T	T	T
0.0802579539884238	0.3240151267583717	0.1638514253037789	T	T	T
0.1977465978926302	0.3681194697211964	0.3035550473514207	T	T	T
0.2323199488515193	0.3286208552823813	0.5229617399537694	T	T	T
0.3870196409032227	0.3258800067437700	0.5114421731804153	T	T	T
0.4358735897328719	0.3687498140620116	0.2986186232814227	T	T	T
0.3195058027673017	0.3270807576204416	0.1680551935962388	T	T	T
0.3572992652177320	0.0599464074949423	0.7088496688980820	T	T	T
0.3004746293942780	0.0691734107150316	0.8854807346129221	T	T	T
0.2005094594468938	0.0529945719738533	0.0166924736947495	T	T	T
0.1009537964710234	0.0724509285909733	0.8866277689383665	T	T	T
0.1041533185349432	0.0541343889661569	0.6885187963177960	T	T	T
0.2296078978626647	0.0290425420369068	0.7296133146705652	T	T	T
0.3593545489389194	0.8290301740524015	0.7392100388439522	T	T	T
0.3033216543316228	0.8391588106900668	0.9149250864941655	T	T	T
0.1904220602290487	0.8524841739741448	0.0166119879472040	T	T	T
0.0866568636671907	0.8303466560221098	0.8992072505071989	T	T	T
0.1026131575549825	0.8411722161634154	0.7038956087317882	T	T	T
0.2296586807326673	0.8572403079008777	0.7522734693390362	T	T	T
0.3208006691718043	0.9483409623129418	0.8049309258760219	T	T	T
0.0901035088039163	0.9512703205488181	0.8151198625090683	T	T	T
0.4316026562718485	0.1236447255384380	0.5747844429005754	T	T	T
0.4171560494434528	0.9919627950492224	0.5603676995593023	T	T	T
0.4003741448540033	0.8594861014008448	0.5558149226369863	T	T	T
0.1955299763592216	0.1278242274114589	0.6037695850010154	T	T	T
0.1810556228000173	0.9996800140326797	0.5494613117647262	T	T	T
0.1917191862284978	0.8653707280339924	0.5606816063872111	T	T	T
0.9921081004030804	0.0418008601059331	0.7794393252868643	T	T	T
0.9856963447967435	0.8739496275405861	0.7881611130197756	T	T	T
0.1426001959966803	0.9420897547576581	0.2119553240852264	T	T	T
0.2008438559482813	0.9270469852870659	0.3873290665697700	T	T	T
0.2978766732316505	0.9417436530767325	0.5240002190370546	T	T	T
0.3946334168176175	0.9279146178789115	0.3885657195820042	T	T	T
0.3963098489528519	0.9485307249228473	0.1914023369845557	T	T	T
0.2702795345152309	0.9717962021103107	0.2316706045397412	T	T	T

Structure files (CONTCAR) involved in this work:

0.1396824302276838	0.1661063847117753	0.2384027558479952	T	T	T
0.1956931189408034	0.1648722400920809	0.4124236722038434	T	T	T
0.3094473358432772	0.1477073287083238	0.5092155951183407	T	T	T
0.4129587807809138	0.1730366942471037	0.3918303751498145	T	T	T
0.3947474041677915	0.1540229411812111	0.1975649082884467	T	T	T
0.2693025248369900	0.1384028680324299	0.2512745042586147	T	T	T
0.1796692567725613	0.0499034100711437	0.3152433291456044	T	T	T
0.4154314904119358	0.0494275648602015	0.3195288279794879	T	T	T
0.0681665672013212	0.8723502540052340	0.0865954161122801	T	T	T
0.0820388272241863	0.0028952428545474	0.0560027915076114	T	T	T
0.0986608724519122	0.1352967167861646	0.0559188065851735	T	T	T
0.3056306511465204	0.8718595152468542	0.1081277595974790	T	T	T
0.3183136598350116	0.9989862616128405	0.0503785855274429	T	T	T
0.3029010710866392	0.1328243148048391	0.0574887081046788	T	T	T
0.5076189988689329	0.9538449960552001	0.2875436893222195	T	T	T
0.5139294035108287	0.1334645763136238	0.2770170974310868	T	T	T
0.6345047484660195	0.5668692102927900	0.2741863091852889	T	T	T
0.6873865504786119	0.5445438277942360	0.0983666234794461	T	T	T
0.7946996906712132	0.5484815416567040	0.9787062622733582	T	T	T
0.8915206659314084	0.5630896346497349	0.1132374047042135	T	T	T
0.8940371586384690	0.5446790390755833	0.3072989775478025	T	T	T
0.7660870718203940	0.5626704403267069	0.2547790172148474	T	T	T
0.6427214475084221	0.3288298243029958	0.2543247068565965	T	T	T
0.7031176037912602	0.3646421677771309	0.0905922971505916	T	T	T
0.8096715945204591	0.3469276607449576	0.9819085060373643	T	T	T
0.9079555281948231	0.3221424607391774	0.1137491862207035	T	T	T
0.9017082747106232	0.3416752778632747	0.3096345791187398	T	T	T
0.7749258694403428	0.3448577441838323	0.2545075067858006	T	T	T
0.6955118298986390	0.4505294769793965	0.2415812671694264	T	T	T
0.9173249165076945	0.4439413668960984	0.1837429819966317	T	T	T
0.5619940996486680	0.6238803874184627	0.4189979841908475	T	T	T
0.5925186924427853	0.4940774213366830	0.4297357126004261	T	T	T
0.6008493305415938	0.3606237379677227	0.4351455076131098	T	T	T
0.8229756344782556	0.6396703535773879	0.3923331650542590	T	T	T
0.7963876463379537	0.5108449318650271	0.4331690497641345	T	T	T
0.8101958551674844	0.3770751836271308	0.4413524167627347	T	T	T
0.0068724858412093	0.5442923172037381	0.2093888656075397	T	T	T
0.0169766125039116	0.3605045145769400	0.2180893012092171	T	T	T
0.8608893527837437	0.4313531758494184	0.7909865895210684	T	T	T
0.8159061896475606	0.4498199299184303	0.6050935712083774	T	T	T
0.7001075128046763	0.4359909852090548	0.5062616352982162	T	T	T
0.5848361826000228	0.4262323705183167	0.6002507258600766	T	T	T
0.6011651996937467	0.4294671636651327	0.7961648809172631	T	T	T
0.7302324081843177	0.4358334800310206	0.7504209351740325	T	T	T
0.8439058731721799	0.6711037179065198	0.7772502734405242	T	T	T
0.8034347529393803	0.6289565882051554	0.5960976172183768	T	T	T
0.6875766736527295	0.6442352729610378	0.4696424910250152	T	T	T
0.5896590112465878	0.6626221464125318	0.6043476163542379	T	T	T
0.5919904023114553	0.6533302274825552	0.8023104773656209	T	T	T
0.7172481445319107	0.6434228235555716	0.7457624912926888	T	T	T
0.8055446932495630	0.5455550130833636	0.7484416302869019	T	T	T
0.5823347968447774	0.5431121743152989	0.6935184632581763	T	T	T
0.9325937203763786	0.3857161768756831	0.9425058361196108	T	T	T

Structure files (CONTCAR) involved in this work:

0.9159642911686270	0.5174137551243688	0.9273120117835308	T	T	T
0.8906678381515011	0.6471632120564548	0.9683903351247787	T	T	T
0.6892023532179576	0.3576634024213333	0.8973771529971160	T	T	T
0.6829986392606592	0.4912403827211547	0.9181968550859346	T	T	T
0.6854746985735916	0.6235289540381731	0.9414524748225085	T	T	T
0.4830065140047582	0.4551035625419321	0.7194891730428857	T	T	T
0.4800093573510755	0.6282622918828588	0.7064853132518972	T	T	T
0.6364353504402493	0.9327072029749953	0.2719247785681775	T	T	T
0.6792998087988906	0.9634566085058914	0.0892421695866493	T	T	T
0.7987092927033513	0.9632878673560866	0.0045425317965739	T	T	T
0.9142471490346232	0.9326257413414344	0.0871408354931938	T	T	T
0.8936130139616796	0.9307295448027298	0.2833967640027986	T	T	T
0.7660709842383728	0.9374204772744928	0.2318516598932402	T	T	T
0.6358134149642602	0.1698898183911592	0.2311302690251949	T	T	T
0.7113031188748430	0.1273922317907361	0.0807569485606389	T	T	T
0.8139235913287552	0.1554789558416354	0.9615535249801238	T	T	T
0.9131412110402912	0.1627921927456104	0.0905292780856633	T	T	T
0.8960331589829374	0.1618978716004371	0.2882989289470594	T	T	T
0.7672150942144979	0.1624210197086897	0.2509931561407965	T	T	T
0.6942296614343052	0.0504443684778736	0.2397691703568954	T	T	T
0.9117613931526113	0.0471657974620459	0.1898486305737752	T	T	T
0.5651693521017443	0.8719318840694616	0.4162863782883659	T	T	T
0.5873079671315931	0.0027369891621739	0.4259353645506798	T	T	T
0.6093549092874345	0.1342443705802968	0.4191323905209909	T	T	T
0.8056909082350847	0.8593859084599926	0.3825643806392641	T	T	T
0.8072996284088172	0.9934946422773302	0.4009181652075862	T	T	T
0.8100603203353337	0.1243070621189104	0.4321331912185097	T	T	T
0.0124528729617567	0.9589099723418768	0.2121698446985514	T	T	T
0.0136267745561423	0.1320185307026581	0.2107764438840308	T	T	T
0.8639365068250942	0.0707221052248184	0.7631358942602854	T	T	T
0.8173776696448054	0.0414682963515278	0.5847236316058204	T	T	T
0.7034043050234451	0.0522864207217850	0.4864908852154626	T	T	T
0.5927527018594744	0.0737800046017697	0.5914165669244200	T	T	T
0.6054556701905142	0.0657186360535131	0.7872537906370224	T	T	T
0.7333300721884035	0.0621732026917879	0.7345727768691452	T	T	T
0.8684986941357083	0.8334176508107199	0.7292275765244253	T	T	T
0.7969463540511443	0.8764786940302173	0.5766270642641529	T	T	T
0.6880594110535950	0.8510670294121292	0.4721738026144444	T	T	T
0.5906592564075120	0.8319382266307773	0.6054312051097717	T	T	T
0.6008297544957228	0.8520246926338496	0.8040715065100421	T	T	T
0.7364553894736461	0.8393960995553144	0.7467792889159197	T	T	T
0.8085466965421860	0.9521858457619888	0.7359576435541765	T	T	T
0.5836816936734424	0.9544483490392794	0.6781856498311867	T	T	T
0.9376577052704682	0.1344029726743955	0.8973159814634971	T	T	T
0.9116466897304137	0.0077923619234903	0.9264457230481120	T	T	T
0.8814823594723101	0.8772099462758668	0.9156277127004208	T	T	T
0.6930603791385395	0.1367491574951767	0.8882329201129191	T	T	T
0.6912737777432031	0.0013177674247886	0.9002157014126074	T	T	T
0.7105027088638726	0.8718430778328092	0.9523571701129154	T	T	T
0.4881606817883338	0.0455013873482299	0.7082677290554376	T	T	T
0.4846644084093554	0.8667083863088522	0.7109772891960624	T	T	T
0.3524481722111399	0.4380528406042135	0.7147269984129779	T	T	T
0.2955204984726892	0.4297687465640282	0.8913739052328818	T	T	T

Structure files (CONTCAR) involved in this work:

0.2002703207916149	0.4443395792813559	0.0305192430776938	T	T	T
0.1051435936185209	0.4286434831359940	0.8920494440035615	T	T	T
0.1007846267476936	0.4429976637610524	0.6949618196739470	T	T	T
0.2256807249150499	0.4721731706502265	0.7353344068252471	T	T	T
0.3565088088371600	0.6691914223906678	0.7391513161157783	T	T	T
0.2996873695846272	0.6627865111084106	0.9132928803247619	T	T	T
0.1912473162039711	0.6455688310012598	0.0250407087578166	T	T	T
0.0929809022924452	0.6693158613559679	0.8963118640766237	T	T	T
0.1004347995998300	0.6562160353261823	0.7013174319559041	T	T	T
0.2273221428914743	0.6383807238067378	0.7510255726292633	T	T	T
0.3191991415719541	0.5504797976320702	0.8108187617272294	T	T	T
0.0843761208381388	0.5487137390090152	0.8164970677278918	T	T	T
0.4297705601672386	0.3742477152783491	0.5850140349566149	T	T	T
0.4143841670494551	0.5059160393174419	0.5673275086062709	T	T	T
0.3944146784566900	0.6382189386824278	0.5549981090705639	T	T	T
0.1965629254180776	0.3716301995034280	0.6104782885191079	T	T	T
0.1763206278598151	0.4982765280746718	0.5545197417732202	T	T	T
0.1907820301763852	0.6323453534470102	0.5594511540050765	T	T	T
0.9905200248993730	0.4533857977231208	0.7960626735835664	T	T	T
0.9833941698851485	0.6349539650206535	0.7950400696530755	T	T	T
0.1377069800649456	0.5592174906460670	0.2150538331197772	T	T	T
0.1963604842496276	0.5671737414659253	0.3893531954543986	T	T	T
0.2946939993237910	0.5520295419583694	0.5230725343462405	T	T	T
0.3942286863728788	0.5660788519725238	0.3920441293229520	T	T	T
0.3963033252785420	0.5515930480127089	0.1950048116903824	T	T	T
0.2678068836212548	0.5340089969578873	0.2312986385737709	T	T	T
0.1436405515412552	0.3262458565272600	0.2386810109464916	T	T	T
0.1944716500630370	0.3407324102343013	0.4172121297786527	T	T	T
0.3098684198954610	0.3520078651181403	0.5107946028457266	T	T	T
0.4167175126199592	0.3274444412030480	0.3989008057319974	T	T	T
0.3969491918503928	0.3374335008998990	0.2024660160320762	T	T	T
0.2719269804053438	0.3565450846211239	0.2569232646569861	T	T	T
0.1789585773352420	0.4474992319728863	0.3017190193173501	T	T	T
0.4136732273140768	0.4462720991823763	0.3147460966243111	T	T	T
0.0661889979692598	0.6248946934530231	0.0807237049643865	T	T	T
0.0794826744813563	0.4927920875430108	0.0626037911730060	T	T	T
0.0982173290219105	0.3609856383731205	0.0591552253036226	T	T	T
0.3103546193151318	0.6292195466640703	0.1051385711653558	T	T	T
0.3185457043207859	0.5001038966672945	0.0545608496701138	T	T	T
0.3056239528527478	0.3662736713588308	0.0635538523035668	T	T	T
0.5077913087503855	0.5388607014138121	0.2924294240912955	T	T	T
0.5160516991567367	0.3632597264243209	0.2795705664403260	T	T	T
0.4408510064542159	0.7483043776097882	0.6416527344648775	T	T	T
0.1920250405121205	0.7484220127595562	0.6507851720957571	T	T	T
0.2723661071962433	0.7503347959171361	0.0559393852467419	T	T	T
0.1079087461439883	0.7489699505196666	0.0520201106437778	T	T	T
0.0599796147231986	0.2473500826032658	0.1384013001740320	T	T	T
0.3044234401301901	0.2481642364667051	0.1500273049913089	T	T	T
0.2281795245704197	0.2503402514645183	0.5553083576165339	T	T	T
0.3920423073277919	0.2490139085946445	0.5513447221236518	T	T	T
0.5618202056933178	0.2474387788125031	0.3504609098635398	T	T	T
0.8173931041749458	0.2504409515698904	0.3805878365760297	T	T	T
0.7194925830033582	0.2472015238350276	0.9952736671737530	T	T	T

Structure files (CONTCAR) involved in this work:

0.9029686150685985	0.2550827063563025	0.9467363910809798	T	T	T
0.9354981108604485	0.7620529268266233	0.8681042002953877	T	T	T
0.6791332332940950	0.7417515372933905	0.8804516403319087	T	T	T
0.6022467398053061	0.7478545192765396	0.4546654673990523	T	T	T
0.7747056473648439	0.6696055525050629	0.0935387572705636	T	T	T
0.6905555719541475	0.7758782821416359	0.1058074454993576	T	T	T
0.8338747383142081	0.7929038896112335	0.1221821950595185	T	T	T
0.7802938109976961	0.7547208436018924	0.4954741848457745	T	T	T
0.9165560370711004	0.6790108284508090	0.8441115118324799	T	T	T
0.6797270441209798	0.8283142274947973	0.8417797392914228	T	T	T
0.7671501839985649	0.6702298847771990	0.4983969995934672	T	T	T
0.6985896419247658	0.7043149611390587	0.0269796413692936	T	T	T
0.7618527818049684	0.8217590549141014	0.0575941889414625	T	T	T
0.8612380101092538	0.7167831879263081	0.0637947592229964	T	T	T
0.9504762483444369	0.7481292237531764	0.1026489420773817	T	T	T
0.8791584970840540	0.6857087032435415	0.3700165709178319	T	T	T
0.9651526973247311	0.7824912026780708	0.0431588041193609	T	T	T
0.9450538414005019	0.7716588243093273	0.1759356738441264	T	T	T
0.9758393577322257	0.6992786819419863	0.1021190778486142	T	T	T
0.8584970284321292	0.7309645979385825	0.3350716141221259	T	T	T
0.9035369246538806	0.6982780185208226	0.4409355284863676	T	T	T
0.9143722318360408	0.6599026813301196	0.3206897213890475	T	T	T
0.7671951755806909	0.6818393110560381	0.1636536609488269	T	T	T

Figure 4(b) Route(a)-Cu ②

Si O Al Cu C H

1.0000000000000000

20.0219993591000005 0.0000000000000000 0.0000000000000000

0.0000000000000000 19.8990001678000006 0.0000000000000000

0.0000000000000000 0.0000000000000000 13.3830003737999998

93 195 3 3 2 7

Selective dynamics

Direct

0.4216990096584527	0.0536412783143162	0.6386414242107189	T	T	T
0.3015056704519398	0.0257838079427732	0.7832165313175240	T	T	T
0.2799489400858635	0.0628700864987200	0.0032963425789192	T	T	T
0.1204714778663976	0.0636879103580606	0.0044804592118124	T	T	T
0.0685427884940817	0.0255917889253163	0.7940725152234667	T	T	T
0.1773205478072953	0.0514521015847618	0.6432805784360499	T	T	T
0.4208254186502187	0.8261654412499060	0.6633682569914257	T	T	T
0.3015260376134509	0.8686203078799609	0.8029326217307325	T	T	T
0.2682799921810527	0.8272574956323896	0.0249226454847813	T	T	T
0.1142295251636113	0.8247351438757058	0.0175770688349864	T	T	T
0.0655038111690092	0.8667156205756088	0.8040847639599621	T	T	T
0.1790267407951253	0.8272742096219944	0.6670149197536099	T	T	T
0.0761761395066571	0.9436008408847022	0.1437597461517921	T	T	T
0.1981032436719837	0.9716089373113229	0.2863683324536687	T	T	T
0.2175387450561778	0.9328186333893800	0.5062963719836692	T	T	T
0.3767110973581506	0.9291533835633037	0.5078855502681019	T	T	T
0.4282521055520294	0.9695098898675047	0.2992654589634857	T	T	T
0.3223136841528501	0.9468623597546929	0.1444902744233885	T	T	T
0.0786785720166512	0.1695572866287999	0.1599230631594719	T	T	T
0.1964364057316401	0.1286304662084781	0.3040228792849245	T	T	T

Structure files (CONTCAR) involved in this work:

0.2303200912064648	0.1717500811871750	0.5213116399384904	T	T	T
0.3849130514211323	0.1724296386892165	0.5068246474862329	T	T	T
0.4335008974490863	0.1264359246940639	0.2973524189585885	T	T	T
0.3176927912461489	0.1678741230215517	0.1653002788970390	T	T	T
0.5765976261547644	0.5572027166428065	0.3568236069434952	T	T	T
0.6932959178697943	0.5284790447711333	0.2158295976855122	T	T	T
0.7142736167664587	0.5487036588098839	0.9876814693339034	T	T	T
0.8734301908199562	0.5644983697123245	0.9981211879208751	T	T	T
0.9303760790511790	0.5245274588737446	0.2061514767425761	T	T	T
0.8161917004407987	0.5602369087959586	0.3416984795484584	T	T	T
0.5790065088966597	0.3241457056359799	0.3308198621689597	T	T	T
0.7012309154958791	0.3715234578966645	0.2130979998397307	T	T	T
0.7305684639644396	0.3281084635202246	0.9920041740783380	T	T	T
0.8867413832976470	0.3281530747768565	0.9961251125242825	T	T	T
0.9348713611080706	0.3675820850561991	0.2068304228497181	T	T	T
0.8243644382542943	0.3290309162968164	0.3505007819760356	T	T	T
0.9237490782451950	0.4455327416229921	0.8614254904632224	T	T	T
0.8021182532307037	0.4675273622398324	0.7221468680377351	T	T	T
0.7801083005784148	0.4409841953841640	0.4963069863085408	T	T	T
0.6200378175006880	0.4298058559022438	0.4917204131777322	T	T	T
0.5621073663910474	0.4640192798571081	0.7024318600474414	T	T	T
0.6759871312471175	0.4284106604390447	0.8401933420004559	T	T	T
0.7923244659863823	0.6234369507839195	0.7091430256698141	T	T	T
0.6084796081152347	0.6702559836966627	0.4939097585100533	T	T	T
0.5582973975197674	0.6217955433662558	0.7053678275596678	T	T	T
0.6691654136199696	0.6667090686219874	0.8373920627845395	T	T	T
0.5743524486653691	0.9398424843083881	0.3537565676290436	T	T	T
0.6924063552977650	0.9708746585542872	0.2108442869049303	T	T	T
0.7150014329285949	0.9543971614795798	0.9870734264657026	T	T	T
0.8749028534874368	0.9485952526175335	0.9856096137762819	T	T	T
0.9326096820636541	0.9680383824835103	0.1964633248793450	T	T	T
0.8160925918363771	0.9292629256654302	0.3276767848643438	T	T	T
0.5795516166549785	0.1703267221283297	0.3214555082399497	T	T	T
0.7014746437273452	0.1272788096406592	0.2006611751520659	T	T	T
0.7344589748753954	0.1679107161760385	0.9816899580100862	T	T	T
0.8913827044426135	0.1763248176611730	0.9763470765267068	T	T	T
0.9343064385036207	0.1260214658307172	0.1953291484385996	T	T	T
0.8225451010087139	0.1734977298368542	0.3366462240740508	T	T	T
0.9232826900608154	0.0647851933041166	0.8403920147780332	T	T	T
0.8045160090941263	0.0294866410134302	0.7024748006106245	T	T	T
0.7831503244304402	0.0527103091950754	0.4755703405132139	T	T	T
0.6232224363275508	0.0654685185217212	0.4820976700330412	T	T	T
0.5665169762701679	0.0344690079281937	0.6922076906583403	T	T	T
0.6807056417144904	0.0690920265142639	0.8269897633498013	T	T	T
0.9124784271177948	0.8317969552194595	0.8347672961326558	T	T	T
0.7991126679504988	0.8720777444920150	0.6995131170593373	T	T	T
0.7671766602667249	0.8297236443006515	0.4846923113398363	T	T	T
0.6110708188089468	0.8249918859301809	0.4914778178723712	T	T	T
0.5638193413201916	0.8762864184188325	0.7034735417451442	T	T	T
0.4189483353866919	0.4427484128047358	0.6471354749113523	T	T	T
0.2988643154494684	0.4723878410697168	0.7890227049277021	T	T	T
0.2799708952368162	0.4346763930356162	0.0110108450686849	T	T	T
0.1211412346530524	0.4328943838011444	0.0107392710338117	T	T	T

Structure files (CONTCAR) involved in this work:

0.0693176019487312	0.4706416341710800	0.7999086977305331	T	T	T
0.1760697765089365	0.4463247504633455	0.6484961286495196	T	T	T
0.4176552613357886	0.6711022874673985	0.6650719708064343	T	T	T
0.3000028895614092	0.6289816028474121	0.8046085048931600	T	T	T
0.2675027695859525	0.6706490687985476	0.0259906340134687	T	T	T
0.1133354344380656	0.6714476259447199	0.0150126853228583	T	T	T
0.0636384046434855	0.6301298523475740	0.8004228667554024	T	T	T
0.1793378758863762	0.6690519509365463	0.6662756798230077	T	T	T
0.0739843418257386	0.5541804279283248	0.1444753877483300	T	T	T
0.1962248470667040	0.5259455599101998	0.2849849697692249	T	T	T
0.2165291918622530	0.5628371550640268	0.5068953521081704	T	T	T
0.3763016081166562	0.5653358740483178	0.5101582374360590	T	T	T
0.4309457017792872	0.5267470098730085	0.3001152614526922	T	T	T
0.3229974486939952	0.5525470140364768	0.1484199517493606	T	T	T
0.0792927845658995	0.3242138857016059	0.1628271888261395	T	T	T
0.1964708847339220	0.3677476431859683	0.3040292374636713	T	T	T
0.2311752285527792	0.3280609920807287	0.5233301107578435	T	T	T
0.3862431549341991	0.3252703609605989	0.5113066922112406	T	T	T
0.4358895535430256	0.3691033628361642	0.2987557511312158	T	T	T
0.3187098385717496	0.3268680301669626	0.1687181129526778	T	T	T
0.3561605062139743	0.0590138447868947	0.7091838414951657	T	T	T
0.2995807797494843	0.0691794163966851	0.8860956251772590	T	T	T
0.2000150811750606	0.0510118513986008	0.0171488383808351	T	T	T
0.0998652800874005	0.0672078587366626	0.8874883437834750	T	T	T
0.1025365435111128	0.0494794049573212	0.6901145267681543	T	T	T
0.2285580668289555	0.0280853031687840	0.7306996445741666	T	T	T
0.3578183948714413	0.8291165406992024	0.7396006640973020	T	T	T
0.3003306006648703	0.8377973316327250	0.9148674784031119	T	T	T
0.1906523300854043	0.8518873280064521	0.0255908379140847	T	T	T
0.0923319734185304	0.8268190493534708	0.9012727714966370	T	T	T
0.1019741756460836	0.8373866358734620	0.7046386757351792	T	T	T
0.2283216077046644	0.8588795235417409	0.7518331116515025	T	T	T
0.3202453818661976	0.9480686104535740	0.8074136131609256	T	T	T
0.0812130799068508	0.9462427245121871	0.8153730949944370	T	T	T
0.4300394825001205	0.1224181481565631	0.5743206927066253	T	T	T
0.4168700729945803	0.9902999606989823	0.5619251039183351	T	T	T
0.3994539185505797	0.8577753834790027	0.5556199057936851	T	T	T
0.1929606419282689	0.1273296613242733	0.6060265453195384	T	T	T
0.1808808144511649	0.9998341668710738	0.5493243665577290	T	T	T
0.1895864792112219	0.8655670001426977	0.5609086595591725	T	T	T
0.9892271521713648	0.0399766344752445	0.7817238716505929	T	T	T
0.9854790016323434	0.8549947642859377	0.7967961955454481	T	T	T
0.1418973572568488	0.9398738680347933	0.2134827477503580	T	T	T
0.2013935639815592	0.9268423656366854	0.3877383221134426	T	T	T
0.2972592411597664	0.9405873572635357	0.5261493656343521	T	T	T
0.3934360822500497	0.9271952300194845	0.3893559828702620	T	T	T
0.3965758583963215	0.9487371182043534	0.1921741723894985	T	T	T
0.2697987066101235	0.9700116476943766	0.2304324408853391	T	T	T
0.1406883236649593	0.1659100786895153	0.2367724260046819	T	T	T
0.1939697601251080	0.1627359769125777	0.4137274228416379	T	T	T
0.3075748317397272	0.1469455884296514	0.5111558826999303	T	T	T
0.4109036901258746	0.1723340174974783	0.3919263554702455	T	T	T
0.3947517751913746	0.1525687661720582	0.1975070511234560	T	T	T

Structure files (CONTCAR) involved in this work:

0.2697165168895884	0.1384533430874495	0.2535783156669589	T	T	T
0.1794125611652141	0.0490296650698940	0.3130598211699943	T	T	T
0.4149433791800097	0.0487726714350546	0.3216117147673921	T	T	T
0.0665701809051829	0.8723217091614435	0.0857110358719491	T	T	T
0.0808300183806615	0.0028685648743507	0.0600969029989932	T	T	T
0.0987549913389588	0.1346332532916346	0.0543971679739528	T	T	T
0.3085901567533976	0.8706653246494213	0.1073609512482614	T	T	T
0.3185829267551598	0.9983049122555079	0.0502445089698187	T	T	T
0.3017208473431031	0.1319132574553735	0.0590097975741239	T	T	T
0.5070788865272365	0.9531678662830428	0.2898333536685486	T	T	T
0.5134414424430724	0.1325355341597237	0.2787803336581219	T	T	T
0.6382397772941276	0.5704397213760931	0.2790974983473127	T	T	T
0.6812305372593542	0.5449121569397944	0.0972535555020882	T	T	T
0.7946931120675668	0.5452585304462179	0.9903732576828365	T	T	T
0.8988602648635692	0.5655340428196159	0.1119800993051886	T	T	T
0.8937430286051083	0.5465133096841963	0.3082420305485163	T	T	T
0.7694699071567325	0.5494342762205285	0.2412200032761955	T	T	T
0.6422193931349389	0.3239195936012899	0.2550043912671351	T	T	T
0.7041500621168012	0.3633531548261752	0.0932459712493472	T	T	T
0.8087812379751202	0.3481218716389730	0.9789424688477887	T	T	T
0.9049733033749418	0.3237273579313056	0.1142742200693656	T	T	T
0.9000361345777695	0.3430078932179352	0.3101280183810777	T	T	T
0.7724715264728194	0.3507852677898702	0.2619396932563763	T	T	T
0.6824052535586227	0.4489787708514918	0.2389728483781237	T	T	T
0.9176673286292939	0.4455438782861987	0.1833384486517238	T	T	T
0.5602698014056754	0.6235194527705830	0.4230091496809991	T	T	T
0.5938467259181733	0.4944180504926370	0.4297291341664091	T	T	T
0.5992653454229265	0.3608154652518772	0.4346376273983544	T	T	T
0.8071451605960037	0.6347635165926500	0.3814660680709011	T	T	T
0.7956082167826561	0.5024462725258613	0.4218224952700603	T	T	T
0.8109314546653973	0.3713186436151125	0.4517591768506541	T	T	T
0.0093474282469918	0.5420215948262495	0.2155248994852260	T	T	T
0.0152146538153097	0.3590686189446287	0.2167751640944916	T	T	T
0.8606010112980099	0.4319183422095710	0.7883820693945629	T	T	T
0.8147606820123813	0.4539384068946126	0.6044363047760675	T	T	T
0.6999229559402240	0.4328230405779706	0.5081342979990517	T	T	T
0.5837975888139573	0.4273991073393141	0.5996814515142339	T	T	T
0.6008618543688454	0.4293011299348546	0.7959163238413828	T	T	T
0.7302540166169134	0.4340031501431588	0.7507690880840746	T	T	T
0.8434740654402925	0.6726146328893780	0.7647906457022031	T	T	T
0.7990768390360533	0.6237024771815425	0.5912437386804095	T	T	T
0.6835026174872915	0.6451393271005696	0.4826297515356832	T	T	T
0.5827478553307471	0.6647475234034043	0.6100229492658309	T	T	T
0.5922447884048342	0.6520633560991134	0.8085618955347297	T	T	T
0.7162768001798984	0.6469486356774582	0.7456841441554227	T	T	T
0.8015803968368000	0.5464861318220527	0.7522650739652197	T	T	T
0.5807684937825280	0.5435959280130105	0.6964015901062115	T	T	T
0.9326202710167694	0.3834443429530474	0.9395854491755790	T	T	T
0.9152083139290046	0.5141957778603831	0.9271480170803578	T	T	T
0.8898239175884027	0.6406349409439146	0.9556385178484641	T	T	T
0.6871635171188932	0.3585833858596214	0.9003129087455410	T	T	T
0.6832088071852802	0.4932771264607584	0.9146923882678052	T	T	T
0.6920502045186585	0.6250385112011982	0.9434935332464346	T	T	T

Structure files (CONTCAR) involved in this work:

0.4825811122139501	0.4539038437782471	0.7206699382002538	T	T	T
0.4778461662722415	0.6282936950451613	0.7173107659501800	T	T	T
0.6358075393359561	0.9323899515018093	0.2748403476645203	T	T	T
0.6758131049888154	0.9639659772043194	0.0917166053124382	T	T	T
0.7953488664108707	0.9589885176291305	0.0104790140861659	T	T	T
0.9137590402735785	0.9346903003184538	0.0888704569522023	T	T	T
0.8921275677534124	0.9303642311826626	0.2847780461650031	T	T	T
0.7648926328251257	0.9363965616496814	0.2320337924745793	T	T	T
0.6354724525526727	0.1693149600077018	0.2328442041911069	T	T	T
0.7090491285638477	0.1269736695700338	0.0798706373664487	T	T	T
0.8135161813712336	0.1536536539394190	0.9641054447355978	T	T	T
0.9140780588247001	0.1611696866526060	0.0902371675901156	T	T	T
0.8965640465506181	0.1622795697495328	0.2884602654438795	T	T	T
0.7679471523432545	0.1610264509412579	0.2482165893937688	T	T	T
0.6939569751577541	0.0502372008551971	0.2406451107168416	T	T	T
0.9126871604264172	0.0472322921234381	0.1933265843006277	T	T	T
0.5647553788544882	0.8721525237392362	0.4194591205183039	T	T	T
0.5866479289263644	0.0028986311300074	0.4279373707486498	T	T	T
0.6090185336955741	0.1342031076079006	0.4207012349827083	T	T	T
0.8040869099187861	0.8588677095750795	0.3841054889370520	T	T	T
0.8054918663818945	0.9931432653437310	0.4008157894576826	T	T	T
0.8095817483912795	0.1239445860898661	0.4308481127997743	T	T	T
0.0119236932293632	0.9570889254042514	0.2153449388801714	T	T	T
0.0146006561340075	0.1323631021395981	0.2107970621431142	T	T	T
0.8619738371975126	0.0707469791521961	0.7625353095308920	T	T	T
0.8170002675448473	0.0407217496518522	0.5842230770861430	T	T	T
0.7028297993911146	0.0526220725230353	0.4884152003066982	T	T	T
0.5920038089877880	0.0738867699560638	0.5929356036799454	T	T	T
0.6043475856847271	0.0675464332618712	0.7882287113150298	T	T	T
0.7318819128307664	0.0605441603315118	0.7335881283713119	T	T	T
0.8651033251000890	0.8299135535814592	0.7372294945822336	T	T	T
0.7974073186586319	0.8727674738736066	0.5787031044549215	T	T	T
0.6877984157995802	0.8489386657176969	0.4747137493586342	T	T	T
0.5902838353541768	0.8329108233991828	0.6081036850424538	T	T	T
0.5970193217425436	0.8508309460822140	0.8062399508945214	T	T	T
0.7338575252214924	0.8396490920060466	0.7491015374075908	T	T	T
0.8084527578966046	0.9508977322178415	0.7353508711792458	T	T	T
0.5831893230393442	0.9550179896139910	0.6826637942062302	T	T	T
0.9367822025350826	0.1363713051764901	0.8949944395635846	T	T	T
0.9056188951868533	0.0129947439154623	0.9307528628899724	T	T	T
0.8799299879526168	0.8825926319480532	0.9159796309246117	T	T	T
0.6936888403277189	0.1392668823090368	0.8857847030962120	T	T	T
0.6908803572528850	0.0056329134412969	0.9031682140943523	T	T	T
0.7051773955831816	0.8754734753721723	0.9503412764733989	T	T	T
0.4870087519976671	0.0457474816987139	0.7092250249693074	T	T	T
0.4826114554017482	0.8682474408632893	0.7106791586869892	T	T	T
0.3522400960210739	0.4369383667974678	0.7149726123731664	T	T	T
0.2961137265076145	0.4298471011870086	0.8925171897668696	T	T	T
0.2003183295855223	0.4451478242405875	0.0306932153138722	T	T	T
0.1052326545839256	0.4311842366731152	0.8921989365835736	T	T	T
0.1011574091283123	0.4450285353123440	0.6948698959138095	T	T	T
0.2259381048309032	0.4717389444884140	0.7366145252691361	T	T	T
0.3545079121146427	0.6704413285648481	0.7404826249297819	T	T	T

Structure files (CONTCAR) involved in this work:

0.2991730949526243	0.6604654897331033	0.9158097077378724	T	T	T
0.1900883408261801	0.6452277374276355	0.0263695118654447	T	T	T
0.0919128224787205	0.6698498413612747	0.8986409274388372	T	T	T
0.1025717134888387	0.6579309374586902	0.7014353708919057	T	T	T
0.2271375184515221	0.6371721734938830	0.7527720106227965	T	T	T
0.3203711941847989	0.5499075680647461	0.8103138345586778	T	T	T
0.0803307386929342	0.5506202615807353	0.8155878428823918	T	T	T
0.4291554531860099	0.3730861982737404	0.5854704927406750	T	T	T
0.4150320228237864	0.5049032082650753	0.5681402301125008	T	T	T
0.3967808764845567	0.6372938850945885	0.5587994046446556	T	T	T
0.1958470763307910	0.3714472851058194	0.6109899708392968	T	T	T
0.1784483588155498	0.4982176382684935	0.5547931432563820	T	T	T
0.1927608953224122	0.6321952757277889	0.5598081968657819	T	T	T
0.9904090201212433	0.4524729630477320	0.7945678648050678	T	T	T
0.9853873476529066	0.6441024131592332	0.7874805012252318	T	T	T
0.140008517857035	0.5595066415001101	0.2137781981874851	T	T	T
0.1971979046766060	0.5671148778706284	0.3895137821850231	T	T	T
0.2965323232188428	0.5526348858733277	0.5217922033482657	T	T	T
0.3978247118334884	0.5669323462490934	0.3935958438253760	T	T	T
0.3973520908950546	0.5522160723962083	0.1964149070622204	T	T	T
0.2693947693594032	0.5313423012262618	0.2338935989276499	T	T	T
0.1420861461101941	0.3264535439994580	0.2389035120449945	T	T	T
0.1932409685661498	0.3400087225552398	0.4176151517950297	T	T	T
0.3088935841934680	0.3509302261241669	0.5110341661938188	T	T	T
0.4159856428873311	0.3277317937745998	0.3988428033615997	T	T	T
0.3958979133087311	0.3387843609097260	0.2028461364108577	T	T	T
0.2706113359247471	0.3555931383488041	0.2574078473503356	T	T	T
0.1782172133505094	0.4472370318410847	0.3030311772832511	T	T	T
0.4160494551220818	0.4471588609370665	0.3158047952929827	T	T	T
0.0647118854865660	0.6242180522323787	0.0827394964788519	T	T	T
0.0793801382318986	0.4931262489446603	0.0640163416248844	T	T	T
0.0980339769492320	0.3615926828121113	0.0585946623622255	T	T	T
0.3089917820433159	0.6278662935958543	0.1077975847483698	T	T	T
0.3197441527366738	0.4989928437750514	0.0566186859350334	T	T	T
0.3042493486411182	0.3653649960122188	0.0638501043805735	T	T	T
0.5105047591799574	0.5399229681013785	0.2911587976892566	T	T	T
0.5156823373362934	0.3616088059759297	0.2781981511226281	T	T	T
0.4408993710668644	0.7479873389044019	0.6455004092948000	T	T	T
0.1950956317077470	0.7483504645244502	0.6508576707166025	T	T	T
0.2727438932284381	0.7490529260795941	0.0572689023617151	T	T	T
0.1071322039238938	0.7479748724064940	0.0568905154279008	T	T	T
0.0607980385870959	0.2471389139286678	0.1359458328157415	T	T	T
0.3050678984674325	0.2476066379167977	0.1508587671057267	T	T	T
0.2262485131331150	0.2496846793545922	0.5556967775070144	T	T	T
0.3909495872517058	0.2482362324469589	0.5509636749341875	T	T	T
0.5601349764454718	0.2464359577384017	0.3529556279030276	T	T	T
0.8160086173873893	0.2499420389222720	0.3772264962686629	T	T	T
0.7202335623817344	0.2474366975358395	0.9960088936529833	T	T	T
0.9009622316398921	0.2548069068892883	0.9487605910684538	T	T	T
0.9159695866997524	0.7581989808065004	0.8929936567123512	T	T	T
0.6790854620215020	0.7421424825349566	0.8859282536680299	T	T	T
0.5982732874583351	0.7478424293305667	0.4582239799383291	T	T	T
0.7939348794496459	0.6777955767668415	0.0900215096724315	T	T	T

Structure files (CONTCAR) involved in this work:

0.7106322150102710	0.7795228277721139	0.1005017302745590	T	T	T
0.8434059508963704	0.7994173086868308	0.0842374114235450	T	T	T
0.7796747898527686	0.7517335738402415	0.4973223988486112	T	T	T
0.9135518466875222	0.6754971602366707	0.8360622500030916	T	T	T
0.6760744949023424	0.8281668505286101	0.8420936275471841	T	T	T
0.7680014822560300	0.6660528544464326	0.4875642180093188	T	T	T
0.7131190093721788	0.7056516776700376	0.0239735793668534	T	T	T
0.7690090930054346	0.8331418699181267	0.0388225031749129	T	T	T
0.8648261048130069	0.7232066156060556	0.0179555669662146	T	T	T
0.9676873313520620	0.7633202174872153	0.2295044206686385	T	T	T
0.9138341953741654	0.7267215229839891	0.2880453063074099	T	T	T
0.9574586798276847	0.7633284864865324	0.1482429110561944	T	T	T
0.9713962522733334	0.8162743772300372	0.2519292282929175	T	T	T
0.0170448355353006	0.7399154934382738	0.2389752878771084	T	T	T
0.8645302736883138	0.7503751903045224	0.2789384025177374	T	T	T
0.9241161096431728	0.7268236432906122	0.3688013907383625	T	T	T
0.9098492647916233	0.6737728021249427	0.2658848581974304	T	T	T
0.7938083605778323	0.6978589286995321	0.1575151611061399	T	T	T

Figure 4(b) Route(a)-Cu ③

Si O Al Cu C H

1.0000000000000000

20.0219993591000005 0.0000000000000000 0.0000000000000000

0.0000000000000000 19.8990001678000006 0.0000000000000000

0.0000000000000000 0.0000000000000000 13.3830003737999998

93 195 3 3 2 7

Selective dynamics

Direct

0.4200713588993181	0.0537725875374975	0.6404400239168185	T	T	T
0.2999882082792739	0.0265221059664171	0.7851589916154417	T	T	T
0.2790487796911720	0.0646516821858637	0.0050047472558419	T	T	T
0.1193914209546678	0.0648114918109091	0.0038091841399310	T	T	T
0.0666314935549508	0.0270712197098328	0.7925235788922972	T	T	T
0.1769109956936092	0.0519993304192624	0.6436012476355435	T	T	T
0.4208503026994875	0.8271308989971713	0.6633588765479688	T	T	T
0.3008049572090393	0.8693326685506547	0.8023552699358050	T	T	T
0.2694922812188389	0.8275471029316899	0.0255328132621111	T	T	T
0.1153513005798932	0.8261266649470488	0.0183761542340544	T	T	T
0.0644470429030578	0.8666759063427324	0.8039710647391791	T	T	T
0.1783762217699373	0.8283402906032328	0.6660406190885113	T	T	T
0.0740258171376920	0.9447242454219978	0.1425261686477884	T	T	T
0.1966950868157832	0.9718891537252540	0.2855127237149366	T	T	T
0.2168381043832301	0.9333850665075618	0.5054295674184014	T	T	T
0.3763986309999632	0.9291312039468302	0.5081936812071999	T	T	T
0.4289163280103137	0.9710636549841186	0.3003857938264083	T	T	T
0.3226430406305829	0.9476094067028754	0.1443136036524429	T	T	T
0.0787660121064964	0.1706397598808410	0.1601087699960229	T	T	T
0.1968903406833579	0.1294718491315463	0.3038227505566921	T	T	T
0.2289397855026365	0.1724006950852278	0.5213607809287670	T	T	T
0.3837724470711961	0.1729170780692988	0.5078856707129229	T	T	T
0.4342024986469886	0.1278342607476420	0.2993879111454581	T	T	T
0.3186367784466532	0.1688983923117248	0.1675349342135481	T	T	T
0.5745243401698904	0.5579165864665441	0.3581206511854053	T	T	T

Structure files (CONTCAR) involved in this work:

0.6934032012812531	0.5280758201539073	0.2200987095967856	T	T	T
0.7102227686333502	0.5456782810011647	0.9904420390361575	T	T	T
0.8681707159646801	0.5594398574073173	0.9892827455005085	T	T	T
0.9293116623173919	0.5274060141947763	0.1960145102345370	T	T	T
0.8187163510736759	0.5638869058737568	0.3405144230328657	T	T	T
0.5796025213460881	0.3267224579165901	0.3290571524707980	T	T	T
0.7012538137850690	0.3712330802221104	0.2106899909658651	T	T	T
0.7334767934434882	0.3299818564463909	0.9910851427321525	T	T	T
0.8885423757383781	0.3269682919591164	0.9929287640655056	T	T	T
0.9350143587987787	0.3705983718831105	0.2030253715878352	T	T	T
0.8241298061660302	0.3303304006747924	0.3479884565984021	T	T	T
0.9251080288684310	0.4410096179386221	0.8564768381361306	T	T	T
0.8056172847954509	0.4669056704654413	0.7198421803632996	T	T	T
0.7812084412178409	0.4442598866391435	0.4933963368287670	T	T	T
0.6213328784918752	0.4318344652232692	0.4904258657874278	T	T	T
0.5641349237173006	0.4617745329955361	0.7004536291906930	T	T	T
0.6766266062360387	0.4285138310066985	0.8389140862579917	T	T	T
0.7948850490960254	0.6208160989303073	0.7027390225287310	T	T	T
0.6078559437541452	0.6740112310966515	0.4878555412720501	T	T	T
0.5667311896375552	0.6202387423038045	0.7026671572215651	T	T	T
0.6738578632391355	0.6673510552431999	0.8459035115172947	T	T	T
0.5746878703986029	0.9434866527949020	0.3569622040416147	T	T	T
0.6953729617854322	0.9742458762490187	0.2200053798790611	T	T	T
0.7119728302898991	0.9524710695908565	0.9900631780337280	T	T	T
0.8720509976623684	0.9455632238856435	0.9848516565995338	T	T	T
0.9285736294276851	0.9717941781900495	0.2000162186408667	T	T	T
0.8174421973600570	0.9327020544523272	0.3411996958550530	T	T	T
0.5792165210071751	0.1734301405242928	0.3281300462163417	T	T	T
0.7027633888234195	0.1304547694021146	0.2086703903683866	T	T	T
0.7345630649305732	0.1683571889622427	0.9886359311878612	T	T	T
0.8899962780207687	0.1749494062500770	0.9860488047487199	T	T	T
0.9350722827693408	0.1291968507669412	0.2025341708215715	T	T	T
0.8242976286626003	0.1754762061546614	0.3427484854024090	T	T	T
0.9236645753204034	0.0643528931786977	0.8467780354849305	T	T	T
0.8040286052935998	0.0343983630156846	0.7125367386157272	T	T	T
0.7819442065330847	0.0571335873678890	0.4853609863786559	T	T	T
0.6216951780880384	0.0689890577471521	0.4878676137558876	T	T	T
0.5646390427934942	0.0366888906026696	0.6989146833965592	T	T	T
0.6768639685473317	0.0690572294711105	0.8363723807830870	T	T	T
0.9122665118165475	0.8273596128231164	0.8375252724998345	T	T	T
0.7973387367067591	0.8776040097092824	0.7075173557013781	T	T	T
0.7679420662703001	0.8285357368327911	0.4921450366325329	T	T	T
0.6092682587533562	0.8260942313307760	0.4945817059279960	T	T	T
0.5631657432323250	0.8782297539910540	0.7079292354494731	T	T	T
0.4202653433186004	0.4437230106680808	0.6450813829293532	T	T	T
0.3000698148358354	0.4729006959322598	0.7882481172433148	T	T	T
0.2809152713047778	0.4337417989537021	0.0084915368246348	T	T	T
0.1220539438025523	0.4319929654132039	0.0080466930969678	T	T	T
0.0710717648798134	0.4708964001907166	0.7992160147184346	T	T	T
0.1773094034611932	0.4482851759278434	0.6467348148502498	T	T	T
0.4230018048161682	0.6714703628464822	0.6653195371167003	T	T	T
0.3037940531733419	0.6295282867707099	0.8044315256899596	T	T	T
0.2695696615862318	0.6715464278580171	0.0257931592956260	T	T	T

Structure files (CONTCAR) involved in this work:

0.1154940925591604	0.6728287179586575	0.0133901976729708	T	T	T
0.0678310564614181	0.6289371987829006	0.8013430301330642	T	T	T
0.1820493176252702	0.6696705151924593	0.6639281389635402	T	T	T
0.0747314377983242	0.5546954560110937	0.1396400621107361	T	T	T
0.1960006487834634	0.5267303362372124	0.2828508271726167	T	T	T
0.2182150854071111	0.5645595530171545	0.5045317063920916	T	T	T
0.3778009288494676	0.5671271320479825	0.5098120100939711	T	T	T
0.4301785715973558	0.5272883485697102	0.3008019636597724	T	T	T
0.3233639528580718	0.5516845783787420	0.1456871836496597	T	T	T
0.0788982063574580	0.3256149841224922	0.1630060798546326	T	T	T
0.1963193785812669	0.3689807606838353	0.3033879705768729	T	T	T
0.2307184025954645	0.3287901542222443	0.5228101941604557	T	T	T
0.3857971972340776	0.3253170580323487	0.5115199440655384	T	T	T
0.4352547639683914	0.3706936934392836	0.3010766580861797	T	T	T
0.3193528258368113	0.3282311457590597	0.1689635604218727	T	T	T
0.3540585695470624	0.0594281870470178	0.7099614416194511	T	T	T
0.2982982325950987	0.0705594348738435	0.8875539889679316	T	T	T
0.1989693315796159	0.0533343909980019	0.0191022522169927	T	T	T
0.1001606715209191	0.0667848717061788	0.8862889456852483	T	T	T
0.1016855600410779	0.0490140612634889	0.6885363115587625	T	T	T
0.2269965921945880	0.0286850233466799	0.7326188877956624	T	T	T
0.3576072037882995	0.8301133796641965	0.7395344793165878	T	T	T
0.2979599006975635	0.8369469113367658	0.9132142462941983	T	T	T
0.1917583520372844	0.8522335642907867	0.0316438128863423	T	T	T
0.0957822500251442	0.8304005122106546	0.9014417567910348	T	T	T
0.1015081994637199	0.8381386230242998	0.7045828639973359	T	T	T
0.2281052162089243	0.8609383137535531	0.7493079820223965	T	T	T
0.3188937233831940	0.9488703164335952	0.8101058125073426	T	T	T
0.0745147152049891	0.9471191928330830	0.8131225185631895	T	T	T
0.4282334744218317	0.1221506534469567	0.5750784692134584	T	T	T
0.4157041892014145	0.9899523176810557	0.5644919485706584	T	T	T
0.3985845120238338	0.8573471917839954	0.5550348826293878	T	T	T
0.1922802471103578	0.1281231514448391	0.6070215576618876	T	T	T
0.1817966538429762	0.0010200843876847	0.5490964977846188	T	T	T
0.1878211439436110	0.8664851328491723	0.5596218948713791	T	T	T
0.9884042363364579	0.0467350973634993	0.7798579924434664	T	T	T
0.9854048244905461	0.8492159921683794	0.7987041808968522	T	T	T
0.1383350076966947	0.9415286902168576	0.2149553281843213	T	T	T
0.1995610711379770	0.9276373018651354	0.3872487937329228	T	T	T
0.2966814976239783	0.9399489913468824	0.5242042227304692	T	T	T
0.3944053775901155	0.9282235619438440	0.3900249951475401	T	T	T
0.3964381486625588	0.9512493856038967	0.1934172711319168	T	T	T
0.2679688921234791	0.9673411353223444	0.2289827903192591	T	T	T
0.1426599396768815	0.1666782664281768	0.2335258499339896	T	T	T
0.1920968079790625	0.1626699824433845	0.4140713646860807	T	T	T
0.3062477412009230	0.1479198174439811	0.5106445284983815	T	T	T
0.4103300956761811	0.1735577678877096	0.3932786850635746	T	T	T
0.3958675255988748	0.1530588442982317	0.1985252302766349	T	T	T
0.2711153680424931	0.1397624473294675	0.2567109315507919	T	T	T
0.1800395192261677	0.0498301887591890	0.3111227368229872	T	T	T
0.4159262190865810	0.0501533893658321	0.3238708915328184	T	T	T
0.0656214879464636	0.8726166719133381	0.0856393198451634	T	T	T
0.0798938207510384	0.0033619277410844	0.0584634232599090	T	T	T

Structure files (CONTCAR) involved in this work:

0.0960821295322574	0.1354273674340014	0.0535323790799971	T	T	T
0.3122247101695714	0.8715498315445365	0.1043433464716159	T	T	T
0.3177188154794434	1.0000105666892596	0.0514995205534068	T	T	T
0.3012783643363829	0.1333076573425373	0.0613559981542402	T	T	T
0.5079169791454260	0.9548609260703109	0.2906401766771322	T	T	T
0.5143655260932068	0.1346516270698346	0.2827258573889492	T	T	T
0.6372169527724562	0.5688272719107385	0.2821648306711961	T	T	T
0.6790504771726784	0.5410922801681619	0.1013738595889639	T	T	T
0.7904061693430844	0.5363502168972973	0.9913861710089916	T	T	T
0.8980827116323530	0.5685730179725551	0.1010395235112168	T	T	T
0.8944272052493898	0.5516527867087754	0.2981010044598011	T	T	T
0.7681008888136426	0.5546324428320777	0.2437931504132874	T	T	T
0.6392998168109889	0.3250885606113403	0.2469320791248016	T	T	T
0.7049750846531251	0.3669802934820026	0.0901517033288971	T	T	T
0.8115036214539034	0.3513104728110856	0.9792389096209387	T	T	T
0.9085890178201229	0.3248177415599411	0.1104195740147722	T	T	T
0.8988622489915767	0.3470471897669675	0.3059071055322661	T	T	T
0.7712343595186648	0.3451919821245871	0.2578482340838187	T	T	T
0.6869886858557567	0.4482666359208443	0.2451494560024106	T	T	T
0.9163840638966313	0.4479445267261982	0.1761185692497048	T	T	T
0.5581147526070891	0.6245494324714779	0.4234704465815877	T	T	T
0.5894234734816305	0.4955347132242982	0.4327777811228929	T	T	T
0.6059305829084584	0.3627597890981524	0.4300851095545141	T	T	T
0.8137318307781972	0.6374885549644294	0.3854649562240697	T	T	T
0.8018287711854035	0.5044547992543298	0.4195454761916712	T	T	T
0.8079339267496531	0.3736323404997179	0.4468291221035081	T	T	T
0.0083941729710606	0.5434323023533540	0.2067829091181290	T	T	T
0.0153739145062979	0.3624394953537477	0.2159284810061753	T	T	T
0.8625100721205339	0.4261137450364128	0.7827629549296148	T	T	T
0.8161011069524495	0.4527135057733694	0.6019570419350073	T	T	T
0.7007503340533058	0.4414589421084000	0.5053668909041471	T	T	T
0.5854043148406809	0.4242402366364910	0.5980266096820794	T	T	T
0.6021212812055375	0.4247378134028163	0.7926446410138857	T	T	T
0.7317017010144157	0.4399469040594390	0.7518276036180080	T	T	T
0.8550619474873052	0.6712744824550168	0.7287152827949731	T	T	T
0.7784374708343360	0.6157964693465288	0.5870249831859726	T	T	T
0.6827596299150476	0.6611579911546087	0.4542809110888710	T	T	T
0.5966774999936411	0.6600522230235719	0.6077890523761481	T	T	T
0.5993076907836644	0.6495397005289195	0.8065355731316720	T	T	T
0.7280881548047127	0.6442883257981611	0.7659077964519667	T	T	T
0.8134400028930604	0.5457255127427673	0.7483379726127545	T	T	T
0.5849222286382374	0.5406908304629453	0.6955161793751782	T	T	T
0.9368911151793061	0.3769507267208132	0.9302905792038445	T	T	T
0.9122461697336349	0.5062893297087969	0.9273176870409054	T	T	T
0.8762198840568030	0.6325773809037893	0.9330792651371009	T	T	T
0.6913819657407771	0.3582642864184840	0.8966121672221083	T	T	T
0.6768490984328147	0.4922891597423684	0.9161641805983253	T	T	T
0.6882590115004397	0.6235556859258703	0.9540193002223146	T	T	T
0.4842356962631502	0.4538733144587732	0.7181237669286129	T	T	T
0.4862424421188054	0.6300144441019240	0.7101943471255202	T	T	T
0.6371406802161576	0.9349153274358379	0.2797919317516279	T	T	T
0.6821396925023717	0.9656680774530066	0.1008923411757400	T	T	T
0.7926760824063478	0.9594338153508634	0.9890558062667199	T	T	T

Structure files (CONTCAR) involved in this work:

0.9009003201624671	0.9368782259163329	0.0974794616319698	T	T	T
0.8932303198131314	0.9364235652543945	0.2957409484813324	T	T	T
0.7671890834730007	0.9402356394433298	0.2450998926668473	T	T	T
0.6376377073161548	0.1724392026801939	0.2435776423720116	T	T	T
0.7066963947170299	0.1305265250762773	0.0878619807621362	T	T	T
0.8130889567497395	0.1491404171423919	0.9747068296021243	T	T	T
0.9124334276342180	0.1682033704032006	0.1018425452557846	T	T	T
0.8994721824636226	0.1623867340972037	0.2996511382305028	T	T	T
0.7710483935612605	0.1632338741314600	0.2522105783010483	T	T	T
0.6955240200235675	0.0534935209996322	0.2494692002272647	T	T	T
0.9113690570261337	0.0510959808266561	0.1947640242178374	T	T	T
0.5656564543353011	0.8770419113328677	0.4247023262794213	T	T	T
0.5860379048148734	0.0078812440790040	0.4287316952493827	T	T	T
0.6066021604184220	0.1389571219918940	0.4300112203727302	T	T	T
0.8070266322647469	0.8608951228953760	0.3945913246681036	T	T	T
0.8062352333186590	0.9948628658764319	0.4168287098669352	T	T	T
0.8082192088029994	0.1269552759839005	0.4366347674960772	T	T	T
0.0079289265422342	0.9575655362473473	0.2102066975802486	T	T	T
0.0157843786521274	0.1331845249134036	0.2142018350179283	T	T	T
0.8596001301534318	0.0766110103338527	0.7754680819093078	T	T	T
0.8150396674589018	0.0500652923382852	0.5951845385939070	T	T	T
0.7014205882349002	0.0564095179780029	0.4945519264030058	T	T	T
0.5900114229680938	0.0746897186263773	0.5984093206118462	T	T	T
0.6014191971068513	0.0726846294095171	0.7934925516195239	T	T	T
0.7295248334505327	0.0587120103007718	0.7451141978058318	T	T	T
0.8621338970647283	0.8334879454654626	0.7443122443823208	T	T	T
0.7906218611151286	0.8751848967100739	0.5871785054047549	T	T	T
0.6878894746012765	0.8400565287314665	0.4725545638258700	T	T	T
0.5936015017175617	0.8385751070332838	0.6118626134970664	T	T	T
0.5928519514181414	0.8482816092200914	0.8099041262850926	T	T	T
0.7320666573088871	0.8520572465686195	0.7639153821851120	T	T	T
0.8147041295387861	0.9555600612739447	0.7390096650952351	T	T	T
0.5829849951355467	0.9575740925033381	0.6940961865889116	T	T	T
0.9380186744875123	0.1306807555128578	0.9138348810800528	T	T	T
0.9113075278951225	0.0030726018651941	0.9255261330906203	T	T	T
0.8873219398246542	0.8722474437849538	0.9342001591412410	T	T	T
0.6928898644589871	0.1390021146804925	0.8943959768000288	T	T	T
0.6805782400755561	0.0044819430995838	0.9115554770792310	T	T	T
0.6893110874717641	0.8741963862895511	0.9641890400745340	T	T	T
0.4846695695968253	0.0467729270809420	0.7126097650008488	T	T	T
0.4816683499435812	0.8712239981256482	0.7089105905940244	T	T	T
0.3536370721966703	0.4388689755465854	0.7132300406951042	T	T	T
0.2971520895419780	0.4284046054238916	0.8900320851918609	T	T	T
0.2012352823686936	0.4440151735427159	0.0275320648817131	T	T	T
0.1055640166762589	0.4283057532333199	0.8897128926353626	T	T	T
0.1023220387532219	0.4476307029512140	0.6927043736239985	T	T	T
0.2274014032223946	0.4731994594200987	0.7349092477272426	T	T	T
0.3627305066978527	0.6683112084015248	0.7458628569707138	T	T	T
0.2995004471919721	0.6625924677315266	0.9144908102060246	T	T	T
0.1919209515483671	0.6470795624192333	0.0287635060706215	T	T	T
0.0972395692508802	0.6718951024533651	0.8958941617514244	T	T	T
0.1061668843763183	0.6552328836354365	0.7008941212039109	T	T	T
0.2331416453880775	0.6389386027801861	0.7467212560357913	T	T	T

Structure files (CONTCAR) involved in this work:

0.3212087214931458	0.5499099107429850	0.8136800836827215	T	T	T
0.0852137325148344	0.5498889632147217	0.8204566167379849	T	T	T
0.4293671686704043	0.3737310071942826	0.5838033845593217	T	T	T
0.4165454883368001	0.5058725356092357	0.5659853871176969	T	T	T
0.3985861879778576	0.6384404516787557	0.5600834038365146	T	T	T
0.1957148061951282	0.3729175595859237	0.6098502820291166	T	T	T
0.1800947527347737	0.5000997255257669	0.5529480825199782	T	T	T
0.1943584285505436	0.6344645716840073	0.5558987742111736	T	T	T
0.9917998965796820	0.4546332960040066	0.7918113926300662	T	T	T
0.9893663631303554	0.6401904411459418	0.7908974477716126	T	T	T
0.1390036597497857	0.5601085096400894	0.2126083499269777	T	T	T
0.1989965747889170	0.5682757622005264	0.3869744139378996	T	T	T
0.2980070805205624	0.5545076352061387	0.5212403869120058	T	T	T
0.3980836894867905	0.5699174483560817	0.3926858082751151	T	T	T
0.3969927828682807	0.5499359477733725	0.1955444955775876	T	T	T
0.2684239357289812	0.5311488488597899	0.2294475740580852	T	T	T
0.1417696620936743	0.3274488597765375	0.2389105731451346	T	T	T
0.1934094917469225	0.3408091759419570	0.4166904950572789	T	T	T
0.3085626743237620	0.3511419087720001	0.5113960491388350	T	T	T
0.4148216761282879	0.3267857180803597	0.3985096286062206	T	T	T
0.3962570866511495	0.3417745369856119	0.2032224589084641	T	T	T
0.2703919155510345	0.3575795669277800	0.2561243228839751	T	T	T
0.1775522784007020	0.4483322272862924	0.3026476992659823	T	T	T
0.4146131385095341	0.4482525204976860	0.3215847185919782	T	T	T
0.0659080730881357	0.6249212982902288	0.0781120654625961	T	T	T
0.0814214659275998	0.4936572911240293	0.0596119254495791	T	T	T
0.0983296301466620	0.3616034437405984	0.0580491285006625	T	T	T
0.3114718365038509	0.6274808509695591	0.1054247375946278	T	T	T
0.3202776745698498	0.4984985152633460	0.0535229691982295	T	T	T
0.3051538352958184	0.3648405505089360	0.0625269190846580	T	T	T
0.5095876487622134	0.5403988278253242	0.2901557861570049	T	T	T
0.5152480505005970	0.3652628910581024	0.2816030106759210	T	T	T
0.4429085995621574	0.7494402759418315	0.6467904317396511	T	T	T
0.1949461836451188	0.7495918913174063	0.6501834121871634	T	T	T
0.2753473280557688	0.7496338312214912	0.0587894404664040	T	T	T
0.1065027261429974	0.7490761625779164	0.0559310185719326	T	T	T
0.0599086765657430	0.2482549199350427	0.1380061180103816	T	T	T
0.3063696774924146	0.2486481101381111	0.1536869653265194	T	T	T
0.2246995043757889	0.2504542268340302	0.5551533768413992	T	T	T
0.3901428613152026	0.2485594887891366	0.5526590329508397	T	T	T
0.5589606367869705	0.2500024802725640	0.3551143128200989	T	T	T
0.8194259911421363	0.2521776831043408	0.3814082001774429	T	T	T
0.7249462102166152	0.2490096260961651	0.9982820467934883	T	T	T
0.8971079668233745	0.2517868167356034	0.9487833516221719	T	T	T
0.9133676271969464	0.7507784128785505	0.8845144516020207	T	T	T
0.6804506318585181	0.7434093963256543	0.8863409360527540	T	T	T
0.5846990789835703	0.7511102377200480	0.4654830751237277	T	T	T
0.7896401521718491	0.6798522979449438	0.0829919467673072	T	T	T
0.6825741487425971	0.7498001065144688	0.1583345135854792	T	T	T
0.8717290805343904	0.7910225408870392	0.0941869168830639	T	T	T
0.7878680068892284	0.7521000440551242	0.5072748562387844	T	T	T
0.9127406874829702	0.6700433757630774	0.8219398614912391	T	T	T
0.6723672815490095	0.8279016038686053	0.8478837296640527	T	T	T

Structure files (CONTCAR) involved in this work:

0.7666905015343879	0.6686740256245826	0.4848077480208828	T	T	T
0.6960954858778716	0.6896356094521354	0.0632633935469806	T	T	T
0.6790974665453940	0.8181626665229634	0.0756135939270929	T	T	T
0.8624213855228066	0.7148508052012434	0.0055331633695487	T	T	T
0.9135260678746259	0.7848925203780037	0.1843297314260155	T	T	T
0.8825951131420229	0.7346941153114247	0.2540287505464109	T	T	T
0.9135798067233845	0.8350446652593907	0.2182224744602277	T	T	T
0.8882342088285911	0.8280679729910159	0.0511281276683018	T	T	T
0.9646918009994677	0.7717481541047420	0.1616268178638952	T	T	T
0.8299949217893068	0.7470937436195536	0.2692739412832319	T	T	T
0.9078436280301110	0.7358581180851502	0.3268114453102697	T	T	T
0.8870773410226310	0.6829096479568503	0.2261198207239172	T	T	T
0.7972111055990186	0.6904872950412545	0.1538242108787562	T	T	T

Figure 4(b) Route(a)-Cu ④

Si O Al Cu C H

1.0000000000000000

20.0219993591000005 0.0000000000000000 0.0000000000000000

0.0000000000000000 19.8990001678000006 0.0000000000000000

0.0000000000000000 0.0000000000000000 13.3830003737999998

93 195 3 3 2 7

Selective dynamics

Direct

0.4196976507880079	0.0536966060173956	0.6422184136613561	T	T	T
0.2985903622438020	0.0265576868907042	0.7851016832762915	T	T	T
0.2775864181741430	0.0641047121682561	0.0058876892958222	T	T	T
0.1178816179310846	0.0647960126969880	0.0058889520939664	T	T	T
0.0644622121670590	0.0249310762032181	0.7956387074872474	T	T	T
0.1736624766120422	0.0512617868899612	0.6451129645596846	T	T	T
0.4200960819439219	0.8272461372936826	0.6619845780440364	T	T	T
0.3021939944607497	0.8691041497673941	0.8039779195488213	T	T	T
0.2689892184398817	0.8279500640675187	0.0261467958796344	T	T	T
0.1145240194477500	0.8257615043121318	0.0163437620335805	T	T	T
0.0643795908014866	0.8644364706719972	0.8005012615678113	T	T	T
0.1809571412084823	0.8269516915959680	0.6657995488112425	T	T	T
0.0738393312209193	0.9438298722166303	0.1435095685296086	T	T	T
0.1959002656971340	0.9721509031460431	0.2861684224714513	T	T	T
0.2158148246666074	0.9339129028314359	0.5062229247555111	T	T	T
0.3747611077491437	0.9306321824993098	0.5087699507782523	T	T	T
0.4281065363358066	0.9714444103162968	0.3008997047733642	T	T	T
0.3215106442864478	0.9477277059001727	0.1461454494044249	T	T	T
0.0771514625833838	0.1705419496815604	0.1610679972412443	T	T	T
0.1957002508553919	0.1295575990406324	0.3036336447902320	T	T	T
0.2274266851873220	0.1715151669770114	0.5223531730673933	T	T	T
0.3824009314087358	0.1723090056228903	0.5099280129917643	T	T	T
0.4328206595294229	0.1283373100218911	0.3005932117790239	T	T	T
0.3176747074875115	0.1688964030439401	0.1673289717501670	T	T	T
0.5721294607962866	0.5564735946452853	0.3566123422796466	T	T	T
0.6914479061918252	0.5267165092041552	0.2179611950634324	T	T	T
0.7111171406214227	0.5461082340678606	0.9891590396255351	T	T	T
0.8686629339411597	0.5636740422450445	0.9875320228047396	T	T	T
0.9312236357282718	0.5305792305646027	0.1941012696982036	T	T	T
0.8184850439502422	0.5619746287467962	0.3350334718125285	T	T	T

Structure files (CONTCAR) involved in this work:

0.5789394782251623	0.3267561714078171	0.3292815495801953	T	T	T
0.7011331138049969	0.3698008465262914	0.2094015033721533	T	T	T
0.7316866439250276	0.3292626011208812	0.9896211892724917	T	T	T
0.8870304223158341	0.3293507165590397	0.9925579198238658	T	T	T
0.9342592847472004	0.3729024480733513	0.2035465100666912	T	T	T
0.8238674207264515	0.3297115863889520	0.3462421687228114	T	T	T
0.9236297631371114	0.4435693906680159	0.8546041660611140	T	T	T
0.8035913125859424	0.4657821743123152	0.7182255882539902	T	T	T
0.7803277788497511	0.4459840489662287	0.4916671529984047	T	T	T
0.6206251560877419	0.4323042709563242	0.4898249086326391	T	T	T
0.5638501555000385	0.4617958761589680	0.6995840605382304	T	T	T
0.6764350767212545	0.4275536139682087	0.8372604908278732	T	T	T
0.7942600584469580	0.6205969847659877	0.7040403100807554	T	T	T
0.6056697418404835	0.6735224301219546	0.4845576870732200	T	T	T
0.5669058197897832	0.6202845130788953	0.7005740623074563	T	T	T
0.6735089225191828	0.6681847091957418	0.8469786598106412	T	T	T
0.5735386726470493	0.9445316447279142	0.3591325531078364	T	T	T
0.6949083151868268	0.9756897807862333	0.2222110512437669	T	T	T
0.7116711689866704	0.9500392665550460	0.9944184789822629	T	T	T
0.8722862275665817	0.9434968665113225	0.9877709591080294	T	T	T
0.9290471238357438	0.9687489130520879	0.1997523266652167	T	T	T
0.8176455322588538	0.9334398901990523	0.3420140247113237	T	T	T
0.5785926545116858	0.1734403068815366	0.3292540170836613	T	T	T
0.7019433289107051	0.1314965899820072	0.2095231094095978	T	T	T
0.7340503754199594	0.1680497759412191	0.9888096698130662	T	T	T
0.8903203517967307	0.1766594981568305	0.9860834298775155	T	T	T
0.9341472281132602	0.1267261434089142	0.2013998888805660	T	T	T
0.8235244648553162	0.1752265093157161	0.3431391454079221	T	T	T
0.9211605282171905	0.0642909329179761	0.8529507227441904	T	T	T
0.8035267004320019	0.0339027307689762	0.7132699805064492	T	T	T
0.7811393879337701	0.0572084437810175	0.4866656918566067	T	T	T
0.6209425895009237	0.0691050665113750	0.4901104017304039	T	T	T
0.5646582196309262	0.0362057011718579	0.6997318208836705	T	T	T
0.6771245062101680	0.0665534374234485	0.8383986032910707	T	T	T
0.9129829504919085	0.8290658878399967	0.8309155175310873	T	T	T
0.7958021821812952	0.8767640685874044	0.7084954074493862	T	T	T
0.7661012174787982	0.8288513237118293	0.4904347383509248	T	T	T
0.6078932920791850	0.8251404707781450	0.4926431835550422	T	T	T
0.5638021771539952	0.8779259550157076	0.7052516938086254	T	T	T
0.4199786615280835	0.4433159200370794	0.6434774135313229	T	T	T
0.3000939041304175	0.4723406505070538	0.7874441386023511	T	T	T
0.2800804938579073	0.4337711550831822	0.0070842674315663	T	T	T
0.1209419013370619	0.4314360292215560	0.0080839571966157	T	T	T
0.0699223307138372	0.4715786358808813	0.7992211387362740	T	T	T
0.1767323541349460	0.4476563210537498	0.6470127164774606	T	T	T
0.4224397046750831	0.6715342760309515	0.6636616428970811	T	T	T
0.3042320583594275	0.6288329149381708	0.8047877766629813	T	T	T
0.2699633751608911	0.6715661916964152	0.0259515918520387	T	T	T
0.1163590498593206	0.6729878475990020	0.0130694282562449	T	T	T
0.0678844823806831	0.6297311133285513	0.8017810226281193	T	T	T
0.1825528218023839	0.6686308695107434	0.6644869153158903	T	T	T
0.0757983030077807	0.5550123601242593	0.1396995785660418	T	T	T
0.1963044263927444	0.5261547582423768	0.2829943578393100	T	T	T

Structure files (CONTCAR) involved in this work:

0.2180716546006865	0.5632176915969702	0.5047040733323107	T	T	T
0.3773464947706289	0.5664096796634485	0.5088173787151722	T	T	T
0.4283409040308068	0.5257142904488700	0.3000264285454332	T	T	T
0.3226193051055995	0.5513253055651831	0.1445553890954075	T	T	T
0.0778252823174030	0.3255616407376882	0.1632081080304513	T	T	T
0.1953456833084236	0.3685407785193951	0.3040013496828788	T	T	T
0.2294515527934760	0.3279188304048708	0.5236861505862983	T	T	T
0.3844620971495152	0.3243958396765148	0.5118123902665278	T	T	T
0.4336547250537700	0.3696127835495510	0.3017951309360851	T	T	T
0.3182309390459863	0.3279976090822563	0.1686701990650030	T	T	T
0.3534904241983908	0.0598261881086836	0.7114271658246056	T	T	T
0.2959716772924060	0.0698105517788082	0.8881512816059353	T	T	T
0.1975525755476814	0.0537418441009828	0.0216693512449739	T	T	T
0.0987095877217988	0.0651474177396912	0.8884258509944722	T	T	T
0.0987847596570294	0.0493385100587785	0.6919351957141288	T	T	T
0.2256774280196677	0.0287946201186061	0.7322414167545594	T	T	T
0.3598590397324649	0.8297322655125566	0.7432517262323799	T	T	T
0.3003353026103547	0.8385000859981607	0.9158752072468300	T	T	T
0.1911060504932673	0.8521275322406674	0.0270796877128157	T	T	T
0.0930825112693454	0.8281136273113434	0.9000340796770274	T	T	T
0.1042134437370103	0.8373186630577228	0.7027607932908665	T	T	T
0.2298890658807746	0.8583947339453983	0.7509082162179002	T	T	T
0.3184554276729341	0.9490446765665431	0.8088052891652470	T	T	T
0.0744830418562753	0.9448384306820429	0.8129215228469018	T	T	T
0.4277164599272952	0.1221022926435995	0.5766737063667852	T	T	T
0.4155704016160185	0.9899872927781010	0.5659809405847103	T	T	T
0.3937988501426580	0.8580100494215319	0.5560777954455708	T	T	T
0.1891220546123095	0.1269239017243529	0.6060123034859257	T	T	T
0.1770427073207789	-0.0012318857912346	0.5521613117183113	T	T	T
0.1917462277979143	0.8648038405924786	0.5595372450866978	T	T	T
0.9853172937809348	0.0414498704040823	0.7876380304909280	T	T	T
0.9866100149520765	0.8445279985392828	0.7861774138199769	T	T	T
0.1392356485313775	0.9404153048114207	0.2139969505923700	T	T	T
0.1979827708974331	0.9282585496827190	0.3882581103184439	T	T	T
0.2954365672885259	0.9450888990116099	0.5231924135314819	T	T	T
0.3939133930327710	0.9287501166471358	0.3910073663002991	T	T	T
0.3957833959485558	0.9511021005559568	0.1939380455228246	T	T	T
0.2680704999170351	0.9689110819640390	0.2318353394474664	T	T	T
0.1413171360618045	0.1673054539662033	0.2341641071719410	T	T	T
0.1919143118770590	0.1627003952797066	0.4139689197682850	T	T	T
0.3049315828589140	0.1471431014936239	0.5140993050017897	T	T	T
0.4081820785675517	0.1732394689030014	0.3949254123238743	T	T	T
0.3948782729594753	0.1542011341173233	0.1997230704726035	T	T	T
0.2698290188577232	0.1397346536756081	0.2560320612386899	T	T	T
0.1781345280165672	0.0500628070164180	0.3108229208994526	T	T	T
0.4145851515362382	0.0505235207240634	0.3237163352918027	T	T	T
0.0658579535941191	0.8726694090109877	0.0842471321921213	T	T	T
0.0783141519323581	0.0040704294872618	0.0617510819227227	T	T	T
0.0947451090997233	0.1361010121247994	0.0539813911691090	T	T	T
0.3095481022875429	0.8713972545623596	0.1082533160327168	T	T	T
0.3160968476061018	-0.0007777417815725	0.0521614696377329	T	T	T
0.3011945484041886	0.1326911716337061	0.0613699596862919	T	T	T
0.5072604851167355	0.9558864898513438	0.2916946972363448	T	T	T

Structure files (CONTCAR) involved in this work:

0.5130346537742680	0.1355015260763465	0.2848684436998054	T	T	T
0.6351937444244785	0.5661697772615831	0.2807798236137091	T	T	T
0.6782948205476697	0.5382777116637901	0.0993387090363538	T	T	T
0.7913202296613030	0.5398633332337164	0.9965749018154851	T	T	T
0.9019509563901215	0.5700082006864926	0.0976525914976606	T	T	T
0.8942011836297498	0.5586152328801486	0.2945515989477985	T	T	T
0.7652826707254867	0.5570683659354949	0.2445725845903358	T	T	T
0.6377295290289388	0.3258404419784771	0.2455191997192739	T	T	T
0.7040963789742469	0.3669346180583956	0.0889598919223264	T	T	T
0.8094663720306123	0.3511522873673358	0.9761147988365748	T	T	T
0.9055798270150475	0.3293164752865650	0.1106466095656067	T	T	T
0.8985405610067994	0.3480863266498773	0.3060268545155220	T	T	T
0.7706766895305884	0.3415690003930327	0.2555081457350983	T	T	T
0.6904667382803806	0.4473268754830597	0.2458291223621521	T	T	T
0.9154605591139545	0.4512013891551527	0.1823264603448261	T	T	T
0.5563772978654312	0.6239767689567179	0.4201816859938067	T	T	T
0.5862844221136762	0.4952107721621549	0.4335269759947764	T	T	T
0.6071313213596308	0.3631833555648258	0.4291147311034624	T	T	T
0.8139794254469087	0.6397425478914037	0.3857429699265893	T	T	T
0.8029801957157314	0.5094505944224637	0.4220893611694229	T	T	T
0.8061187174784059	0.3767524502434876	0.4411223289029557	T	T	T
0.0098569960471399	0.5454116488293886	0.2093389640591412	T	T	T
0.0145389065487676	0.3643261538698798	0.2141208120708036	T	T	T
0.8617574360383994	0.4266219155509995	0.7803270046609119	T	T	T
0.8154595578041396	0.4534156473477155	0.5997248206863975	T	T	T
0.7000363188570605	0.4458242086703388	0.5011532916142105	T	T	T
0.5870542632915539	0.4231625040036455	0.5986936390112382	T	T	T
0.6011503776531348	0.4265243317130244	0.7937869211993436	T	T	T
0.7305935318651290	0.4351946689127136	0.7475702141320241	T	T	T
0.8573298851763083	0.6677329472597425	0.7263149183880461	T	T	T
0.7771820149219205	0.6157588595981632	0.5875015057384173	T	T	T
0.6809645179970890	0.6605049295103981	0.4493274954133293	T	T	T
0.5973289138677799	0.6590894617814764	0.6046708573712140	T	T	T
0.6001051779231703	0.6482011216206647	0.8043552969727794	T	T	T
0.7291710238486885	0.6482043664499848	0.7665569149992660	T	T	T
0.8077841253433315	0.5444296632446289	0.7484794522867366	T	T	T
0.5841765534904314	0.5406061008328255	0.6920095139213100	T	T	T
0.9345818392121380	0.3809826563072514	0.9314150695854418	T	T	T
0.9101299055055834	0.5106884876153701	0.9210409506089949	T	T	T
0.8742518290008844	0.6374097299830087	0.9338447458550163	T	T	T
0.6888420553058613	0.3573137947910515	0.8958161899199835	T	T	T
0.6815653425811978	0.4919933205156998	0.9125825393527124	T	T	T
0.6881976592895108	0.6232581373397436	0.9538594462132655	T	T	T
0.4840447477174986	0.4532236152431314	0.7163574818767842	T	T	T
0.4866079803438479	0.6310893590994633	0.7077211669425637	T	T	T
0.6368997243787206	0.9372154239330180	0.2838488832719369	T	T	T
0.6809728215069509	0.9677135101124563	0.1035637652982640	T	T	T
0.7922796723082655	0.9528079251886259	0.9955341982457956	T	T	T
0.9032136808295240	0.9307477283789211	0.0988766918755175	T	T	T
0.8932029541324277	0.9358723827183721	0.2969393870391795	T	T	T
0.7666701368133855	0.9418420302709324	0.2474617037403057	T	T	T
0.6361263966704914	0.1730050968775998	0.2433555885883870	T	T	T
0.7067515468858497	0.1308023416586675	0.0888422746692185	T	T	T

Structure files (CONTCAR) involved in this work:

0.8130833470436786	0.1519158032677093	0.9748355771967178	T	T	T
0.9124329642054729	0.1678882814493105	0.1019041659702005	T	T	T
0.8976354820547321	0.1588004191287532	0.2989361590237089	T	T	T
0.7693298814023678	0.1662059276482665	0.2531930183288462	T	T	T
0.6955495378681238	0.0550508481037835	0.2521224509280649	T	T	T
0.9119426687647025	0.0483666846653824	0.1908141991931796	T	T	T
0.5642269922975974	0.8771744134620350	0.4252087050986572	T	T	T
0.5832820925248176	0.0080330985950853	0.4333952530769049	T	T	T
0.6065949085553682	0.1386965823997106	0.4304945351847389	T	T	T
0.8069698215232373	0.8616129494424795	0.3959056809265432	T	T	T
0.8070301709414287	0.9949372539713449	0.4193897320343348	T	T	T
0.8057153942456985	0.1274305302048349	0.4369282216042031	T	T	T
0.0085221657412487	0.9554416913202678	0.2131894497936884	T	T	T
0.0147525461162713	0.1322180013330402	0.2150927946011350	T	T	T
0.8582091962862158	0.0753280218390118	0.7786638909088727	T	T	T
0.8144532322470300	0.0520938477335709	0.5965107008091051	T	T	T
0.7004947167006781	0.0548650932555598	0.4952030257306865	T	T	T
0.5903659582518721	0.0767048406318930	0.6012783683062701	T	T	T
0.6011243979816411	0.0691764157326696	0.7969306438851973	T	T	T
0.7285248039265734	0.0570640364676006	0.7453719205400505	T	T	T
0.8615209738763704	0.8318532533680554	0.7380263416561341	T	T	T
0.7842004132429264	0.8734209619483436	0.5886036179621270	T	T	T
0.6864500026353342	0.8361539443156962	0.4667780851325755	T	T	T
0.5955660755616924	0.8369769842709273	0.6108673600324038	T	T	T
0.5922389777010935	0.8492481256627992	0.8085296463643492	T	T	T
0.7323057976680638	0.8527508614719039	0.7704442208170097	T	T	T
0.8149261045485742	0.9548067700474773	0.7358900379991961	T	T	T
0.5829344900924560	0.9572469603563674	0.6891498016039299	T	T	T
0.9377245735281993	0.1343072398222983	0.9105776653904881	T	T	T
0.9052063907350366	0.0108646315364377	0.9416090126524039	T	T	T
0.8936532272545552	0.8812161949213060	0.9183041127474423	T	T	T
0.6928928845615481	0.1371896415112454	0.8952200072890487	T	T	T
0.6831976380761566	0.0025545566647944	0.9135472099214318	T	T	T
0.6850087102481046	0.8732450946863335	0.9693993305351940	T	T	T
0.4846037234070120	0.0464244091119150	0.7137739062672274	T	T	T
0.4823796954920421	0.8709045387149243	0.7031436212528361	T	T	T
0.3534785572097379	0.4386229999628148	0.7117951818391095	T	T	T
0.2971673602944238	0.4274431721711276	0.8889383489334952	T	T	T
0.2002529265379902	0.4437758290964998	0.0252139503752493	T	T	T
0.1029502355281999	0.4284054525429269	0.8902951395123765	T	T	T
0.1018540763060206	0.4480826143362733	0.6932753882444527	T	T	T
0.2272837328300561	0.4727902659371118	0.7344638209623279	T	T	T
0.3628515305925916	0.6676123220745021	0.7452945969230412	T	T	T
0.3004854892655967	0.6618178505577672	0.9150091930910249	T	T	T
0.1925288171176274	0.6465345505260195	0.0287876267331254	T	T	T
0.0988766550353219	0.6722389397586979	0.8954520039983427	T	T	T
0.1063356786234621	0.6550117901987973	0.7007463355907297	T	T	T
0.2332013835456597	0.6377352312684210	0.7478487357933520	T	T	T
0.3216704002987676	0.5491313649849481	0.8135494626700158	T	T	T
0.0843962923811413	0.5503718400120866	0.8210583896991481	T	T	T
0.4288761050760956	0.3733799041864166	0.5821693709349746	T	T	T
0.4169752692481593	0.5054709021882987	0.5643598698857406	T	T	T
0.3978115168455053	0.6377891984017784	0.5589612774261645	T	T	T

Structure files (CONTCAR) involved in this work:

0.1943479343513024	0.3719648622870670	0.6108271153671488	T	T	T
0.1796528598614721	0.4986474840251137	0.5521869575150283	T	T	T
0.1944730257303886	0.6328045089322061	0.5567905006052394	T	T	T
0.9906183824879615	0.4556848294589229	0.7900800592382312	T	T	T
0.9895840944259539	0.6420809262759308	0.7930053240728521	T	T	T
0.1401153440959534	0.5603664425232054	0.2121914749915461	T	T	T
0.1992292877331918	0.5677430313775796	0.3870195969472498	T	T	T
0.2978282506406336	0.5526592357457664	0.5213056678775291	T	T	T
0.3970036043422802	0.5694625614140654	0.3913166017214519	T	T	T
0.3963361163616510	0.5477275753136767	0.1938362949873103	T	T	T
0.2685622062622000	0.5297914395391635	0.2291301116683813	T	T	T
0.1401510463399146	0.3275383940426999	0.2400172796047327	T	T	T
0.1925057892046494	0.3403695784603686	0.4173054952924798	T	T	T
0.3073100828226090	0.3504590093152317	0.5124966068719246	T	T	T
0.4129638068178055	0.3250581553600630	0.3983829910078207	T	T	T
0.3952347722159629	0.3411233870927954	0.2032125417692187	T	T	T
0.2692127110467504	0.3569062345200434	0.2561462689569400	T	T	T
0.1769266368645489	0.4480438622235505	0.3030802592238704	T	T	T
0.4124325874383470	0.4470189001916464	0.3228097825860630	T	T	T
0.0667285892536749	0.6244275851938661	0.0768950819956007	T	T	T
0.0804825345678257	0.4924809745098897	0.0620190567796243	T	T	T
0.0981658495918141	0.3606321063861995	0.0578599989326472	T	T	T
0.3114837168146870	0.6277760049886464	0.1066738577834268	T	T	T
0.3184734104167510	0.4995281848981027	0.0507935412457648	T	T	T
0.3044363785147880	0.3656164053896971	0.0629189494392567	T	T	T
0.5078538583717270	0.5381953111714834	0.2884764650413950	T	T	T
0.5139385059605532	0.3651264027624666	0.2836085225905350	T	T	T
0.4413438908716345	0.7494796252214350	0.6433087052076218	T	T	T
0.1968462485467089	0.7480753001232735	0.6496343775248087	T	T	T
0.2749469059487196	0.7497553780386338	0.0582499354386472	T	T	T
0.1073874837839448	0.7489109592722418	0.0562837626789495	T	T	T
0.0576483651238399	0.2483338752501481	0.1400996644136906	T	T	T
0.3050470339335827	0.2485895011461073	0.1522565935000026	T	T	T
0.2232713836112278	0.2496641029351923	0.5561592456696629	T	T	T
0.3889503005239438	0.2480901319423769	0.5543492956642420	T	T	T
0.5590772349491110	0.2502336753271665	0.3568969742164287	T	T	T
0.8216323092440037	0.2522692498172857	0.3829754177955835	T	T	T
0.7224818706405907	0.2486548465345721	0.9976397315791458	T	T	T
0.8984075604503299	0.2540703711413342	0.9512064497804960	T	T	T
0.9117061004843610	0.7537613445542597	0.8829219984465072	T	T	T
0.6774338539216622	0.7438852702297231	0.8871202439030741	T	T	T
0.5821257779995767	0.7503920117586265	0.4633290239251569	T	T	T
0.7910944019642487	0.6852450842456185	0.0905635777702575	T	T	T
0.6768360636776363	0.7469142963102228	0.1634700049179411	T	T	T
0.8386088108041664	0.7982155210461294	0.0763171599102083	T	T	T
0.7889321769194757	0.7520208774025186	0.5022751082481482	T	T	T
0.9128000525342557	0.6725790315225642	0.8228859329866645	T	T	T
0.6707375513136735	0.8287062356252304	0.8518911448945091	T	T	T
0.7607602012572164	0.6708242379594355	0.4923379279393181	T	T	T
0.6961369397834457	0.6869019480288565	0.0696838961379330	T	T	T
0.6772462534178680	0.8150310683449231	0.0796840032129675	T	T	T
0.8550750434858334	0.7225260463703664	0.0006297866561403	T	T	T
0.9614409579216338	0.7703265304797604	0.2653920717295573	T	T	T

Structure files (CONTCAR) involved in this work:

0.9342230318444126	0.7381369526252559	0.3429124281165976	T	T	T
0.9437702865469967	0.8202033051528805	0.2440192846021572	T	T	T
0.8806916667271660	0.8191435052636350	0.0968454606070801	T	T	T
1.0034741064553401	0.7498941794467781	0.2230653424041949	T	T	T
0.8944066645271085	0.7617535645227776	0.3867812408584483	T	T	T
0.9539647946649860	0.6897564508136351	0.3682079690668428	T	T	T
0.8463395962470923	0.6727591713997414	0.3596258122217481	T	T	T
0.7957614632045485	0.7236959504856809	0.1376088907543052	T	T	T

Figure 4(b) Route(b-i)-Cu ① as same as Route(a)-Cu ①**Figure 4(b) Route(b-i)-Cu ②**

Si	O	Al	Cu	C	H
1.0000000000000000					
20.0219993591000005	0.0000000000000000	0.0000000000000000			
0.0000000000000000	19.8990001678000006	0.0000000000000000			
0.0000000000000000	0.0000000000000000	13.3830003737999998			
93	195	3	3	2	7

Selective dynamics

Direct

0.4212072609358669	0.0540010671253087	0.6370878790300027	T	T	T
0.3018925895133980	0.0255313408034822	0.7830385895282836	T	T	T
0.2798085066307228	0.0632952529237287	0.0026186067337974	T	T	T
0.1203765489161211	0.0642082918196617	0.0017633628790486	T	T	T
0.0709655095024086	0.0311679780012813	0.7899646557561035	T	T	T
0.1801295468006815	0.0531225071128875	0.6413995012773167	T	T	T
0.4210897858077832	0.8265816924586431	0.6631875193502413	T	T	T
0.3001798783997887	0.8680887266516291	0.8012537962056300	T	T	T
0.2666399171022699	0.8276014261264905	0.0229131189675899	T	T	T
0.1117322388306568	0.8260620062364051	0.0154703893184195	T	T	T
0.0625423298299136	0.8748411993657458	0.8044862155882935	T	T	T
0.1745479515237454	0.8286280462894179	0.6683759994272166	T	T	T
0.0757459070854119	0.9451607239839732	0.1416133772013898	T	T	T
0.1974000626189226	0.9720136287299854	0.2869354179904726	T	T	T
0.2164198601038866	0.9322647807710183	0.5057621758728179	T	T	T
0.3764738525035108	0.9288187199106618	0.5060532306293052	T	T	T
0.4287666667912344	0.9692264492879188	0.2972977969987394	T	T	T
0.3211681434360141	0.9469823280783433	0.1445512837903113	T	T	T
0.0772471092872630	0.1687893879065435	0.1605313779226057	T	T	T
0.1956208534589852	0.1288739233016728	0.3046716750861832	T	T	T
0.2325956656736490	0.1731696044420647	0.5190889353988375	T	T	T
0.3869495942065275	0.1735045556491943	0.5048213880475276	T	T	T
0.4345877973613569	0.1267490511799509	0.2951431821729105	T	T	T
0.3168325458927583	0.1681692369991720	0.1647928443673291	T	T	T
0.5747477333635468	0.5568806353524803	0.3552899763853870	T	T	T
0.6969043332542472	0.5327781633921760	0.2195492701646232	T	T	T
0.7154660546795913	0.5519733750003535	0.9868563115806953	T	T	T
0.8735865228438484	0.5642613347408453	0.9939890585787243	T	T	T
0.9288494380240283	0.5200308386858408	0.2035399037382453	T	T	T
0.8209867451308149	0.5608044292405157	0.3492659182649943	T	T	T
0.5798864365941663	0.3262432704197215	0.3287784419880709	T	T	T
0.7056050243059491	0.3743059525450958	0.2123154686561447	T	T	T
0.7308739831076030	0.3288290482851717	0.9924709218350212	T	T	T
0.8890400169104550	0.3254720395906460	0.9955227164148341	T	T	T

Structure files (CONTCAR) involved in this work:

0.9363062872417258	0.3624477720310325	0.2092402903164486	T	T	T
0.8248691578554147	0.3260015187441329	0.3491840386180561	T	T	T
0.9240661605051358	0.4445025357208092	0.8615194714111353	T	T	T
0.8026998788231798	0.4664716615917742	0.7238290820885489	T	T	T
0.7807210025316006	0.4408253398787039	0.4973469046255291	T	T	T
0.6199432849052089	0.4303240567394142	0.4909248883705630	T	T	T
0.5632494918184765	0.4646727575387367	0.7022838632801810	T	T	T
0.6754175938802860	0.4309812973038420	0.8431279580903090	T	T	T
0.7940222793036503	0.6242789014317955	0.7179839511167146	T	T	T
0.6123091071004797	0.6694217834891155	0.4890842082031094	T	T	T
0.5600859413419580	0.6223019425433444	0.7005842453335934	T	T	T
0.6677532512224577	0.6667145754866979	0.8365282795941275	T	T	T
0.5753964356937821	0.9382753769549080	0.3483895240686534	T	T	T
0.6931808522552479	0.9676586426499849	0.2036999884573287	T	T	T
0.7198104378474394	0.9533339851557185	0.9789793731218699	T	T	T
0.8752618691394619	0.9477890471464531	0.9816165235111883	T	T	T
0.9314939650014907	0.9698347038054295	0.1952650393530314	T	T	T
0.8166922771851214	0.9291010147033887	0.3254101520775715	T	T	T
0.5803402742188487	0.1708665469646880	0.3176505677279716	T	T	T
0.7016954282114385	0.1252330706267984	0.1985352620070745	T	T	T
0.7323404720806950	0.1699537643009235	0.9801057189132647	T	T	T
0.8899598082065221	0.1752727636655428	0.9757537669881973	T	T	T
0.9313239531676899	0.1271569734029608	0.1962138024087017	T	T	T
0.8213820947858624	0.1724077570881485	0.3393490609057179	T	T	T
0.9255636869660591	0.0611688509665172	0.8363997185537343	T	T	T
0.8022270314256449	0.0293234636086242	0.7036876983732563	T	T	T
0.7831778101307031	0.0511612830080967	0.4756932906625361	T	T	T
0.6228989719141378	0.0646006356007069	0.4777862765809969	T	T	T
0.5663595071554097	0.0338819815776893	0.6888287567102714	T	T	T
0.6788444021295952	0.0702246200939510	0.8273316046731553	T	T	T
0.9143676470855296	0.8336931757261514	0.8299053814590764	T	T	T
0.7978799788004030	0.8726523082509163	0.6944257255944312	T	T	T
0.7667804344268351	0.8330859626472842	0.4824464874117284	T	T	T
0.6120054141678671	0.8257810179813809	0.4897889522289486	T	T	T
0.5639746448761229	0.8758489563482073	0.7021518494196706	T	T	T
0.4192416313503870	0.4442167183768732	0.6456198794766564	T	T	T
0.2985132255545628	0.4730850262525065	0.7877744109995062	T	T	T
0.2800749891690701	0.4341813143291202	0.0091135262500189	T	T	T
0.1212141478634091	0.4319525746126570	0.0091340508319079	T	T	T
0.0690973308128588	0.4682841752888210	0.7990163486338648	T	T	T
0.1757662386450183	0.4465377546304953	0.6471679736763616	T	T	T
0.4176134234380348	0.6713081477811318	0.6619117154848096	T	T	T
0.2990223383216790	0.6300341991214782	0.8024183525648225	T	T	T
0.2659320676844713	0.6715325036696728	0.0236832941249443	T	T	T
0.1115044745187461	0.6717957916780279	0.0119545501427479	T	T	T
0.0605948110233772	0.6266856601548000	0.8000657526054491	T	T	T
0.1758030326228911	0.6692128491121118	0.6652351355452149	T	T	T
0.0731765410659573	0.5540219692332867	0.1411071675313726	T	T	T
0.1948567821737300	0.5260969323029761	0.2836337151725130	T	T	T
0.2144692840214027	0.5637139828108108	0.5062743988895271	T	T	T
0.3739934125553186	0.5660743061057517	0.5090219080474009	T	T	T
0.4281468764955969	0.5268811452779555	0.2990956543668403	T	T	T
0.3215317216229482	0.5529894883831785	0.1459254394601251	T	T	T

Structure files (CONTCAR) involved in this work:

0.0803490740107373	0.3232141618090562	0.1630519480932879	T	T	T
0.1975539774955523	0.3680076273035288	0.3021484549042937	T	T	T
0.2326909761529153	0.3291200575340615	0.5214804332984689	T	T	T
0.3874613037416178	0.3262568080220889	0.5100025699227445	T	T	T
0.4360692958242571	0.3694679563738522	0.2970376547186878	T	T	T
0.3194298972180361	0.3270974487611949	0.1671415864771354	T	T	T
0.3562803679637444	0.0589838273993591	0.7089277443001591	T	T	T
0.3005203400162442	0.0689747366753764	0.8858385237672866	T	T	T
0.1998122344278268	0.0514613079010201	0.0147747366088054	T	T	T
0.1001530030829642	0.0726859388865954	0.8851926859866263	T	T	T
0.1050431739331023	0.0546666775894344	0.6861597936697842	T	T	T
0.2289987224347975	0.0280977246425611	0.7305939723613699	T	T	T
0.3563144826876167	0.8292282283997244	0.7365095071895542	T	T	T
0.2998016029868282	0.8372518534162858	0.9134011492320614	T	T	T
0.1886837920961120	0.8517043134404931	0.0206603258819585	T	T	T
0.0853898647431549	0.8321730784793377	0.9017626285634270	T	T	T
0.0977269564789254	0.8409450816437496	0.7066990037985128	T	T	T
0.2263310552253337	0.8579762801562932	0.7518814392037625	T	T	T
0.3192500690894303	0.9474429155005285	0.8066035732152272	T	T	T
0.0863871899443877	0.9524649782855727	0.8132022995339945	T	T	T
0.4301973555811449	0.1234853735616912	0.5747193986077385	T	T	T
0.4140851112698172	0.9919894205150144	0.5586575423111889	T	T	T
0.4020165535886759	0.8588379971418041	0.5549039619137387	T	T	T
0.1980653924467443	0.1285787403534432	0.6056838271776485	T	T	T
0.1832769974495267	1.0014487709513944	0.5475820280329948	T	T	T
0.1854129596560521	0.8671205329684322	0.5623298538991899	T	T	T
0.9922780997180253	0.0463934676349900	0.7726374054313169	T	T	T
0.9813454569923439	0.8752898819661777	0.7992185204702601	T	T	T
0.1411625097629318	0.9425560389463108	0.2119405108627477	T	T	T
0.1991452511358187	0.9260533944776296	0.3873399315797111	T	T	T
0.2965046370583291	0.9362019997709446	0.5240833537191351	T	T	T
0.3936163242790309	0.9274202189352098	0.3876843292998442	T	T	T
0.3956550432318540	0.9481555457452263	0.1912073497864120	T	T	T
0.2692906812934509	0.9698672928420911	0.2316466573117771	T	T	T
0.1382456961076549	0.1647860380833492	0.2389644976114609	T	T	T
0.1938234483753085	0.1641642521805068	0.4135121455925448	T	T	T
0.3094853902574741	0.1486059443556255	0.5049651653829256	T	T	T
0.4145087844212529	0.1727229494260839	0.3908791906142940	T	T	T
0.3937252778629184	0.1527995712899099	0.1972319865882695	T	T	T
0.2682536771486778	0.1388399144990074	0.2523067454576547	T	T	T
0.1796851088841925	0.0492317302993105	0.3157834877686600	T	T	T
0.4167998009002480	0.0488547213349109	0.3193020433071392	T	T	T
0.0657186640102649	0.8716384196383371	0.0897165447003542	T	T	T
0.0813700684434617	0.0009758695382916	0.0529266593674449	T	T	T
0.0980838127678431	0.1332292627832861	0.0562536011377660	T	T	T
0.3057594372841677	0.8713663489682453	0.1061612648693117	T	T	T
0.3177572179898561	0.9989610761052660	0.0510767711537338	T	T	T
0.3010541481716584	0.1325680503638978	0.0581735346018800	T	T	T
0.5072604036842366	0.9518763974708997	0.2863505212908758	T	T	T
0.5140258433416606	0.1341600469380479	0.2734629406358338	T	T	T
0.6344807652682956	0.5680596581897742	0.2745641758320022	T	T	T
0.6901151705598939	0.5446009295300489	0.1004887447338667	T	T	T
0.7955068625431704	0.5460261155849986	0.9747783861150608	T	T	T

Structure files (CONTCAR) involved in this work:

0.8907195553077881	0.5556482947427034	0.1116317587149996	T	T	T
0.8953244565866811	0.5457196357367986	0.3079960811513031	T	T	T
0.7666566738521331	0.5653499398774691	0.2607276793940552	T	T	T
0.6433614595728844	0.3311300290304015	0.2540183313668044	T	T	T
0.7062097979004089	0.3677975492326017	0.0921892078716718	T	T	T
0.8103997258845015	0.3428840317289791	0.9798809817531896	T	T	T
0.9081156043023120	0.3210207407263271	0.1135628062064392	T	T	T
0.9018159065038670	0.3344490418258085	0.3108655547696267	T	T	T
0.7755473222673480	0.3458673128777321	0.2568538384595240	T	T	T
0.6974747903425936	0.4526749720676911	0.2447482307505660	T	T	T
0.9163781037758045	0.4405702080257854	0.1929746423375794	T	T	T
0.5615890963370737	0.6247335983300640	0.4196376411237170	T	T	T
0.5925081005384364	0.4948519441416305	0.4296610332981138	T	T	T
0.5984660522751863	0.3613137212015987	0.4346731341092676	T	T	T
0.8265709500658396	0.6381031417813154	0.4020312474917307	T	T	T
0.7991041323370898	0.5082862071351794	0.4337020323833853	T	T	T
0.8122427434090703	0.3746043917845702	0.4444471251702476	T	T	T
0.0068574056863290	0.5410502183505963	0.2089563700045425	T	T	T
0.0168399725513359	0.3574208225643634	0.2196405522501280	T	T	T
0.8599828595347969	0.4293931611102318	0.7905754648393548	T	T	T
0.8143195986527959	0.4486338593325382	0.6066291775360317	T	T	T
0.7004502796587654	0.4341863547583752	0.5023512051632022	T	T	T
0.5865787011755085	0.4271963468973374	0.6006765885695835	T	T	T
0.6004022932441425	0.4304502837389024	0.7975199046776708	T	T	T
0.7290731486206741	0.4379608734423807	0.7528378058339711	T	T	T
0.8410241635441631	0.6718786349581655	0.7829876832769183	T	T	T
0.8032659914906306	0.6313497812963719	0.6001080115625725	T	T	T
0.6869345202068691	0.6409152718887549	0.4734602178030869	T	T	T
0.5881485281180362	0.6636495566778264	0.6055610803156896	T	T	T
0.5909504169152374	0.6540431012023475	0.8041682921696048	T	T	T
0.7154351865559548	0.6421086194386955	0.7473270337582204	T	T	T
0.8068137124714003	0.5455747697878836	0.7486798918900871	T	T	T
0.5824309746737345	0.5439040597033710	0.6940977770249041	T	T	T
0.9330736617926557	0.3830800022150672	0.9410273468807313	T	T	T
0.9174635270661403	0.5141510003586622	0.9249519641118082	T	T	T
0.8954751124804453	0.6418044186170002	0.9682954683772658	T	T	T
0.6890131388691774	0.3602593488412003	0.9000653361944208	T	T	T
0.6807446520726003	0.4945246528582521	0.9195133684134068	T	T	T
0.6869630118757148	0.6255211840955095	0.9431035215541000	T	T	T
0.4833464759448019	0.4553948889203749	0.7180093961851776	T	T	T
0.4793306952558464	0.6279780368803042	0.7081491852876254	T	T	T
0.6361951862361193	0.9297852215857753	0.2685528127852251	T	T	T
0.6802169630148042	0.9564239935793709	0.0848509084388377	T	T	T
0.7988700429204764	0.9721961329561198	-0.0008602783909552	T	T	T
0.9125137973062996	0.9367272496956250	0.0873013002712568	T	T	T
0.8932774476003816	0.9295605744329725	0.2834873120062594	T	T	T
0.7667605738233149	0.9374634783602742	0.2297461243345212	T	T	T
0.6366540373051971	0.1690844489592387	0.2299669173737361	T	T	T
0.7113226640506963	0.1272376762091777	0.0785050630235170	T	T	T
0.8113798111649690	0.1586847961326142	0.9578626163659789	T	T	T
0.9083958148884275	0.1612749832999563	0.0918036369990516	T	T	T
0.8956177670737275	0.1645685839074914	0.2901088535237774	T	T	T
0.7673183983615205	0.1572087590425044	0.2514786775010762	T	T	T

Structure files (CONTCAR) involved in this work:

0.6914148465020843	0.0474580328314122	0.2326819648027998	T	T	T
0.9093556635210954	0.0483420239080488	0.1955749320248903	T	T	T
0.5656809379175586	0.8706540719765482	0.4147041985074401	T	T	T
0.5879636366012769	0.0016221213386860	0.4221911534146534	T	T	T
0.6080309908637400	0.1337435674583664	0.4172918955810148	T	T	T
0.8040046267633418	0.8578091912531270	0.3798284004937323	T	T	T
0.8064224031349962	0.9915410941233752	0.4014666470805513	T	T	T
0.8114228920016782	0.1222475378362203	0.4332336392862551	T	T	T
0.0113665629651460	0.9612650269333705	0.2116347283492754	T	T	T
0.0118277720939603	0.1328081270892675	0.2090369682288215	T	T	T
0.8619591331716161	0.0676435740911365	0.7632478593107526	T	T	T
0.8152262333035972	0.0392018316564103	0.5853677202907905	T	T	T
0.7026814166135941	0.0526740170067460	0.4844988063683429	T	T	T
0.5911811327733156	0.0725446374720997	0.5883797174677232	T	T	T
0.6034433724458571	0.0681743965408906	0.7842567548765864	T	T	T
0.7315668658397033	0.0638894787915874	0.7350141777436664	T	T	T
0.8652068017873348	0.8345890415840328	0.7348398969063120	T	T	T
0.8014628081938744	0.8754285913917208	0.5732557305658414	T	T	T
0.6879250711342899	0.8539814308322354	0.4771953059953369	T	T	T
0.5871264206361313	0.8321633671755911	0.6046405380401436	T	T	T
0.5997512199117857	0.8515124350603808	0.8031736857354561	T	T	T
0.7326690612446390	0.8341990123268695	0.7329650347020537	T	T	T
0.8020240139471672	0.9505480457183064	0.7360876011912997	T	T	T
0.5828502192255948	0.9544549802503389	0.6789610202092562	T	T	T
0.9348118008808659	0.1292403198545638	0.9016551504118270	T	T	T
0.9170422866087810	-0.0009583524111916	0.9145115865668488	T	T	T
0.8735880593665550	0.8727283985157188	0.9263355383839187	T	T	T
0.6900970665061531	0.1411055774172282	0.8858479205159617	T	T	T
0.6878016198452722	0.0070225761022620	0.9031682049915101	T	T	T
0.7191382267544503	0.8775341960040878	0.9313978261843736	T	T	T
0.4867603717392131	0.0445109034269364	0.7062486226057033	T	T	T
0.4826869246641671	0.8674995784842775	0.7133062584714920	T	T	T
0.3528035061431731	0.4386051915896444	0.7141671346007489	T	T	T
0.2959224972135344	0.4296672464968525	0.8905408376717883	T	T	T
0.2003687994087349	0.4438270256817476	0.0293006720529592	T	T	T
0.1051429169609854	0.4282774156588565	0.8908818688766584	T	T	T
0.1010477344523070	0.4431424970768814	0.6937317470817930	T	T	T
0.2257544656348798	0.4722227069922494	0.7348467723805249	T	T	T
0.3557748900070549	0.6695003845137348	0.7398802155812297	T	T	T
0.2971037449774474	0.6626170313172611	0.9130122714517008	T	T	T
0.1883896233279177	0.6463439840639561	0.0245001561747413	T	T	T
0.0897728214937799	0.6687697582111163	0.8961088350098867	T	T	T
0.0995409183599120	0.6546661382972322	0.7005319395353800	T	T	T
0.2266754963226517	0.6389397083034216	0.7490831563833085	T	T	T
0.3184139850659561	0.5507855909214189	0.8106239958407693	T	T	T
0.0810664795499829	0.5479340726478542	0.8162858180906558	T	T	T
0.4299079642050926	0.3745222138031005	0.5840948782289215	T	T	T
0.4140063974782529	0.5061854000317136	0.5663717157853397	T	T	T
0.3943665383658753	0.6385832756667571	0.5558158146525102	T	T	T
0.1970766275741430	0.3723713540128828	0.6087938254823754	T	T	T
0.1762097573822240	0.4992334669000243	0.5542852233609363	T	T	T
0.1899739314535591	0.6334063763151923	0.5577575590126432	T	T	T
0.9903024239888095	0.4496417248323616	0.7929321007237063	T	T	T

Structure files (CONTCAR) involved in this work:

0.9817442467871302	0.6363867103756354	0.7900731363042609	T	T	T
0.1373690709209057	0.5593093776881487	0.2139922884260082	T	T	T
0.1959365266056652	0.5670354148206156	0.3883925460632308	T	T	T
0.2943383329359847	0.5533038274105280	0.5227102236862369	T	T	T
0.3938411867734240	0.5667375903204133	0.3917779346485083	T	T	T
0.3955669263600791	0.5527934478784786	0.1949638992109880	T	T	T
0.2673543068518348	0.5325363830451429	0.2310418404943824	T	T	T
0.1441673632731051	0.3252271912875551	0.2371604919687609	T	T	T
0.1946073773934193	0.3406398554780348	0.4158336910856423	T	T	T
0.3102498584472637	0.3522737628545927	0.5090290745977896	T	T	T
0.4172522545972749	0.3281276266188392	0.3975396089058444	T	T	T
0.3967631575610342	0.3380257595736480	0.2012411953392156	T	T	T
0.2718586450709468	0.3573695350181928	0.2554771672198189	T	T	T
0.1775829726077077	0.4471373143769129	0.3008467205827209	T	T	T
0.4140184536499130	0.4470460689894367	0.3134228795106021	T	T	T
0.0635973691478200	0.6249852642481035	0.0820022106640737	T	T	T
0.0800687945216563	0.4936507696791085	0.0602008599840564	T	T	T
0.0973452537204283	0.3617129601414767	0.0592847095294876	T	T	T
0.3075965120488613	0.6280337671815925	0.1043281421003861	T	T	T
0.3189984674159118	0.4989471615549942	0.0548476364883839	T	T	T
0.3053450706353754	0.3651863212603600	0.0618258639879753	T	T	T
0.5076254836418269	0.5402130999920642	0.2924691812701125	T	T	T
0.5160062475694938	0.3632604105089564	0.2768323690374962	T	T	T
0.4406076111011915	0.7483611253727712	0.6441436798703049	T	T	T
0.1879284007904062	0.7492793899678770	0.6508874251503608	T	T	T
0.2708759701419990	0.7496268097761913	0.0567687980957385	T	T	T
0.1037715060567874	0.7487074786671880	0.0522476464920155	T	T	T
0.0610488476379990	0.2465660471919081	0.1353142186979196	T	T	T
0.3043876982049870	0.2479869710720685	0.1507583982264573	T	T	T
0.2285107831165475	0.2508757684948082	0.5541645876250741	T	T	T
0.3924942595656672	0.2492500615029050	0.5495319235307573	T	T	T
0.5629040931403063	0.2477921356508896	0.3478284189627787	T	T	T
0.8122718346436115	0.2485176330135890	0.3818256208687157	T	T	T
0.7158659682215495	0.2488605101605577	0.9985709497898543	T	T	T
0.9060450430405198	0.2527781905688393	0.9468900153574639	T	T	T
0.9318889697086704	0.7610957329092983	0.8726029558707885	T	T	T
0.6793721276841046	0.7427841838924566	0.8801262951944431	T	T	T
0.6058346770740722	0.7477591196428612	0.4559189248297612	T	T	T
0.7754481152753003	0.6665696242188954	0.0916429040583840	T	T	T
0.7309053920125373	0.7852014909845513	0.0790474733658979	T	T	T
0.8689057341452135	0.7957228632135106	0.1208731655052078	T	T	T
0.7768075444270043	0.7542426361592451	0.4945253351423793	T	T	T
0.9153462039359102	0.6769743724521731	0.8462193330182839	T	T	T
0.6798854022656901	0.8282313230788745	0.8349472236591338	T	T	T
0.7657861600948035	0.6695227955238950	0.5005994231419669	T	T	T
0.7180635303792636	0.7094802433838848	0.0154009682853719	T	T	T
0.7964670061055394	0.8270229945608689	0.0081057638572996	T	T	T
0.8591735212161119	0.7063300674893184	0.0670271974999197	T	T	T
0.9299920528573191	0.7785908311049217	0.1003710574437188	T	T	T
0.8907539114238706	0.6740748507681678	0.4162344954553279	T	T	T
0.9535659016534888	0.7940035570020201	0.0302142328842273	T	T	T
0.9613359367736845	0.7600411436035207	0.1621818551275373	T	T	T
0.8912595033169647	0.6707453902496225	0.2219547641735423	T	T	T

Structure files (CONTCAR) involved in this work:

0.8843443916593021	0.7244084876109920	0.3845744670154735	T	T	T
0.9006019577822472	0.6767097295704334	0.4967402594708876	T	T	T
0.9303366989977114	0.6461518548350338	0.3782984983319315	T	T	T
0.8538734814224840	0.6767310933712296	0.2189557242544931	T	T	T

Figure 4(b) Route(b-i)-Cu ③

Si O Al Cu C H

1.0000000000000000

20.0219993591000005 0.0000000000000000 0.0000000000000000

0.0000000000000000 19.8990001678000006 0.0000000000000000

0.0000000000000000 0.0000000000000000 13.3830003737999998

93 195 3 3 2 7

Selective dynamics

Direct

0.4218810154674882	0.0530630867885262	0.6392992292675597	T	T	T
0.3016707852526536	0.0249112695757572	0.7837850688551905	T	T	T
0.2810858695628370	0.0629763040811560	0.0035291874728230	T	T	T
0.1219798504263162	0.0638761079509459	0.0039144927598909	T	T	T
0.0706921769157205	0.0254517392878039	0.7943830315643926	T	T	T
0.1781618042083158	0.0501365568928884	0.6429817657964665	T	T	T
0.4237963064486335	0.8255199838934638	0.6642495320437326	T	T	T
0.3030974911593799	0.8677279973189153	0.8020644649570727	T	T	T
0.2696051809054640	0.8264782207153292	0.0238287447290451	T	T	T
0.1151411770630510	0.8239326878859307	0.0145773627273685	T	T	T
0.0669142571636613	0.8678797456931906	0.8022025123060529	T	T	T
0.1802740410616612	0.8266517451416270	0.6651509027400124	T	T	T
0.0755398223626459	0.9429165293085257	0.1407098783943699	T	T	T
0.1971923200701655	0.9703874795634205	0.2849083553158388	T	T	T
0.2188687301134542	0.9317360578167106	0.5050534833119200	T	T	T
0.3782914380761125	0.9281003341287396	0.5085275957027408	T	T	T
0.4289817580183023	0.9695394883983384	0.3004184566906447	T	T	T
0.3230048818903760	0.9467113135022844	0.1437320889209479	T	T	T
0.0779639883760596	0.1682617895720021	0.1597001529949425	T	T	T
0.1958020931024729	0.1275710208501410	0.3036401864344318	T	T	T
0.2300233722022075	0.1706281567223689	0.5211338036378896	T	T	T
0.3846247345628224	0.1720912018976960	0.5080020924092180	T	T	T
0.4337010260309820	0.1262280442055011	0.2993456462835542	T	T	T
0.3180506666327518	0.1674461850136418	0.1660315919533012	T	T	T
0.5759685700856974	0.5550148492012653	0.3589639662122363	T	T	T
0.6956751011213510	0.5268888250957942	0.2214728808652046	T	T	T
0.7114975360564275	0.5470964203724872	0.9908212255041359	T	T	T
0.8702525092760564	0.5681164733875987	0.9971377940858263	T	T	T
0.9291909227581603	0.5246614052651370	0.2034438007584565	T	T	T
0.8187986125757656	0.5617000280753741	0.3464763899600743	T	T	T
0.5798441712423043	0.3243270337497730	0.3306917153593844	T	T	T
0.7042505230371500	0.3697249677503811	0.2160029384956291	T	T	T
0.7311715359191112	0.3267455521880180	0.9944586763739313	T	T	T
0.8881841132847644	0.3284200950902098	0.9971977377405027	T	T	T
0.9344462368803074	0.3681161793461150	0.2070327822827890	T	T	T
0.8266626384781200	0.3269733089095094	0.3547262288533106	T	T	T
0.9235449433916075	0.4479096061979127	0.8648276809618696	T	T	T
0.8031833585100534	0.4654445643913887	0.7249117203658302	T	T	T
0.7814355734094492	0.4410035651813091	0.4985071249201715	T	T	T

Structure files (CONTCAR) involved in this work:

0.6214804533566231	0.4285478414242153	0.4934097683491594	T	T	T
0.5633366995695244	0.4614891801871489	0.7032069069705147	T	T	T
0.6762477903477525	0.4263038497731532	0.8423435725587354	T	T	T
0.7928328286491775	0.6208483276001371	0.7125089447363806	T	T	T
0.6088101640094332	0.6712886613455462	0.4899441476556855	T	T	T
0.5618813081146186	0.6193637692641101	0.7026734081422514	T	T	T
0.6676163240795358	0.6655604341853847	0.8442104559973872	T	T	T
0.5752868999601513	0.9409436837609755	0.3550042327685127	T	T	T
0.6947245950368881	0.9711403981801824	0.2145503023299699	T	T	T
0.7169385382854535	0.9517762313553702	0.9873794190435985	T	T	T
0.8740355596105314	0.9489517592411396	0.9816465203028019	T	T	T
0.9291606270806912	0.9660527722959452	0.1942409737747191	T	T	T
0.8172875070874264	0.9285578988273258	0.3346532511396608	T	T	T
0.5802900031371611	0.1699887352872233	0.3226203876968128	T	T	T
0.7040987481094607	0.1274075345561733	0.2071797337285308	T	T	T
0.7356827447496057	0.1679858416843742	0.9868702545339550	T	T	T
0.8931218695789024	0.1784951072559957	0.9760318346752980	T	T	T
0.9333843442382584	0.1238168914644511	0.1930976222596376	T	T	T
0.8257849761670187	0.1719415155827141	0.3439161104246880	T	T	T
0.9264827676861672	0.0632878297619987	0.8461193141632696	T	T	T
0.8033858421484812	0.0285485578830881	0.7108948415533346	T	T	T
0.7845591935240445	0.0520496021803034	0.4830447248111664	T	T	T
0.6242917640509481	0.0664094006387417	0.4845942107987644	T	T	T
0.5666946330523676	0.0355193063287260	0.6949415445993661	T	T	T
0.6785893949483236	0.0665943958497025	0.8342347529279409	T	T	T
0.9144449351847320	0.8336862300802952	0.8280619898003270	T	T	T
0.7972489620293512	0.8715668857049987	0.7021864486695545	T	T	T
0.7676411136772262	0.8274779942705380	0.4878974329911756	T	T	T
0.6101834021472852	0.8239745649492649	0.4917558203407775	T	T	T
0.5674185309475858	0.8768019689949119	0.7065001943078050	T	T	T
0.4194430369024352	0.4425402822481483	0.6471378019561197	T	T	T
0.2989031626970194	0.4713874086789064	0.7888603893371772	T	T	T
0.2804614346576443	0.4335528289426777	0.0108164441655354	T	T	T
0.1218542022778126	0.4308572160443501	0.0106658719645388	T	T	T
0.0703407193635993	0.4701370939601656	0.8017909613637829	T	T	T
0.1754661075745644	0.4453189380180405	0.6485269257236156	T	T	T
0.4195448227664066	0.6701056280327351	0.6645790549616123	T	T	T
0.3014207677834090	0.6282826534211274	0.8047677641623374	T	T	T
0.2699709453871738	0.6701290899670556	0.0277476078857778	T	T	T
0.1165370303916138	0.6709070062243492	0.0158278694865589	T	T	T
0.0658283354149097	0.6288612951560095	0.8040911178510378	T	T	T
0.1793592675049205	0.6681134318601141	0.6660284080781734	T	T	T
0.0743299696454198	0.5530555029616733	0.1425110842936254	T	T	T
0.1960441764060340	0.5252215778354261	0.2844381415425377	T	T	T
0.2162082239846983	0.5616640336033339	0.5068806271546428	T	T	T
0.3758235434839308	0.5652112979546133	0.5108731118457758	T	T	T
0.4303574287804738	0.5248737357376329	0.3025402303500257	T	T	T
0.3237975629380616	0.5513538521006430	0.1481121595188728	T	T	T
0.0786950181225456	0.3231827646692992	0.1633038676176686	T	T	T
0.1962481096819124	0.3669440455901162	0.3036677536891301	T	T	T
0.2302509278064703	0.3272206982175146	0.5236094185945978	T	T	T
0.3852564473410402	0.3243915577040238	0.5127406575260669	T	T	T
0.4352399629192342	0.3681541376831404	0.3017617515403603	T	T	T

Structure files (CONTCAR) involved in this work:

0.3193633995057881	0.3264843767866643	0.1692220143347063	T	T	T
0.3559325360483803	0.0579024515262331	0.7090320051737508	T	T	T
0.2998175414147695	0.0690427398820712	0.8860110537282373	T	T	T
0.2012769306065732	0.0507560324032599	0.0187083424091089	T	T	T
0.1025953804050524	0.0680356303463856	0.8865820631161583	T	T	T
0.1031611067668805	0.0480435945694725	0.6887275535894223	T	T	T
0.2287303771568616	0.0267145159496154	0.7312411619722632	T	T	T
0.3608550776660867	0.8292280261266315	0.7405916753540478	T	T	T
0.3006888843119824	0.8356608090673423	0.9131695528236142	T	T	T
0.1915899003377434	0.8505350299550889	0.0243735733265526	T	T	T
0.0925273855488928	0.8256154236579133	0.8987021055494921	T	T	T
0.1037421655963112	0.8387359914141614	0.7029435548940908	T	T	T
0.2307235898127273	0.8576918225461784	0.7487568784083326	T	T	T
0.3205212547327410	0.9473842252227626	0.8091854144495602	T	T	T
0.0852331511162928	0.9466736354554489	0.8176252254837019	T	T	T
0.4297432110599619	0.1218861956843628	0.5750061873336338	T	T	T
0.4176470789976672	0.9897186037688187	0.5625692155407542	T	T	T
0.4018543655814507	0.8571953570259625	0.5567379724754998	T	T	T
0.1934866188632968	0.1262338847747046	0.6065534141137882	T	T	T
0.1825903314088352	-0.0012423085219397	0.5488047373282924	T	T	T
0.1908433289517894	0.8641000054142934	0.5584090055857278	T	T	T
0.9913433416191205	0.0401868497613381	0.7831758251219270	T	T	T
0.9870492071545516	0.8603736944176393	0.7913048844627482	T	T	T
0.1391326629922816	0.9386448096663150	0.2147366628091746	T	T	T
0.2019983899282799	0.9261913263885092	0.3865998142508574	T	T	T
0.2985690511053103	0.9388492452109156	0.5252540897005837	T	T	T
0.3950186522890769	0.9261779904122504	0.3900066400353923	T	T	T
0.3965290503544504	0.9488778761237072	0.1937700727479363	T	T	T
0.2681442565800311	0.9682534874353512	0.2271593634671495	T	T	T
0.1392632389101471	0.1649501239337647	0.2378823978909229	T	T	T
0.1933968333292674	0.1606539225957792	0.4139774093517322	T	T	T
0.3073711022325567	0.1463750030230482	0.5108289897976059	T	T	T
0.4110041751705636	0.1726062442660006	0.3933038121731855	T	T	T
0.3948338399596051	0.1518706414762318	0.1992800002725812	T	T	T
0.2689532680650739	0.1381204595559035	0.2530570138841722	T	T	T
0.1789400185397028	0.0478980097959466	0.3110273539944898	T	T	T
0.4148819146111632	0.0485919555365922	0.3238067767625513	T	T	T
0.0666879051684731	0.8714089881253427	0.0823434346478197	T	T	T
0.0821043504286078	0.0025692888382384	0.0583815349414483	T	T	T
0.0998717579308194	0.1346904462559567	0.0539924591848372	T	T	T
0.3102254118337717	0.8708003821184249	0.1046497460865813	T	T	T
0.3204377635045524	0.9988540287216390	0.0503329468347283	T	T	T
0.3027491678370948	0.1321007425530208	0.0590638588886308	T	T	T
0.5080657376525166	0.9544388340610670	0.2907401874254647	T	T	T
0.5137239753447349	0.1322162466778590	0.2813513074538348	T	T	T
0.6375086046853057	0.5667126178740923	0.2808705009000711	T	T	T
0.6825173521472023	0.5388116923381973	0.1023866696102118	T	T	T
0.7919581398330349	0.5479705814546756	0.9890701744814273	T	T	T
0.8954769769687395	0.5668114682556140	0.1118752567229796	T	T	T
0.8950002912591807	0.5469060655718752	0.3072080707591158	T	T	T
0.7693231753182896	0.5561743264026655	0.2472927827599613	T	T	T
0.6405071050178847	0.3256286641030887	0.2503241628971319	T	T	T
0.7096109572357687	0.3656153515166843	0.0957612192966107	T	T	T

Structure files (CONTCAR) involved in this work:

0.8096719426768616	0.3430185164150137	0.9756015894529375	T	T	T
0.9032877981997056	0.3233879544346113	0.1165139974077794	T	T	T
0.9008632554991722	0.3452609681541819	0.3119408812974898	T	T	T
0.7723377863293749	0.3415977373919905	0.2664161270101509	T	T	T
0.6920687824025664	0.4474154341995901	0.2490000003912013	T	T	T
0.9167417581935343	0.4457929654959846	0.1811544687886684	T	T	T
0.5601545572484808	0.6219687686097694	0.4235122654373312	T	T	T
0.5931562024897804	0.4929793129465356	0.4332039599156721	T	T	T
0.6033084813920226	0.3596690524605509	0.4340721165470224	T	T	T
0.8154678029032586	0.6360295710513065	0.3894074509048114	T	T	T
0.7982360502169001	0.5024644977499533	0.4240102064125347	T	T	T
0.8110951930125476	0.3710736588300454	0.4533430419397678	T	T	T
0.0080952740564958	0.5428132773350188	0.2106516326264264	T	T	T
0.0149152976282058	0.3597719103971168	0.2155953165649268	T	T	T
0.8618332958568845	0.4297773558904243	0.7911083071971516	T	T	T
0.8160618421700588	0.4521311313049147	0.6069840740197245	T	T	T
0.7011467664918036	0.4344298965646798	0.5100277737081511	T	T	T
0.5849985762038973	0.4239108962888244	0.6010118649786731	T	T	T
0.6013455084018148	0.4263086109115589	0.7969671266114434	T	T	T
0.7312243327098088	0.4319711144468907	0.7537783145835258	T	T	T
0.8494166933404185	0.6685794456538142	0.7576808020358248	T	T	T
0.7883242623432899	0.6191666717723462	0.5944950943807716	T	T	T
0.6847045134978539	0.6553548452694822	0.4648076501035858	T	T	T
0.5914939371871771	0.6598632539183185	0.6086061472799189	T	T	T
0.5922638978984981	0.6510820464404264	0.8066766941601325	T	T	T
0.7202786914129006	0.6447104898735901	0.7611117957228709	T	T	T
0.8037290865170702	0.5440291807792987	0.7554119600238866	T	T	T
0.5833748038265425	0.5406177513169863	0.6975221005605271	T	T	T
0.9322390569487987	0.3878188830074386	0.9467642328963063	T	T	T
0.9128134883564790	0.5184430982975149	0.9258756010249831	T	T	T
0.8846230574210004	0.6463708791843444	0.9610352456548621	T	T	T
0.6869468261500966	0.3567471664473840	0.9034260128932502	T	T	T
0.6826173667876736	0.4908356300739168	0.9172808686472114	T	T	T
0.6807573051448661	0.6213960908058551	0.9520096851672892	T	T	T
0.4834550955029572	0.4528396342207276	0.7201392285008140	T	T	T
0.4811977849414057	0.6262426606505500	0.7096677660576577	T	T	T
0.6365747766144308	0.9328956945442428	0.2758458170079628	T	T	T
0.6814603977709025	0.9634603069166596	0.0952497693107876	T	T	T
0.7962322181894889	0.9693585727113644	0.9958915634455677	T	T	T
0.9035489713718999	0.9272227933417173	0.0919855689047432	T	T	T
0.8928846230027290	0.9309434563280817	0.2888731675331270	T	T	T
0.7663064892551644	0.9352780886906011	0.2387576339746944	T	T	T
0.6358124528412986	0.1677202248429459	0.2333437745471658	T	T	T
0.7173486893302657	0.1265855417588097	0.0878621634073622	T	T	T
0.8145166318578403	0.1600418138617608	0.9603636357018667	T	T	T
0.9120775488545678	0.1624632347642525	0.0914808796834263	T	T	T
0.8974045469014199	0.1572226229002364	0.2898524808243917	T	T	T
0.7670930427599597	0.1633040304291526	0.2609414013422163	T	T	T
0.6971212716408567	0.0500591193626241	0.2463196133847205	T	T	T
0.9104958962623416	0.0451694137061901	0.1851006159875461	T	T	T
0.5653726738076310	0.8739857644228608	0.4219083558616650	T	T	T
0.5885123913356241	0.0040941284631930	0.4286173191511876	T	T	T
0.6102657574099073	0.1350753654139925	0.4225999337740791	T	T	T

Structure files (CONTCAR) involved in this work:

0.8073277682317486	0.8570814100074950	0.3891228434795110	T	T	T
0.8064602612859795	0.9912048558376549	0.4096742970794837	T	T	T
0.8138235141601735	0.1219397713474893	0.4377254929531775	T	T	T
0.0087176271370447	0.9546470113727984	0.2072921375704559	T	T	T
0.0139800388608232	0.1286805205638439	0.2070138344123468	T	T	T
0.8623287754840067	0.0659303941337536	0.7733538578115232	T	T	T
0.8167504878226942	0.0411612282778405	0.5929729383734255	T	T	T
0.7040297032554766	0.0540975575082216	0.4924976389764785	T	T	T
0.5919562646529585	0.0743378428902839	0.5947556286232211	T	T	T
0.6033691828004850	0.0702033273513321	0.7905506621520433	T	T	T
0.7318331491869930	0.0612953455699464	0.7426320304079674	T	T	T
0.8676372967021228	0.8337548648478740	0.7294185781508981	T	T	T
0.7885486987709450	0.8756526254195168	0.5819001725296593	T	T	T
0.6879802957396086	0.8390414486165365	0.4659787032070054	T	T	T
0.5960743431562416	0.8359844204863627	0.6098784120024023	T	T	T
0.6003162026348100	0.8514180521057397	0.8092642249845617	T	T	T
0.7368576316044094	0.8345845831990558	0.7577062114915746	T	T	T
0.8040685289906326	0.9497782903751271	0.7411021839736406	T	T	T
0.5844118811271279	0.9562928644958978	0.6873848646571145	T	T	T
0.9384146073990685	0.1363125428195565	0.8972400168438394	T	T	T
0.9161455902229735	0.0117960568607175	0.9400895462904582	T	T	T
0.8822663505540205	0.8835757249914186	0.9124072614208339	T	T	T
0.6923050528004805	0.1350518897940005	0.8971854188184323	T	T	T
0.6831594638421118	-0.0007863374097341	0.9041650785003043	T	T	T
0.7080870402907712	0.8710927683402133	0.9603816460279251	T	T	T
0.4868530005660136	0.0458145967752434	0.7104754259185291	T	T	T
0.4861523335784589	0.8667461208793482	0.7111212657187200	T	T	T
0.3528868062392254	0.4364790144514820	0.7153319273004692	T	T	T
0.2958484700480664	0.4285931969150826	0.8921614559670235	T	T	T
0.2008267799201940	0.4431846153944383	0.0317457181912439	T	T	T
0.1065421438892344	0.4287521656463112	0.8920580166391168	T	T	T
0.1006153715452532	0.4448940577878774	0.6954452581621149	T	T	T
0.2261560425521645	0.4703965540619410	0.7358255387810015	T	T	T
0.3586692380163308	0.6686007387268205	0.7443609665712493	T	T	T
0.2987997284436168	0.6596159037607198	0.9160928713259904	T	T	T
0.1925309725302565	0.6447945145872976	0.0335901303867531	T	T	T
0.0989954957651662	0.6692005814622617	0.8985155252350834	T	T	T
0.1028752386078399	0.6564100590573164	0.7028999685203783	T	T	T
0.2295363831625003	0.6374247029238735	0.7503628205657626	T	T	T
0.3200687106364983	0.5488315565074595	0.8111116713580603	T	T	T
0.0840384522500041	0.5495230694224782	0.8188879706703761	T	T	T
0.4289284424945271	0.3730945164430896	0.5845719356445177	T	T	T
0.4152201103619067	0.5052424884172865	0.5690435576631769	T	T	T
0.3949550480369902	0.6376352800499915	0.5590842143493012	T	T	T
0.1941095623450566	0.3700974444152887	0.6111299352379524	T	T	T
0.1781797318058828	0.4968076501643530	0.5542831720032836	T	T	T
0.1916321224174782	0.6308347660487666	0.5594502890187273	T	T	T
0.9909410505698274	0.4542463428548415	0.7993603165242821	T	T	T
0.9872675875940674	0.6414806298800181	0.8001946253338607	T	T	T
0.1389178552347177	0.5586477254227697	0.2144019082397094	T	T	T
0.1973287296189203	0.5660240793493959	0.3892354215954693	T	T	T
0.2961546244587058	0.5516092667563869	0.5223276905874891	T	T	T
0.3973000295283502	0.5669436080454715	0.3941831906401342	T	T	T

Structure files (CONTCAR) involved in this work:

0.3976352563768086	0.5484133384023732	0.1973113336511698	T	T	T
0.2686978640801569	0.5315347597402130	0.2321501585498135	T	T	T
0.1414640878835876	0.3253907052981052	0.2394867574464040	T	T	T
0.1930757013213316	0.3396872798238270	0.4174345357099108	T	T	T
0.3079979803094775	0.3503360184717243	0.5129941499311761	T	T	T
0.4143452699724171	0.3251167515577104	0.3997627084747928	T	T	T
0.3963148957999437	0.3389404744354477	0.2040895695251327	T	T	T
0.2703573159476313	0.3550148603663928	0.2569320197779625	T	T	T
0.1781461768172302	0.4464694426078676	0.3017552046445927	T	T	T
0.4145395449684511	0.4457597013175396	0.3214808971759883	T	T	T
0.0658676367546795	0.6236145661103161	0.0808634457669721	T	T	T
0.0802131039076152	0.4918307791147880	0.0628313458292176	T	T	T
0.0981755610205881	0.3598222196635145	0.0587329912970022	T	T	T
0.3128590812173931	0.6274084770301896	0.1079677390829573	T	T	T
0.3196373682566224	0.4985122731380420	0.0555462457385292	T	T	T
0.3056691829357427	0.3646825981121586	0.0638810487130983	T	T	T
0.5099988188191019	0.5371779692989647	0.2934273177926709	T	T	T
0.5152315164622494	0.3621782793314445	0.2826490104438628	T	T	T
0.4427350125575352	0.7470811334900862	0.6461070328405542	T	T	T
0.1945055195498081	0.7473719860671020	0.6494629607599423	T	T	T
0.2749862346907744	0.7486937232719653	0.0581678190631124	T	T	T
0.1072229001339688	0.7476039878259463	0.0566368235688666	T	T	T
0.0590854589249559	0.2460261806936779	0.1381677916241075	T	T	T
0.3058052468860302	0.2472173341815499	0.1518345539436584	T	T	T
0.2252583149372024	0.2486618030344487	0.5547191535871585	T	T	T
0.3900063359071709	0.2476162353190728	0.5535549441918827	T	T	T
0.5613162180666462	0.2465239695720050	0.3522990723086035	T	T	T
0.8247936717762285	0.2482556879073001	0.3861728082076284	T	T	T
0.7170395673749125	0.2466851395885079	1.0026162253701134	T	T	T
0.9082315031583408	0.2564344596127627	0.9493701231817789	T	T	T
0.9191651019625321	0.7611019848694447	0.8829860081114490	T	T	T
0.6751215488014980	0.7404681946874450	0.8927551574920908	T	T	T
0.5878392077367768	0.7482901790688389	0.4626667960192272	T	T	T
0.7716599562720772	0.6837270543649963	0.0885854442327139	T	T	T
0.6685584347313346	0.7683459580534492	0.1210018814360252	T	T	T
0.8334237611292655	0.8059978236212951	0.0945260915027301	T	T	T
0.7875225863489533	0.7515844505773547	0.5070001024653072	T	T	T
0.9141300369916077	0.6777995060720557	0.8387863454001571	T	T	T
0.6779667775230821	0.8261027130874696	0.8499359921458096	T	T	T
0.7691687698069058	0.6672834175064498	0.4903441251250351	T	T	T
0.6834611438357080	0.6983782522041393	0.0441128759136347	T	T	T
0.7390996208826645	0.8168237175491067	0.0802367498433188	T	T	T
0.8618317388356950	0.7262504543845602	0.0352083147750339	T	T	T
0.9408917529558908	0.7332719758018937	0.1358682541093923	T	T	T
0.9136840303705787	0.7227176867180902	0.2363545033301750	T	T	T
0.9602928779980876	0.7830786000949697	0.1163535971297172	T	T	T
0.8641242688263173	0.8448930036101749	0.0910507640700082	T	T	T
0.9668453646045583	0.6912205016744817	0.0997066324519481	T	T	T
0.8834304414755928	0.7643613013620576	0.2651174660065908	T	T	T
0.9581621165691757	0.7183504921505093	0.2862893243412329	T	T	T
0.8876952455213146	0.6746312249668209	0.2461419864375438	T	T	T
0.7727221521269032	0.6731779616713146	0.1603356765627051	T	T	T

Structure files (CONTCAR) involved in this work:

Figure 4(b) Route(b-i)-Cu ④ as same as Route(a)-Cu ④

Figure 4(c) Route(a)-Ga ①

Si Al O Ga H C

1.0000000000000000
20.0219999999999985 0.0000000000000000 0.0000000000000000
0.0000000000000000 19.8990000000000009 0.0000000000000000
0.0000000000000000 0.0000000000000000 13.3829999999999991
93 3 192 1 6 2

Selective dynamics

Direct

0.4221071774181942	0.0570654300672522	0.6480840841697946	T	T	T
0.3010211488180128	0.0269205629121908	0.7891703822096132	T	T	T
0.2794712148953420	0.0606234734094796	0.0124524089759440	T	T	T
0.1197481404295355	0.0641237514264353	0.0134395261118472	T	T	T
0.0670745692429643	0.0300778997520221	0.8002802306835569	T	T	T
0.1761863502714669	0.0562820050090883	0.6515130210927764	T	T	T
0.4194199778021160	0.8271194331424816	0.6703261642330556	T	T	T
0.3015937302751821	0.8685147889561939	0.8092992292208628	T	T	T
0.2669330625539724	0.8286017011829691	0.0296525095458094	T	T	T
0.1119570972808493	0.8268273461199545	0.0171057957326647	T	T	T
0.0614784005269742	0.8709557653865311	0.8028768631609898	T	T	T
0.1787680768223640	0.8280905927807607	0.6734697765542776	T	T	T
0.0747767047505262	0.9431257714504971	0.1506998424075154	T	T	T
0.1956970014568172	0.9733111960100003	0.2932414360663649	T	T	T
0.2164601472471281	0.9373213221152662	0.5146667135218490	T	T	T
0.3759853626014070	0.9339376508217537	0.5157629435626719	T	T	T
0.4295305724517121	0.9694811469618191	0.3047726381862769	T	T	T
0.3201914539266543	0.9450646620991477	0.1551964930042142	T	T	T
0.0780617555673728	0.1733617559977931	0.1657787226452125	T	T	T
0.1955824400206506	0.1306545185912638	0.3076434151479559	T	T	T
0.2312511397829851	0.1733842164381794	0.5250594217863827	T	T	T
0.3859119993434958	0.1738606165357864	0.5126695576741127	T	T	T
0.4360319068886225	0.1277590255168499	0.3019744388456446	T	T	T
0.3183688228051246	0.1676456649044067	0.1711764921437272	T	T	T
0.5821970215917917	0.5551876372754486	0.3504597297897309	T	T	T
0.6961025386444485	0.5280969055955385	0.1904537443013983	T	T	T
0.7109514846614663	0.5660022926105474	0.9777296309092249	T	T	T
0.8698672060626182	0.5607572265488119	0.9759038031801265	T	T	T
0.9335198158185574	0.5294783272394566	0.1870006120751367	T	T	T
0.5756979852234090	0.3295215489867676	0.3357915124917010	T	T	T
0.7062705010642366	0.3731416070510387	0.2160148461177902	T	T	T
0.7313703298732966	0.3275842534364657	0.9978257136241457	T	T	T
0.8827211916240651	0.3284770451376517	0.9837239183195164	T	T	T
0.9354603907833565	0.3729316250097252	0.1992833152873351	T	T	T
0.9250794016222197	0.4380758127848636	0.8388952531048430	T	T	T
0.7762531558099544	0.4394077731022539	0.4802519146765489	T	T	T
0.6177620044080578	0.4319933338246700	0.4926639897835602	T	T	T
0.5679294293735602	0.4673646001305481	0.7091983824587872	T	T	T
0.6704023427105303	0.4349794886819298	0.8624687712485434	T	T	T
0.9180056626493259	0.6730001858954158	0.8295630654751994	T	T	T
0.8000907108688066	0.6334000174062880	0.6976034578419590	T	T	T
0.7671726665015915	0.6680505641040005	0.4795121172605308	T	T	T

Structure files (CONTCAR) involved in this work:

0.6116368758141112	0.6706991355598307	0.4867600157160623	T	T	T
0.5633866347162411	0.6258413763159411	0.7042708427956135	T	T	T
0.6806797344978270	0.6815625540129998	0.8248221870619740	T	T	T
0.5742625015600310	0.9432672847955257	0.3650373313617605	T	T	T
0.6944414728083902	0.9733158344644344	0.2227938670017124	T	T	T
0.7175408649888826	0.9421335512591769	1.0000539855363706	T	T	T
0.8774730501221005	0.9344869658511639	0.9961273341886041	T	T	T
0.9301130375424602	0.9702846232567220	0.2072128460774037	T	T	T
0.8199083102756868	0.9420288092634866	0.3572268092927329	T	T	T
0.5795969988347008	0.1746656378275241	0.3358523028238520	T	T	T
0.6971202390048912	0.1309310053154298	0.2010702283649617	T	T	T
0.7303920685578623	0.1717599026130268	0.9798291550271279	T	T	T
0.8848722548277989	0.1738394505557354	0.9946967071192198	T	T	T
0.9336382804828186	0.1286814463071913	0.2061666730021711	T	T	T
0.8186166289472604	0.1697444203872800	0.3406097271000184	T	T	T
0.9230072506398691	0.0579716613982753	0.8627667849126679	T	T	T
0.8036220757437521	0.0292712005579399	0.7225884105811141	T	T	T
0.7798780658104820	0.0590500670488559	0.4979988730830973	T	T	T
0.6201661479195659	0.0675634203882549	0.4943737746732852	T	T	T
0.5671433445727934	0.0321465675839655	0.7030308406668118	T	T	T
0.6768589476785736	0.0567820141514625	0.8553651941759617	T	T	T
0.9175294327605589	0.8258571648449914	0.8408588799382062	T	T	T
0.8020935863632405	0.8735038110837064	0.7049066515946841	T	T	T
0.7671654352347262	0.8293997827225764	0.4872141233613119	T	T	T
0.6122376233846408	0.8259007055489114	0.4979220151538690	T	T	T
0.5621201944368610	0.8755326560526669	0.7043290713584981	T	T	T
0.6775237054184540	0.8378825944472709	0.8384164875775653	T	T	T
0.4232405842109724	0.4453944986128165	0.6407360700691332	T	T	T
0.3041556784828695	0.4743494942001369	0.7883038571888028	T	T	T
0.2858828875459426	0.4337391115502907	0.0069464144961968	T	T	T
0.1284724340795137	0.4320034045573775	0.0039952647693241	T	T	T
0.0751112983515536	0.4719556321044563	0.7974136613211396	T	T	T
0.1825178570866778	0.4500130288337920	0.6455898488188588	T	T	T
0.4233261455546181	0.6722855685738913	0.6637227865229409	T	T	T
0.3012741792887495	0.6307501641994997	0.7993709360818815	T	T	T
0.2696141230269165	0.6726679721019292	0.0180427460453907	T	T	T
0.1155070260205147	0.6738027892640901	0.0077043832858355	T	T	T
0.0653462313726336	0.6294270129739885	0.7989706230586875	T	T	T
0.1790879507570032	0.6693463695334690	0.6631481902700257	T	T	T
0.0796493110174731	0.5537806442948227	0.1341997854852083	T	T	T
0.2004252979566593	0.5287403610277048	0.2803988728818504	T	T	T
0.2221363703436275	0.5678923036493636	0.5016817650311479	T	T	T
0.3831547082237574	0.5695208824876445	0.5040845976725595	T	T	T
0.4350118056334198	0.5282196025660494	0.2945760073335696	T	T	T
0.3278374651746296	0.5531465154130271	0.1422584372477540	T	T	T
0.0810391066327898	0.3285107556394837	0.1575122494502642	T	T	T
0.1965142546788453	0.3704701281429371	0.3034431361367034	T	T	T
0.2328361913886945	0.3302095907736904	0.5226258269660788	T	T	T
0.3873342069446528	0.3273219307790266	0.5095493942261929	T	T	T
0.4345158087757026	0.3706776929472911	0.2947682137012026	T	T	T
0.3174820358896316	0.3261199450429331	0.1660853891513273	T	T	T
0.8107405473549001	0.5622554079302269	0.3271184770931332	T	T	T
0.8300223324664895	0.3295384500569837	0.3530763507703451	T	T	T

Structure files (CONTCAR) involved in this work:

0.7929559999283350	0.4738812783096356	0.7278235402628412	T	T	T
0.3566193684352517	0.0623873956885495	0.7189614308670964	T	T	T
0.2993736246879967	0.0658942412893390	0.8954848074214554	T	T	T
0.1993409700545223	0.0515074300867072	0.0274671820273214	T	T	T
0.1004122028138240	0.0672722419202641	0.8961896298606261	T	T	T
0.1014393974044997	0.0578930857241076	0.6984463058519933	T	T	T
0.2277808331600782	0.0326631460054590	0.7382846400707548	T	T	T
0.3572933508626502	0.8263316341305381	0.7481499902477331	T	T	T
0.3039136561364517	0.8436081813975548	0.9243197676096829	T	T	T
0.1892087990672908	0.8522757790824150	0.0207614038271721	T	T	T
0.0839746719617765	0.8323709998043075	0.9041469697969677	T	T	T
0.1013968472315272	0.8382321719986557	0.7083880694105641	T	T	T
0.2276437621985262	0.8546717795597150	0.7625966127894792	T	T	T
0.3193818771430462	0.9480153153867932	0.8037709553591790	T	T	T
0.0802109999690839	0.9498789550895101	0.8116639688845757	T	T	T
0.4303668254953922	0.1265662046431919	0.5853449866473792	T	T	T
0.4162208782396836	0.9948050909681108	0.5696929715859171	T	T	T
0.3966770689230869	0.8627830253822099	0.5664024474219798	T	T	T
0.1938564097648041	0.1312081140815514	0.6120409741060280	T	T	T
0.1783908218512706	0.0029716459005855	0.5594212158163452	T	T	T
0.1923572705939882	0.8689863841406014	0.5704725416628422	T	T	T
0.9879254303392772	0.0464674733166199	0.7921866384356677	T	T	T
0.9814574851869217	0.8618152791630901	0.7870830682615561	T	T	T
0.1405971972173207	0.9391921796531207	0.2207919042999849	T	T	T
0.1974436349642991	0.9312308002208065	0.3972126136877999	T	T	T
0.2964219012198525	0.9472176516605865	0.5300618293876661	T	T	T
0.3952304330502755	0.9301680870090613	0.3983511461817101	T	T	T
0.3951322400767785	0.9452301674949223	0.2009918620469543	T	T	T
0.2688809008189719	0.9703497859914586	0.2415250588922258	T	T	T
0.1411457748941882	0.1710652461157579	0.2415960222218225	T	T	T
0.1938640429089759	0.1625288195661298	0.4188598498221237	T	T	T
0.3084726808028208	0.1484027454336693	0.5160325037337141	T	T	T
0.4131184375573117	0.1709286123139205	0.3989737608797170	T	T	T
0.3956788473538392	0.1555004014178744	0.2044767008541470	T	T	T
0.2698276574388089	0.1393050106096518	0.2596135759622911	T	T	T
0.1761397531810045	0.0514670646255260	0.3131790868761286	T	T	T
0.4177343336547774	0.0494827697575912	0.3212973246343444	T	T	T
0.0668224838366092	0.8718135684643751	0.0922300315490497	T	T	T
0.0801316550844068	0.0030076982905899	0.0681445005041613	T	T	T
0.0977377295995625	0.1353139326414441	0.0624307788682180	T	T	T
0.3025917284433959	0.8691917195480209	0.1197763661693801	T	T	T
0.3167488181629828	0.9953055490622870	0.0595255331769367	T	T	T
0.3037137356739738	0.1292155274375612	0.0666640230646019	T	T	T
0.5084063731190485	0.9523376690581860	0.2957101969576522	T	T	T
0.5158512435198432	0.1366212460747711	0.2846317872147698	T	T	T
0.6467864823838136	0.5559004287665932	0.2784320447085427	T	T	T
0.6778278776259284	0.5690119392102257	0.0882319710311843	T	T	T
0.7906390378254265	0.5484280106982181	0.9856139102572306	T	T	T
0.9048730216634766	0.5627351781402391	0.0862780132861187	T	T	T
0.9014339830309378	0.5681724347137167	0.2901785808940182	T	T	T
0.7729476201871571	0.5433809822350713	0.2167098422449574	T	T	T
0.6428558644088656	0.3378638606403528	0.2713787395400160	T	T	T
0.7227633471289188	0.3266880023776682	0.1181971151663162	T	T	T

Structure files (CONTCAR) involved in this work:

0.8063727748828595	0.3552591674153233	0.9694108253052028	T	T	T
0.9063687859315269	0.3379395917732259	0.0982228992308337	T	T	T
0.9087007396284401	0.3393837865463897	0.2998478564700087	T	T	T
0.7693766433221346	0.3764366637811964	0.2903505649767101	T	T	T
0.6835524977597309	0.4475237341264500	0.1764724103600358	T	T	T
0.9125448387105733	0.4522997203783349	0.1957114017993564	T	T	T
0.5717377647366292	0.6285757429263945	0.4014092714575729	T	T	T
0.5927557966475501	0.5011385541292191	0.4407461915139793	T	T	T
0.5808361699920226	0.3679059803279186	0.4432250383128427	T	T	T
0.7992490639934072	0.6402018206134152	0.3782803129825016	T	T	T
0.8033996535618670	0.4993905479374501	0.4140459780019325	T	T	T
0.8290778762623029	0.3734868597181110	0.4752847823563722	T	T	T
0.0127807112849282	0.5419583598624913	0.2012708941776843	T	T	T
0.0170086855751473	0.3717955975495754	0.1944818179134530	T	T	T
0.8731158708864726	0.4292927411100808	0.7420771051623339	T	T	T
0.7987778184573974	0.4587313079393115	0.5972889385770271	T	T	T
0.6980702649029735	0.4227601925792945	0.4771697704923400	T	T	T
0.6010179203060213	0.4334558086817303	0.6104395041165248	T	T	T
0.5977662830939395	0.4301920355618348	0.8072787329185471	T	T	T
0.7302915528214002	0.4300486448164808	0.7824332052393524	T	T	T
0.8634612323875861	0.6762140112655974	0.7406593133437892	T	T	T
0.8062405740253896	0.6360657436238247	0.5762458510168368	T	T	T
0.6888519687216967	0.6461533301245143	0.4901920354629629	T	T	T
0.5782212657538990	0.6577634701229349	0.5952087209948647	T	T	T
0.6041191500295583	0.6659756333872433	0.7907136035866046	T	T	T
0.7298142536352237	0.6693738464030364	0.7293529660548164	T	T	T
0.8026329525634954	0.5585996995724963	0.7436959354047249	T	T	T
0.5854686784278563	0.5473008819752899	0.7082240604913382	T	T	T
0.9298384890854486	0.3705071198385136	0.9057429040794975	T	T	T
0.9011424588697012	0.4995441561063579	0.9094242702216286	T	T	T
0.8885977063262954	0.6320316598397668	0.9250334792753639	T	T	T
0.6757987724710163	0.3747009882088633	0.9444691581411471	T	T	T
0.6724278332576084	0.5079160479739739	0.9167060422821867	T	T	T
0.7022192114510466	0.6372949356905409	0.9211389639494467	T	T	T
0.4875512371911073	0.4575025320794756	0.7111924144065095	T	T	T
0.4832815107752048	0.6343464875015247	0.7241484052401729	T	T	T
0.6395375705672164	0.9373652912382252	0.2939257714111833	T	T	T
0.6951389155207582	0.9352197014132695	0.1157234866754294	T	T	T
0.7980928913143925	0.9499158724028008	0.9887143590073592	T	T	T
0.9002999375624173	0.9291679840188364	0.1120327951153671	T	T	T
0.8946324267788239	0.9449628116077353	0.3097362983296508	T	T	T
0.7683332348908657	0.9667246225864847	0.2712361708130884	T	T	T
0.6412418398731869	0.1755295472246785	0.2579676216840320	T	T	T
0.6953379573252605	0.1529587669235103	0.0849236876495986	T	T	T
0.8082380239268103	0.1474966572422507	0.9846290823734063	T	T	T
0.9085999779658843	0.1723927715369998	0.1104143545454434	T	T	T
0.8959088428026458	0.1546140260684704	0.3059442545494729	T	T	T
0.7705046454454678	0.1430442239379601	0.2492569844042238	T	T	T
0.6758171442106784	0.0521735803988705	0.2101608389110554	T	T	T
0.9172317601640360	0.0496963546733995	0.1868568226951799	T	T	T
0.5658800610928697	0.8743936595782239	0.4292828329541666	T	T	T
0.5791094458681860	0.0065618168913035	0.4416581775343326	T	T	T
0.6017595583462806	0.1376979086937307	0.4390515487448943	T	T	T

Structure files (CONTCAR) involved in this work:

0.8035953278739387	0.8654052983205801	0.3923914413121150	T	T	T
0.8153832367504023	0.9918087587429522	0.4533100735014843	T	T	T
0.8043162873712933	0.1258717472250845	0.4410806507358582	T	T	T
0.0095309260570661	0.9551332566479761	0.2200568323242316	T	T	T
0.0140830153051251	0.1382969464079234	0.2194669970299958	T	T	T
0.8574816165281863	0.0677488178456260	0.7928206664802024	T	T	T
0.8016266917384154	0.0656004544839408	0.6144490492586597	T	T	T
0.6993230033771547	0.0509594836709026	0.4865105904499752	T	T	T
0.5980633209099905	0.0752935580869932	0.6106659728581026	T	T	T
0.6024183491321131	0.0530508949956691	0.8077027649165441	T	T	T
0.7293899921309662	0.0321177481679217	0.7705612556623981	T	T	T
0.8544788993005391	0.8265038196275594	0.7650798648775426	T	T	T
0.8044278996518628	0.8531470666064992	0.5885330366842275	T	T	T
0.6890756182573534	0.8523169029865095	0.4912820698812269	T	T	T
0.5869154777509212	0.8275809477692250	0.6132644887718410	T	T	T
0.6006889811050286	0.8538159645787753	0.8061726825555557	T	T	T
0.7269725075274015	0.8637726671409480	0.7492495294317396	T	T	T
0.8263297751289591	0.9510574551976900	0.7154993597904160	T	T	T
0.5794312693708881	0.9531295803794514	0.6774190015071957	T	T	T
0.9334352359563084	0.1262939941528691	0.9277677194644074	T	T	T
0.9168722723593519	0.9946970735123806	0.9391407939719270	T	T	T
0.8971540376413190	0.8633285713152232	0.9443090431626303	T	T	T
0.6925872198965440	0.1334476593016123	0.8889007301207315	T	T	T
0.6814904174863079	0.0080844752800075	0.9527450927206376	T	T	T
0.6939877156317515	0.8746357849352072	0.9431686225897340	T	T	T
0.4878775675279570	0.0471105073783575	0.7170065164881119	T	T	T
0.4820208224360906	0.8667959834382966	0.7209505630221655	T	T	T
0.3574119105578711	0.4428799923052145	0.7109224332330196	T	T	T
0.3041090069223517	0.4288780136849501	0.8890388260271248	T	T	T
0.2066005641701170	0.4499391585006630	0.0214187707610871	T	T	T
0.1106000789868137	0.4286985515246536	0.8856238356315135	T	T	T
0.1064059576939741	0.4532252035713787	0.6887244136581361	T	T	T
0.2307095779534331	0.4726075031098928	0.7368652194494342	T	T	T
0.3554301005332979	0.6673950854891291	0.7290381909823554	T	T	T
0.3007837228408628	0.6687702597793849	0.9063085472899326	T	T	T
0.1921967175817027	0.6469250741780327	0.0150938275104474	T	T	T
0.0917321336818588	0.6748006578645965	0.8917633715117974	T	T	T
0.1019151831540961	0.6545712138888863	0.6967280156332388	T	T	T
0.2277994903935112	0.6362240039750209	0.7475280555014253	T	T	T
0.3211475374280532	0.5521626074413409	0.8155429662231011	T	T	T
0.0840147418217123	0.5512895420263644	0.8218082473897583	T	T	T
0.4319704313930857	0.3744786567769999	0.5823305477552411	T	T	T
0.4170105954630250	0.5049614953984257	0.5582234004760439	T	T	T
0.4108858191370595	0.6380297580397999	0.5548765456157914	T	T	T
0.1969670745323919	0.3736335665356573	0.6101930023295169	T	T	T
0.1894197396535695	0.5004661142264740	0.5506850389819647	T	T	T
0.1920773933111853	0.6348397822971480	0.5547124747864326	T	T	T
0.9965739125614307	0.4530126618140310	0.7879480196133766	T	T	T
0.9850838443110561	0.6363065334342488	0.7861419170994000	T	T	T
0.1430339555736394	0.5605652245451741	0.2085313457821517	T	T	T
0.2013291658144233	0.5708417666795824	0.3844649095179936	T	T	T
0.3024455679420052	0.5649649568734637	0.5165138473674754	T	T	T
0.4037119031149665	0.5707070580018715	0.3872909162597354	T	T	T

Structure files (CONTCAR) involved in this work:

0.4016945438984491	0.5563489335978137	0.1918999279010117	T	T	T
0.2728723687010206	0.5344600428760099	0.2276388814317116	T	T	T
0.1382407007542061	0.3317825704630006	0.2430319510817599	T	T	T
0.1947721653947718	0.3427262418552281	0.4171641239389792	T	T	T
0.3102076497366693	0.3539973333088717	0.5118007945048396	T	T	T
0.4141948697610320	0.3299445589036863	0.3955571730465771	T	T	T
0.3941179939723294	0.3398728631801997	0.1998212753008866	T	T	T
0.2688788763230768	0.3563970870908473	0.2528651664990477	T	T	T
0.1819077185770091	0.4508308854375760	0.3028212467438251	T	T	T
0.4155461456276305	0.4494589054853247	0.3099058107024489	T	T	T
0.0688354961129952	0.6232325517435264	0.0727298964512890	T	T	T
0.0851008351742099	0.4915789468694979	0.0563161299821688	T	T	T
0.1098061159669497	0.3599839591601287	0.0532905886989875	T	T	T
0.3117017293679963	0.6260242320443448	0.0941527407437690	T	T	T
0.3277564681700472	0.4950540998868656	0.0567245546337432	T	T	T
0.3033228155991305	0.3623618861772702	0.0591941117888207	T	T	T
0.5153353293776887	0.5370030391406180	0.2870013150666936	T	T	T
0.5136298184030009	0.3615206600087979	0.2724453637649988	T	T	T
0.4412345623208611	0.7505813992111928	0.6451215162432603	T	T	T
0.1928067094944359	0.7490919889540913	0.6520133167889174	T	T	T
0.2725957488380912	0.7494766862980285	0.0574221309982358	T	T	T
0.1079474311224964	0.7488554505635912	0.0531670365300108	T	T	T
0.0609082621623042	0.2508832247134067	0.1377072580906136	T	T	T
0.3038688317207037	0.2466788975985355	0.1521532774203691	T	T	T
0.2275909944688028	0.2521632851416664	0.5554561037812321	T	T	T
0.3912825625404821	0.2509517444188012	0.5513385262657832	T	T	T
0.5598907501568190	0.2515608596875539	0.3615770722365857	T	T	T
0.8071325737574175	0.2469787999594117	0.3665726542627889	T	T	T
0.7244487446380511	0.2512680334780305	0.9563202594263347	T	T	T
0.8901001593395695	0.2501576404004718	0.9527267948278128	T	T	T
0.9364165619321355	0.7483426839651849	0.8670742224207895	T	T	T
0.6871580805143072	0.7588607056271470	0.8594193345444952	T	T	T
0.7735432112851759	0.7492286471834253	0.4780551624157132	T	T	T
0.6061152307772458	0.7495311676043896	0.4572327972029409	T	T	T
0.8861965202252914	0.4177097406311394	0.5891139768335818	T	T	T
0.9279006798435809	0.5981443418505317	0.4343027384719297	T	T	T
0.9287985463568657	0.6636680840643657	0.3423300811798353	T	T	T
0.9945220601156707	0.6011478833827080	0.3438959745197431	T	T	T
0.9691693332712055	0.4491184329458511	0.4580047677263077	T	T	T
0.9764528633540576	0.5010895045735582	0.5690399522616334	T	T	T
0.0142205591670544	0.4195496225292821	0.5670772864116815	T	T	T
0.9416036415111060	0.6111338727700533	0.3573338790502392	T	T	T
0.9723468060942797	0.4496382615551152	0.5397629375454224	T	T	T

Figure 4(c) Route(a)-Ga ②

Si Al O Ga H C

1.0000000000000000

20.0219999999999985 0.0000000000000000 0.0000000000000000

0.0000000000000000 19.8990000000000009 0.0000000000000000

0.0000000000000000 0.0000000000000000 13.3829999999999991

93 3 192 1 6 2

Selective dynamics

Direct

Structure files (CONTCAR) involved in this work:

0.4220993912416267	0.0570915799211128	0.6481584173291383	T	T	T
0.3009465986688014	0.0268468933036698	0.7889556911062999	T	T	T
0.2800549100919146	0.0606397563641511	0.0125509379935314	T	T	T
0.1203857187728303	0.0634485524198498	0.0129021865153198	T	T	T
0.0671939573367541	0.0296160116186259	0.8000459080827309	T	T	T
0.1759903843257318	0.0558201206093852	0.6510611328795586	T	T	T
0.4192151807614708	0.8270891595228328	0.6704124167515578	T	T	T
0.3012168422932548	0.8683940822142567	0.8089133875711835	T	T	T
0.2667830819751045	0.8282751357297525	0.0294024577246896	T	T	T
0.1117761764056524	0.8263684527644711	0.0173948668650647	T	T	T
0.0608534077762666	0.8702333770108608	0.8029731473605073	T	T	T
0.1783210906525387	0.8277133047172476	0.6734341024403273	T	T	T
0.0747253804509591	0.9428643225857284	0.1504930280925255	T	T	T
0.1958625719299395	0.9727231725554197	0.2931178844288369	T	T	T
0.2164512921144761	0.9367544998252230	0.5145860276442952	T	T	T
0.3759469776465512	0.9337531655904191	0.5160914367628867	T	T	T
0.4295384773722445	0.9694987620628470	0.3050762343872312	T	T	T
0.3205085276079575	0.9447232795157061	0.1549723476178479	T	T	T
0.0784430646746263	0.1727489325583820	0.1647932864493001	T	T	T
0.1960241078045465	0.1301336060252064	0.3070554007567651	T	T	T
0.2310365393104124	0.1728091148787915	0.5245985517651833	T	T	T
0.3855678476291564	0.1737321507144335	0.5126009074422470	T	T	T
0.4362357254179273	0.1277902763251612	0.3023060316603638	T	T	T
0.3189766994918742	0.1677018059052510	0.1710269328151278	T	T	T
0.5797899449465485	0.5579371908446552	0.3494000460155156	T	T	T
0.6935014543287893	0.5330666156575029	0.1914967288739388	T	T	T
0.7128586424779095	0.5651276458106778	0.9759256617205838	T	T	T
0.8714079157858928	0.5574123925147915	0.9723559941237024	T	T	T
0.9343951013880246	0.5296889091984388	0.1875135951561323	T	T	T
0.5763387478709530	0.3294256537831641	0.3384083865886321	T	T	T
0.7063949251662427	0.3761989907794003	0.2226436313779737	T	T	T
0.7345801959009298	0.3305582959624593	1.0023150707367714	T	T	T
0.8864961755324727	0.3279010732984630	0.9809588246010967	T	T	T
0.9394841840052444	0.3729709824727955	0.1969014824873502	T	T	T
0.9244118773264000	0.4362350172964186	0.8300705176658194	T	T	T
0.7768315139755521	0.4461643783815307	0.4677120736303624	T	T	T
0.6193465542776344	0.4339785708474902	0.4904083669160792	T	T	T
0.5698754897931303	0.4673964181343145	0.7086962116161121	T	T	T
0.6742874539050387	0.4342943477391616	0.8576828867766795	T	T	T
0.9172602886423790	0.6723946584871784	0.8277278102422257	T	T	T
0.7980961601706095	0.6342539656224593	0.6980880133871822	T	T	T
0.7668893409918606	0.6679944759740515	0.4794469761797183	T	T	T
0.6114075341690565	0.6706867406041090	0.4880942416250683	T	T	T
0.5643696973149506	0.6263043172644106	0.7072972093536288	T	T	T
0.6805925834419803	0.6825275839331760	0.8286783142120803	T	T	T
0.5741389767623504	0.9433124982001998	0.3661865353318198	T	T	T
0.6951748533817713	0.9740873978541353	0.2257110062944746	T	T	T
0.7167901562103687	0.9444762478562260	1.0007886558856947	T	T	T
0.8769376675294647	0.9343006989558763	0.9964729226135469	T	T	T
0.9298343115680094	0.9703452974367655	0.2085113716762382	T	T	T
0.8206369025420789	0.9392830779856653	0.3585267570414434	T	T	T
0.5798691623527971	0.1749287947451869	0.3379332352682402	T	T	T
0.6982900564136553	0.1327157548674218	0.2051102088834873	T	T	T

Structure files (CONTCAR) involved in this work:

0.7304364408690157	0.1733320891573844	0.9831178917330393	T	T	T
0.8849977449282866	0.1734842816152583	0.9954997709321740	T	T	T
0.9335495024233703	0.1291575981039216	0.2075333699114759	T	T	T
0.8203421401062517	0.1704767465374570	0.3448122439291744	T	T	T
0.9232634678414867	0.0579719780865854	0.8634070961815808	T	T	T
0.8036319740255659	0.0307438624939448	0.7248547076651078	T	T	T
0.7806733685765239	0.0570000257637800	0.4987023038236990	T	T	T
0.6208019729205203	0.0670410045897400	0.4957108420105459	T	T	T
0.5672918236777443	0.0330569036128658	0.7048223264495135	T	T	T
0.6765514293605260	0.0605510310005626	0.8564924163880027	T	T	T
0.9165853390136934	0.8252156773714659	0.8420842479211048	T	T	T
0.8006432008579186	0.8745716091696620	0.7086089496521063	T	T	T
0.7666458547640115	0.8295619242510794	0.4910320939462716	T	T	T
0.6120526766806964	0.8262667813277143	0.4988445212395002	T	T	T
0.5616406335385086	0.8760104433018601	0.7058463013553655	T	T	T
0.6757810783505117	0.8384896746327759	0.8417239747913000	T	T	T
0.4249021004474428	0.4453833079881150	0.6381279267728315	T	T	T
0.3052365063486197	0.4730504824402561	0.7863809459252520	T	T	T
0.2861284941960854	0.4322331195863877	0.0033234586811394	T	T	T
0.1271115284287157	0.4311703779759997	-0.0004166553548457	T	T	T
0.0736189315916192	0.4718905509185384	0.7931823874636383	T	T	T
0.1828578269146041	0.4492526862256043	0.6438287942045359	T	T	T
0.4238077937283811	0.6721137209014062	0.6634927751057346	T	T	T
0.3015132139048847	0.6299437288406100	0.7990124830668547	T	T	T
0.2692121228075154	0.6721392408911192	0.0172535298340749	T	T	T
0.1147825038135760	0.6730000698342059	0.0077629714554121	T	T	T
0.0644706380136876	0.6295853756797504	0.7978466783761626	T	T	T
0.1794349160272844	0.6689217898316174	0.6627240265968647	T	T	T
0.0797726646147772	0.5524490543689957	0.1342245831471410	T	T	T
0.2008277009890213	0.5274599893707264	0.2798500687330259	T	T	T
0.2231309149790758	0.5677031346638954	0.5010846074414319	T	T	T
0.3837572475697671	0.5697692300086069	0.5035358513694612	T	T	T
0.4331895661169353	0.5279549215627125	0.2935973068519150	T	T	T
0.3267069806802922	0.5519993723624060	0.1408016503652250	T	T	T
0.0830340409291342	0.3276925982066145	0.1560497048935270	T	T	T
0.1989347304878369	0.3697141081302192	0.3013059247662878	T	T	T
0.2323450142466567	0.3293011672606737	0.5208617658209951	T	T	T
0.3865910176169837	0.3271140314651718	0.5080178897098637	T	T	T
0.4347672469788777	0.3704746791130782	0.2943184495012240	T	T	T
0.3194168486664034	0.3263737208738272	0.1653573049590811	T	T	T
0.8187221131207006	0.5708568279418493	0.3165916395024473	T	T	T
0.8322902314950696	0.3280438587993421	0.3504838689172403	T	T	T
0.7902105857284651	0.4763314335347697	0.7206587923524531	T	T	T
0.3565520771727151	0.0624546519687770	0.7188581934687119	T	T	T
0.2995899996304203	0.0656855135958713	0.8954229797547283	T	T	T
0.1999795407509425	0.0514045921980028	0.0279689722835261	T	T	T
0.1016559356717009	0.0663961607942689	0.8954164040637034	T	T	T
0.1012116578545772	0.0572578287487796	0.6978510264614821	T	T	T
0.2277238235986030	0.0329068929920007	0.7380541880326851	T	T	T
0.3569038123213763	0.8260733443422067	0.7478914405524040	T	T	T
0.3034539937726477	0.8436563821274708	0.9239240866592622	T	T	T
0.1890396977591391	0.8520397467130381	0.0214658374661282	T	T	T
0.0839892047896197	0.8322466426154433	0.9043194818852012	T	T	T

Structure files (CONTCAR) involved in this work:

0.1009288700582628	0.8375851816205855	0.7085014345456701	T	T	T
0.2272575862576761	0.8546150701801707	0.7622996956379148	T	T	T
0.3191624326247571	0.9478891882608008	0.8030963718498322	T	T	T
0.0791689211957104	0.9493089211109685	0.8109567347755234	T	T	T
0.4302504198731239	0.1265122593499762	0.5850685902486106	T	T	T
0.4163220878742084	0.9945333591139138	0.5702699707753260	T	T	T
0.3965642911099768	0.8624172461108865	0.5661728452396351	T	T	T
0.1932014751749458	0.1308026606412477	0.6112572762941951	T	T	T
0.1783899179298088	0.0024968429829186	0.5591049291159024	T	T	T
0.1920016075919065	0.8685832416440119	0.5704139533672360	T	T	T
0.9882354165046203	0.0470748355771005	0.7929005161194758	T	T	T
0.9808054456086617	0.8606150873121470	0.7880400149861304	T	T	T
0.1403989719162225	0.9390431836753592	0.2209551700702167	T	T	T
0.1977902923448943	0.9305842562875783	0.3970294110860337	T	T	T
0.2963617221082752	0.9468525228756605	0.5305752405460018	T	T	T
0.3950905527747297	0.9303743947252042	0.3986373330428220	T	T	T
0.3953222171889643	0.9449354623380157	0.2013466931559683	T	T	T
0.2689239930641571	0.9697204088553051	0.2410521989089990	T	T	T
0.1413310399534364	0.1700157203723232	0.2408684034872510	T	T	T
0.1940068867675178	0.1623403740778429	0.4181016033730267	T	T	T
0.3082700878519921	0.1478829965957950	0.5161431652297187	T	T	T
0.4127216337541029	0.1710073777186178	0.3988933039653333	T	T	T
0.3963191586177866	0.1553638505438253	0.2042924954469263	T	T	T
0.2702522264971098	0.1391400843343220	0.2591123187717705	T	T	T
0.1768345024647930	0.0509624048972851	0.3134802485660989	T	T	T
0.4177909715269870	0.0495542608721646	0.3213459967049978	T	T	T
0.0666026763271924	0.8714259618127677	0.0925253751181596	T	T	T
0.0807284684475569	0.0022841318032867	0.0672111792202448	T	T	T
0.0978521971347957	0.1345837770486619	0.0615221851956155	T	T	T
0.3030230992400074	0.8689491280934013	0.1190378602216813	T	T	T
0.3175350586119222	0.9955091428114156	0.0598300888025552	T	T	T
0.3043055581395043	0.1295087203098050	0.0662501872452807	T	T	T
0.5084941478415940	0.9528033465737002	0.2965435955310222	T	T	T
0.5162209535659722	0.1369092112435418	0.2864097609177455	T	T	T
0.6412758402685672	0.5641890049380167	0.2729480411522537	T	T	T
0.6733748627778886	0.5628002331783779	0.0814378910661283	T	T	T
0.7922162910034938	0.5484999501516273	0.9905545700972965	T	T	T
0.9148796965988486	0.5523280127523322	0.0731924231928162	T	T	T
0.9008699487220444	0.5715597905238151	0.2752370227600938	T	T	T
0.7682538922546502	0.5542324645212379	0.2151283620213935	T	T	T
0.6436341668165725	0.3368809006301535	0.2735004891205218	T	T	T
0.7262088649523289	0.3333195989049544	0.1226378956370973	T	T	T
0.8102034030284372	0.3558772114502296	0.9733139559132925	T	T	T
0.9169404377261147	0.3380990546038177	0.0912546986556255	T	T	T
0.9091112498470656	0.3358732476459481	0.2935687357359036	T	T	T
0.7690764087723002	0.3770651777863295	0.2996146159966312	T	T	T
0.6828896508578814	0.4511436105448024	0.1909861210908702	T	T	T
0.9150381909325287	0.4502507634027179	0.1952034677175054	T	T	T
0.5672847444635383	0.6288520146515439	0.4068737287547177	T	T	T
0.5938578090029192	0.5014384087390992	0.4355176082909672	T	T	T
0.5829131151900756	0.3681047681894813	0.4454998873759186	T	T	T
0.8018075127712545	0.6446843831127049	0.3792026099331566	T	T	T
0.8060024355342460	0.5033515790082280	0.4010221760673126	T	T	T

Structure files (CONTCAR) involved in this work:

0.8328950689450834	0.3778514637059521	0.4728541485661945	T	T	T
0.0153707113711841	0.5371367179778281	0.2021630689464923	T	T	T
0.0211483125393431	0.3702428571542653	0.2018097102508085	T	T	T
0.8727058954373559	0.4266368666330276	0.7288314789319802	T	T	T
0.7991380407908788	0.4672184472647128	0.5873825723363986	T	T	T
0.6999501597462716	0.4254321261074619	0.4730473763096149	T	T	T
0.6050680736208981	0.4371457903175845	0.6087659478155126	T	T	T
0.6008469496733001	0.4285426806813812	0.8049939613741730	T	T	T
0.7328520981754532	0.4252877140937747	0.7747744802292170	T	T	T
0.8626231696792444	0.6760947129635599	0.7388568944698016	T	T	T
0.8026928248024888	0.6330111729356255	0.5771964273762941	T	T	T
0.6881514376900125	0.6451907262594554	0.4845305955916247	T	T	T
0.5818053575830754	0.6581649423820384	0.5992884693416417	T	T	T
0.6038993607519934	0.6659776556594454	0.7955707647873523	T	T	T
0.7289105111429947	0.6713990047820038	0.7317976064778392	T	T	T
0.7998717721673558	0.5592918536163538	0.7454830435241004	T	T	T
0.5856477572285168	0.5475077154261758	0.7122521901067760	T	T	T
0.9294173629360964	0.3680642523717814	0.8944153294231127	T	T	T
0.8940214108084931	0.4967599179848146	0.8942621769190333	T	T	T
0.8889572111431336	0.6289133965018571	0.9209699759150529	T	T	T
0.6806229064222336	0.3777389264412894	0.9452166163501841	T	T	T
0.6792997740592169	0.5093681960436408	0.9036538811536218	T	T	T
0.7042606049320749	0.6380583669706946	0.9236196524218763	T	T	T
0.4898220814909412	0.4552273933781331	0.7084021085602433	T	T	T
0.4838710479791548	0.6344292834650531	0.7239677562219856	T	T	T
0.6394524529093936	0.9380367814712797	0.2951405228078364	T	T	T
0.6939769314407213	0.9393941321623466	0.1163532457996683	T	T	T
0.7974895826517088	0.9494998457249351	0.9890167712269615	T	T	T
0.8997923506412662	0.9305503622945215	0.1123943956340901	T	T	T
0.8952392457463374	0.9431082396634884	0.3106508253715318	T	T	T
0.7690488972888337	0.9636167637343710	0.2722104148474768	T	T	T
0.6412072741737093	0.1771922088895393	0.2594444083443463	T	T	T
0.6964727174109048	0.1522132839085680	0.0879919330193696	T	T	T
0.8080719154966129	0.1482014957909047	0.9841629968706137	T	T	T
0.9073042576959124	0.1724479300628538	0.1118883902915798	T	T	T
0.8972890286532869	0.1568452772831514	0.3077386478710257	T	T	T
0.7713569304597441	0.1484973196421250	0.2520762865637107	T	T	T
0.6791136949471914	0.0539011697963199	0.2190063213977560	T	T	T
0.9159941177864472	0.0501292995457731	0.1914459589991217	T	T	T
0.5653541084716510	0.8742371857240367	0.4296631023040725	T	T	T
0.5791581373902556	0.0062606430279680	0.4436055357084307	T	T	T
0.6028800878544698	0.1372589909100858	0.4400794323035396	T	T	T
0.8044644708784494	0.8629733952141007	0.3950689246916319	T	T	T
0.8155928095288134	0.9897344841040520	0.4538817467125813	T	T	T
0.8058343933586208	0.1235522257911589	0.4415600149454570	T	T	T
0.0095183836249861	0.9561085071916897	0.2193806219633059	T	T	T
0.0141276417621317	0.1382584341468143	0.2184283480751161	T	T	T
0.8581631037739329	0.0698430528332382	0.7932085694110709	T	T	T
0.8031957096278257	0.0639419519220276	0.6145882893099471	T	T	T
0.6999530700563608	0.0501996292095294	0.4878715325335166	T	T	T
0.5987427872092527	0.0753257448613416	0.6119134331877298	T	T	T
0.6020281482695976	0.0556045153763711	0.8092711890628410	T	T	T
0.7291342608185341	0.0378652687217860	0.7706970208528010	T	T	T

Structure files (CONTCAR) involved in this work:

0.8532870096270873	0.8266758862010686	0.7667046195016539	T	T	T
0.8026717314734334	0.8574380494154060	0.5912117356658478	T	T	T
0.6886063308378984	0.8532711398655348	0.4910262048302754	T	T	T
0.5869270830766382	0.8289147917571378	0.6142824517328382	T	T	T
0.5989398474436634	0.8529969625361857	0.8080599737834551	T	T	T
0.7255716968888581	0.8638236137832853	0.7526812076620146	T	T	T
0.8245570702916725	0.9519673769077246	0.7237907199268412	T	T	T
0.5798622483779441	0.9538371329083696	0.6816114064016061	T	T	T
0.9340081924396495	0.1252598443598673	0.9306972951387886	T	T	T
0.9161931432981247	0.9939982171962878	0.9379925596554576	T	T	T
0.8968669056109250	0.8628589792322083	0.9457936295093307	T	T	T
0.6908678650148650	0.1374085206563891	0.8915570162472483	T	T	T
0.6828443998315086	0.0113354596967511	0.9528724184413062	T	T	T
0.6907951533981641	0.8773617256713921	0.9452933766222341	T	T	T
0.4878757815574926	0.0477921422346942	0.7172568200996109	T	T	T
0.4813610562534163	0.8675406755781618	0.7208615369598019	T	T	T
0.3588907318897613	0.4436136101242819	0.7078961910172724	T	T	T
0.3074589772348498	0.4269534895023386	0.8864438908854009	T	T	T
0.2062202075668181	0.4459147773670560	0.0117454010160210	T	T	T
0.1059144218696164	0.4271289867817777	0.8818701618229376	T	T	T
0.1060774049019335	0.4540296310585665	0.6849644918723511	T	T	T
0.2312387900447916	0.4691804232231949	0.7361422915981555	T	T	T
0.3557939619855129	0.6662171227938323	0.7283876486820813	T	T	T
0.3017452951767468	0.6675838036613924	0.9062503801027531	T	T	T
0.1918707307195539	0.6468386511648867	0.0120776763756233	T	T	T
0.0901561555460868	0.6738058434975783	0.8918638676786760	T	T	T
0.1023443481324042	0.6536381800883876	0.6961166290934759	T	T	T
0.2279693702213144	0.6358621813696038	0.7474028140136194	T	T	T
0.3204380938561267	0.5510317692784369	0.8143183281800660	T	T	T
0.0812866501187250	0.5506755456803506	0.8198380299139360	T	T	T
0.4322511090663696	0.3746699332036165	0.5787368235342369	T	T	T
0.4196294523422717	0.5057151964492849	0.5566717082611625	T	T	T
0.4116917337066702	0.6383386182313627	0.5540801988031125	T	T	T
0.1945973775705728	0.3728236713837152	0.6066428229790713	T	T	T
0.1902129235311352	0.5002082770828276	0.5499246180385858	T	T	T
0.1927953855278625	0.6344697406258599	0.5543004933891221	T	T	T
0.9947066722480504	0.4528043192148946	0.7761517517887943	T	T	T
0.9846249215179026	0.6374107757510642	0.7819211035752789	T	T	T
0.1450878096671604	0.5589446693669667	0.2058543090714315	T	T	T
0.2026690083367989	0.5699506604392660	0.3838168425509508	T	T	T
0.3032398069337628	0.5642602151642191	0.5185370208069150	T	T	T
0.4015289610832029	0.5708312730209438	0.3857478002312006	T	T	T
0.4008659667515963	0.5548059116948241	0.1895097801807703	T	T	T
0.2736801779883105	0.5316072933940293	0.2278181042852150	T	T	T
0.1440321930827621	0.3300531515026700	0.2355811713715358	T	T	T
0.1951327420914493	0.3403556250677342	0.4142598742231968	T	T	T
0.3095249110790655	0.3540938680561380	0.5119996468693567	T	T	T
0.4124676095949875	0.3288224444272210	0.3934522657687315	T	T	T
0.3965949325539700	0.3398135720854867	0.1970554925114902	T	T	T
0.2726080810422052	0.3578831176955990	0.2536384372297246	T	T	T
0.1820523770564517	0.4495827375573216	0.3039195740315170	T	T	T
0.4149141074565532	0.4489408017344771	0.3099955684220732	T	T	T
0.0691970309332143	0.6226883163859426	0.0739896885190096	T	T	T

Structure files (CONTCAR) involved in this work:

0.0872873295937986	0.4925012080335179	0.0519272928772899	T	T	T
0.1071073640256365	0.3597078769834606	0.0496745162336739	T	T	T
0.3100513722449243	0.6253874201614585	0.0948939264444816	T	T	T
0.3254086270118561	0.4950896274160126	0.0535610625490539	T	T	T
0.3042271863640647	0.3619603047043016	0.0583742446862273	T	T	T
0.5131156297895821	0.5378627550496655	0.2872477066355643	T	T	T
0.5143919942994513	0.3618279214761977	0.2755372517806856	T	T	T
0.4414802148064980	0.7505878596138614	0.6458649866657076	T	T	T
0.1927377471579205	0.7487427092781275	0.6521313072474031	T	T	T
0.2726095634809245	0.7490440070893191	0.0563653311503158	T	T	T
0.1078552740758128	0.7483439901738229	0.0525135312774927	T	T	T
0.0618714571806419	0.2502675455869394	0.1365956131758669	T	T	T
0.3047800651060465	0.2469351130958012	0.1531041110109293	T	T	T
0.2274230876591170	0.2515829232993715	0.5552130619761467	T	T	T
0.3905647373023332	0.2509815507320006	0.5509276485408084	T	T	T
0.5600086452539194	0.2516713609442134	0.3650435388344034	T	T	T
0.8100844376397152	0.2471874171937993	0.3775641606924167	T	T	T
0.7254729210915162	0.2536100138955598	0.9647506470758840	T	T	T
0.8913286224691095	0.2492548170502989	0.9512846565747123	T	T	T
0.9345635948020138	0.7474242867711580	0.8677480673408724	T	T	T
0.6860774869217329	0.7597356951796409	0.8645223407145500	T	T	T
0.7714076613511434	0.7492564589274917	0.4899733719812824	T	T	T
0.6054430254935617	0.7496919170990854	0.4595285860718298	T	T	T
0.8777911523024265	0.4144471876569951	0.5867424579824929	T	T	T
0.0095714680372874	0.5523423258991506	0.5768885677438552	T	T	T
0.9306494422050824	0.5566744618167248	0.5142479773237453	T	T	T
0.0047002746148379	0.5484273545381430	0.4436373700683653	T	T	T
0.9442288391642695	0.4358440615470517	0.4556192977816908	T	T	T
0.9708217902510220	0.4377973183949976	0.5960237936138700	T	T	T
0.0249450944765215	0.4304285213374029	0.5027597248789772	T	T	T
0.9803140685052978	0.5331927711095684	0.5137532852218730	T	T	T
0.9769803673448650	0.4566439150492762	0.5151692735857669	T	T	T

Figure 4(c) Route(a)-Ga ③

Si Al O Ga H C

1.0000000000000000

20.0219999999999985 0.0000000000000000 0.0000000000000000

0.0000000000000000 19.8990000000000009 0.0000000000000000

0.0000000000000000 0.0000000000000000 13.3829999999999991

93 3 192 1 6 2

Selective dynamics

Direct

0.4219626230215113	0.0567513904863388	0.6481548509937602	T	T	T
0.3007552433478632	0.0266299310588254	0.7890627785587563	T	T	T
0.2795502829789430	0.0601981584710684	0.0123216491537948	T	T	T
0.1198763788617179	0.0630701131616185	0.0130293417265753	T	T	T
0.0671870469137781	0.0295372418394528	0.8001110202383743	T	T	T
0.1757762108126537	0.0554695222449708	0.6510460531522514	T	T	T
0.4188440016666573	0.8270698626417033	0.6701558419019981	T	T	T
0.3012074642522059	0.8683372202021428	0.8094268011447036	T	T	T
0.2668482164430409	0.8281462767632198	0.0295698193243022	T	T	T
0.1119405795630758	0.8264276210477618	0.0173216500064827	T	T	T
0.0614689080933624	0.8707004570687840	0.8029449505357701	T	T	T

Structure files (CONTCAR) involved in this work:

0.1786049000355601	0.8277133864286529	0.6737608711211438	T	T	T
0.0744606048741096	0.9425291242948850	0.1507522156563506	T	T	T
0.1956959052735539	0.9726256238862372	0.2933476040958400	T	T	T
0.2162774011336450	0.9366219283877412	0.5146402227934154	T	T	T
0.3755861905240897	0.9339250937244702	0.5156976390081713	T	T	T
0.4289559070151339	0.9698127099191077	0.3049457655608896	T	T	T
0.3201422926552737	0.9446697544431475	0.1546928102197665	T	T	T
0.0781977376240023	0.1721735766266688	0.1651736854221263	T	T	T
0.1957283687344923	0.1299822899597489	0.3076416393020749	T	T	T
0.2305932202944705	0.1728510342182732	0.5249261747117475	T	T	T
0.3852933401177732	0.1736968994377234	0.5134393817963196	T	T	T
0.4358411020937040	0.1279219914105003	0.3028821709904895	T	T	T
0.3185492380014671	0.1673201359294242	0.1711757825436308	T	T	T
0.5823408582613753	0.5534336333851329	0.3515420464287576	T	T	T
0.6929664732789029	0.5297533449864693	0.1893971271065833	T	T	T
0.7172666519901180	0.5651121492893207	0.9754880502834405	T	T	T
0.8754158329897080	0.5663285090947897	0.9892324336946017	T	T	T
0.9335659838410250	0.5325620591703398	0.1964307947126834	T	T	T
0.5751344418107579	0.3291778958247457	0.3363008521908699	T	T	T
0.6976520018837972	0.3750874164560322	0.2054013091493983	T	T	T
0.7309348291499572	0.3268129980016914	0.9911716389474882	T	T	T
0.8825427886103359	0.3267121277093831	0.9854733308682468	T	T	T
0.9356906111236187	0.3759132262385746	0.1931071832659737	T	T	T
0.9302981027685975	0.4436898272819830	0.8589884360486731	T	T	T
0.7831456875590095	0.4414955372522335	0.4884810355419810	T	T	T
0.6254038994410946	0.4297957828123341	0.4943299534958293	T	T	T
0.5673197929811871	0.4690719642573347	0.7066145665466077	T	T	T
0.6710336585950855	0.4344404794011569	0.8565397547354063	T	T	T
0.9180350114122765	0.6725299365299786	0.8292545316093621	T	T	T
0.7983222085007151	0.6344321929266640	0.6935733102130501	T	T	T
0.7673782321183616	0.6687926904917090	0.4754365519456263	T	T	T
0.6116539951254176	0.6704923987203864	0.4880278112186794	T	T	T
0.5640253530941278	0.6274528035447364	0.7054799132552841	T	T	T
0.6821811083670000	0.6812256298641174	0.8245818285102394	T	T	T
0.5736163121964761	0.9429233618359018	0.3652230025487260	T	T	T
0.6932221658567749	0.9728393556407107	0.2224055356271291	T	T	T
0.7171550550936644	0.9409034317060438	1.0004295695705003	T	T	T
0.8770812242984317	0.9331993093989872	0.9949725825801126	T	T	T
0.9295068536802007	0.9695291511127031	0.2057850238986972	T	T	T
0.8190196766685317	0.9432714928830012	0.3568217195838820	T	T	T
0.5793443248238097	0.1742055964293246	0.3369730930578757	T	T	T
0.6958644988982345	0.1291248480225440	0.2003671576376837	T	T	T
0.7303489817171321	0.1709246536246408	0.9795686565508087	T	T	T
0.8846821504768632	0.1730432386398095	0.9939367081668399	T	T	T
0.9335066707047716	0.1276815409556321	0.2046149613478730	T	T	T
0.8176216259608448	0.1669360738344714	0.3370125047563698	T	T	T
0.9229268346583603	0.0572712321738816	0.8625130023332134	T	T	T
0.8033509423409447	0.0295709578828917	0.7229563951700417	T	T	T
0.7799351610014362	0.0601502319429198	0.4980772435839789	T	T	T
0.6200921930241022	0.0672141209377654	0.4950403019322660	T	T	T
0.5670571362189866	0.0309467885018013	0.7034851169677493	T	T	T
0.6763048215836827	0.0557476689767571	0.8562866151721611	T	T	T
0.9175257886591986	0.8258972734913840	0.8384756845824288	T	T	T

Structure files (CONTCAR) involved in this work:

0.8012807754320851	0.8738864690780267	0.7047804484500183	T	T	T
0.7656684602275396	0.8300996339350378	0.4865223143344637	T	T	T
0.6107419531078536	0.8248831309364523	0.4963903310280747	T	T	T
0.5615943182423352	0.8742678804966630	0.7036909602330140	T	T	T
0.6768829105554807	0.8369590902790517	0.8390101346969848	T	T	T
0.4229024311327279	0.4454046255738621	0.6397194840249334	T	T	T
0.3041437233834068	0.4735448074518076	0.7882849642959613	T	T	T
0.2865470102970513	0.4334770966442323	0.0076394066102147	T	T	T
0.1286811958264299	0.4325105045974350	0.0077425896841234	T	T	T
0.0770174900086408	0.4732553462129891	0.8011992448648021	T	T	T
0.1815923102543218	0.4493275698883118	0.6460636713838568	T	T	T
0.4233312021245348	0.6723822844907584	0.6643631930927560	T	T	T
0.3009980511935704	0.6302764785738054	0.7993850188655811	T	T	T
0.2696022782773698	0.6720998701202840	0.0181700821438943	T	T	T
0.1153133926319383	0.6734867535485475	0.0090262255808193	T	T	T
0.0651121671794475	0.6301783168311343	0.8006637044452297	T	T	T
0.1785227172202920	0.6691878666426078	0.6637121676677198	T	T	T
0.0791007101860240	0.5542794765220861	0.1384006737018757	T	T	T
0.2014039395744993	0.5284010370319917	0.2805223497362211	T	T	T
0.2213470707969329	0.5675811539258493	0.5032077523047008	T	T	T
0.3815998325260834	0.5697720801794701	0.5055203997148597	T	T	T
0.4318319565151377	0.5269676704145648	0.2983610226635542	T	T	T
0.3286866215941383	0.5528681217948366	0.1429331273912779	T	T	T
0.0813602753723386	0.3270520963715324	0.1584526053588477	T	T	T
0.1973780984024809	0.3700152749378510	0.3028720990529151	T	T	T
0.2309985734625756	0.3296301967725089	0.5240865380811224	T	T	T
0.3848254026365496	0.3269141545012710	0.5126016080832264	T	T	T
0.4306767627741359	0.3709135164072404	0.2989986680147012	T	T	T
0.3184546529779005	0.3255832416835913	0.1656968471405408	T	T	T
0.8160389329512768	0.5623488239235180	0.3287627038562281	T	T	T
0.8213171347093648	0.3275413155046751	0.3287804184388823	T	T	T
0.7912127273418446	0.4732693849463002	0.7289045518174623	T	T	T
0.3565292831704550	0.0620345671555166	0.7190715599340955	T	T	T
0.2990349146282586	0.0658499389944217	0.8952158059598552	T	T	T
0.1994727704281029	0.0509497160006968	0.0277260370846212	T	T	T
0.1008152043367850	0.0667669298832080	0.8957311696833337	T	T	T
0.1010847439597101	0.0574596273080949	0.6980411655982239	T	T	T
0.2276282138651070	0.0321830081059252	0.7376931557248088	T	T	T
0.3566236350581453	0.8261693694841927	0.7476980582091092	T	T	T
0.3038841568284957	0.8432449861611107	0.9242653068682986	T	T	T
0.1892068362970006	0.8521844555420737	0.0205702240292041	T	T	T
0.0834589663666166	0.8321343516635470	0.9045059531404940	T	T	T
0.1012299247626931	0.8376307568279765	0.7085864414152002	T	T	T
0.2271755359279793	0.8547231776940863	0.7629785271884136	T	T	T
0.3191976821234551	0.9478117606534073	0.8040305322109833	T	T	T
0.0808523034441482	0.9495045573699141	0.8115758720035771	T	T	T
0.4299690294608054	0.1264471571694105	0.5858538073688535	T	T	T
0.4160718066861628	0.9947807440537813	0.5693250366033374	T	T	T
0.3963732284727720	0.8628059437423240	0.5661803752829667	T	T	T
0.1932632443206614	0.1303791244917576	0.6114720940086016	T	T	T
0.1777109359872826	0.0020967488339247	0.5590826113890226	T	T	T
0.1923883396326778	0.8683248635831787	0.5705915296447557	T	T	T
0.9879934958252594	0.0458206456302278	0.7923482557281502	T	T	T

Structure files (CONTCAR) involved in this work:

0.9814189421454680	0.8628125646912919	0.7862130263381165	T	T	T
0.1400303409503146	0.9391018379095685	0.2213931011938294	T	T	T
0.1978916189744661	0.9302177778511529	0.3970076577730694	T	T	T
0.2961026239240606	0.9472766778080381	0.5306755640898744	T	T	T
0.3945161020359051	0.9302540042023545	0.3981662166307371	T	T	T
0.3949566828241899	0.9455443407272058	0.2009277897067996	T	T	T
0.2685479303375950	0.9698982983855586	0.2406276348502744	T	T	T
0.1409776017159104	0.1696320794859767	0.2413194045544761	T	T	T
0.1935540416297201	0.1624935896044980	0.4184393950066536	T	T	T
0.3078852206928195	0.1481173853798718	0.5157906868983915	T	T	T
0.4131625623075497	0.1712596720977858	0.3999758443242634	T	T	T
0.3957980681637365	0.1556345027204377	0.2051265529483851	T	T	T
0.2698784570116159	0.1391348996011862	0.2595662452129337	T	T	T
0.1767280188176591	0.0507893084951375	0.3143810668303385	T	T	T
0.4170461271864217	0.0497625068361422	0.3221013188451413	T	T	T
0.0667484499130045	0.8712342094218476	0.0925769842192304	T	T	T
0.0802018316498989	0.0019697226580676	0.0674546314467669	T	T	T
0.0975328238633724	0.1340781598517702	0.0619811609757859	T	T	T
0.3028443541084098	0.8686995856411880	0.1195526798833203	T	T	T
0.3169293722530877	0.9947752922886361	0.0587999590500867	T	T	T
0.3040668945554742	0.1285881635890420	0.0668655638904964	T	T	T
0.5079146836928210	0.9532772608412403	0.2960395354417833	T	T	T
0.5157519960318983	0.1362923851482242	0.2852165039141635	T	T	T
0.6384341503465574	0.5618185173784389	0.2666298406122088	T	T	T
0.6821024821445496	0.5699275873181496	0.0838235141632577	T	T	T
0.7968187085763415	0.5473763472692018	0.9861046218411159	T	T	T
0.9057608089533113	0.5752486843262661	0.0998746908239794	T	T	T
0.9004488325733162	0.5547310795946948	0.2992380689719882	T	T	T
0.7676619687829717	0.5386816664128461	0.2276951780904663	T	T	T
0.6358723371577214	0.3361291263952931	0.2586595025817114	T	T	T
0.7178529549536088	0.3282627884270575	0.1099765768137351	T	T	T
0.8068207131669667	0.3547262533752911	0.9673862410024578	T	T	T
0.9047474633199917	0.3316449045571644	0.1011012978327353	T	T	T
0.9027512303606785	0.3498218706259414	0.2961307787960853	T	T	T
0.7604875244849968	0.3779273983839096	0.2798311488639872	T	T	T
0.6745168348154449	0.4499493506435234	0.1708135619489555	T	T	T
0.9192724756326912	0.4537492846011366	0.1686786665404708	T	T	T
0.5697526377358274	0.6240710977102829	0.4097822293351453	T	T	T
0.6065222424509195	0.4972155863375408	0.4331372042337533	T	T	T
0.5921407866707943	0.3643583211273363	0.4432385162671619	T	T	T
0.7983711902904899	0.6416185671928493	0.3741668325906468	T	T	T
0.8025875888761819	0.5054614494248681	0.4279713493804651	T	T	T
0.8318024667850388	0.3742014898328299	0.4520931509456315	T	T	T
0.0143961137153083	0.5433374410450159	0.2078305445223536	T	T	T
0.0165432413090683	0.3671378359950619	0.1991015659089421	T	T	T
0.8751870016033566	0.4420513454836798	0.7642466587495774	T	T	T
0.8153455623200210	0.4484082091470909	0.6037727032516075	T	T	T
0.7068973123729072	0.4183403837229444	0.4973477257656840	T	T	T
0.5998013407633744	0.4342731343788065	0.6083016601863384	T	T	T
0.5969178225535243	0.4339927483107448	0.8065769650550870	T	T	T
0.7275826913836996	0.4257795432013070	0.7710575420981491	T	T	T
0.8628667629350105	0.6727750879644304	0.7412874202252967	T	T	T
0.8064535687480107	0.6376464427938392	0.5732723178869407	T	T	T

Structure files (CONTCAR) involved in this work:

0.6888616886851338	0.6467290056947251	0.4888960202259416	T	T	T
0.5802808130037995	0.6621174725586670	0.5990225010552318	T	T	T
0.6050387967172968	0.6639317468626513	0.7951788501624990	T	T	T
0.7291509395777721	0.6721859455292862	0.7258110696667861	T	T	T
0.7966326891703398	0.5581515009919186	0.7350999233967369	T	T	T
0.5852200785390875	0.5486533838528974	0.7036628384496934	T	T	T
0.9320061628319973	0.3719330534898748	0.9143160537990422	T	T	T
0.9152391570033562	0.5046618644623736	0.9326761806693467	T	T	T
0.8899231489989150	0.6347699993807141	0.9278197780569194	T	T	T
0.6757450848378955	0.3722959458162814	0.9346937759800106	T	T	T
0.6814246254357826	0.5058456183651644	0.9124802077248001	T	T	T
0.7084538950740689	0.6356780483001673	0.9167227988578401	T	T	T
0.4871738887754695	0.4584855962372145	0.7097298839883749	T	T	T
0.4838762331672178	0.6357466950266926	0.7252824480982906	T	T	T
0.6387640275904720	0.9365754867495225	0.2938912497553985	T	T	T
0.6956332244096759	0.9336738613868882	0.1163564458275290	T	T	T
0.7975952578083255	0.9480275788817734	0.9874844381816117	T	T	T
0.8999290435876912	0.9281122206163863	0.1108407052164309	T	T	T
0.8934275673260094	0.9451501158299019	0.3081632942716168	T	T	T
0.7668633511391718	0.9692168356185767	0.2722369632879592	T	T	T
0.6420563265184352	0.1743838027400599	0.2606581133598074	T	T	T
0.6952966977098932	0.1549235242394508	0.0857972322217934	T	T	T
0.8080891103179357	0.1462474729754520	0.9845617333103738	T	T	T
0.9081025184761730	0.1723792702192434	0.1099125871498868	T	T	T
0.8954205070544984	0.1527750311110601	0.3048994009442176	T	T	T
0.7701040066083679	0.1362688877036414	0.2482983258958600	T	T	T
0.6723125488468805	0.0509615229532016	0.2058729850277178	T	T	T
0.9170116389589635	0.0489956033390785	0.1840684665275101	T	T	T
0.5641896660895412	0.8739061290389052	0.4286613619127861	T	T	T
0.5795217173756344	0.0060026110602221	0.4422193142334896	T	T	T
0.6005927939869851	0.1375872252905876	0.4409287818103216	T	T	T
0.8017420345253909	0.8671461890264984	0.3922696753448631	T	T	T
0.8163175277558887	0.9938411177923409	0.4523522757465029	T	T	T
0.8037520268068984	0.1281126635500756	0.4421049604843086	T	T	T
0.0089323603590843	0.9548711260156828	0.2193730247798917	T	T	T
0.0137269312420065	0.1378851722986348	0.2188449693313310	T	T	T
0.8575507787883165	0.0681767009071245	0.7925348250299780	T	T	T
0.8012873889532451	0.0659606587635934	0.6147403308498941	T	T	T
0.6994618912183345	0.0517957222283301	0.4858493724516129	T	T	T
0.5986978183941483	0.0741518194655915	0.6117059804068222	T	T	T
0.6019063300330620	0.0514582460540648	0.8086903605398308	T	T	T
0.7291745037649441	0.0325685094886024	0.7710910991616744	T	T	T
0.8543982515871920	0.8264493821156232	0.7628119236367734	T	T	T
0.8021503285133457	0.8551165350952512	0.5879269763901516	T	T	T
0.6872547414076635	0.8521306889170855	0.4900971622839674	T	T	T
0.5855208564342088	0.8265174573798713	0.6119331505797849	T	T	T
0.6001252103628389	0.8515956468392830	0.8051035665352211	T	T	T
0.7267309456883644	0.8637011517185874	0.7509878797495895	T	T	T
0.8258396512925382	0.9513314536693485	0.7167095073212015	T	T	T
0.5793707360963043	0.9519878559094765	0.6778835788933317	T	T	T
0.9336398266440231	0.1253390576497366	0.9281696403352601	T	T	T
0.9160957781010113	0.9938117700969229	0.9382231195006890	T	T	T
0.8968845602712421	0.8622306378041196	0.9427600696229022	T	T	T

Structure files (CONTCAR) involved in this work:

0.6912751191931693	0.1324285143389088	0.8903245048448658	T	T	T
0.6815613299165718	0.0073688573312043	0.9538143702163061	T	T	T
0.6918238372418070	0.8740444153926308	0.9439090975573888	T	T	T
0.4878535361007388	0.0465173729863489	0.7167071446029435	T	T	T
0.4814485785112724	0.8664937718221232	0.7211079006388208	T	T	T
0.3575310061676064	0.4424898715404428	0.7107462345283460	T	T	T
0.3041743623252896	0.4286384098327872	0.8894572975210830	T	T	T
0.2072713080264665	0.4487606667182049	0.0238768922780314	T	T	T
0.1114314886220331	0.4293197165051425	0.8886811670167262	T	T	T
0.1058954150462465	0.4540725001213922	0.6914199910829789	T	T	T
0.2307195577033007	0.4701433902276817	0.7367680196981652	T	T	T
0.3553685324206955	0.6668636240554311	0.7293435929855441	T	T	T
0.3011076688602899	0.6679333237828370	0.9065393264888788	T	T	T
0.1922097812829909	0.6466727468585043	0.0138229605648287	T	T	T
0.0903254603833071	0.6758561764114064	0.8933320260679496	T	T	T
0.1014062006810690	0.6550081838497127	0.6981930961247672	T	T	T
0.2274904591120892	0.6356915413010703	0.7475088998885679	T	T	T
0.3203986270208110	0.5515062293466217	0.8147224640144856	T	T	T
0.0853635386375353	0.5523759464775834	0.8245492049570098	T	T	T
0.4319846736684771	0.3742948530203220	0.5815652676833666	T	T	T
0.4164476214705962	0.5045294361132429	0.5566002664324691	T	T	T
0.4112637392163919	0.6375378663405969	0.5558589376826393	T	T	T
0.1920065475850244	0.3726226642363012	0.6092749056430484	T	T	T
0.1879610681663111	0.5000820160626656	0.5516424243602912	T	T	T
0.1901516633313708	0.6343394355299081	0.5552054188693870	T	T	T
0.9974738877244972	0.4539725348505847	0.7921681713349991	T	T	T
0.9846818903796122	0.6343474577119421	0.7860561773018250	T	T	T
0.1453033039705377	0.5609870536035093	0.2079916612379067	T	T	T
0.2025667382871112	0.5696505980472961	0.3855090954129468	T	T	T
0.3012717066850364	0.5652399648811219	0.5226443793842038	T	T	T
0.3988878473912347	0.5715244622727356	0.3876347932987126	T	T	T
0.4027435372288335	0.5557865988367700	0.1929010989978085	T	T	T
0.2743945630027033	0.5337118653523528	0.2289925008171533	T	T	T
0.1393266113694555	0.3306862407165931	0.2427686959976363	T	T	T
0.1958866354437159	0.3419923905330814	0.4164951671572387	T	T	T
0.3082504812911798	0.3546587680493785	0.5200311229091067	T	T	T
0.4076726694849604	0.3285054475669673	0.3967435732957565	T	T	T
0.3951006168741776	0.3388933805607195	0.2005092753333373	T	T	T
0.2696949074462355	0.3560455461402647	0.2521714891345559	T	T	T
0.1826161397006635	0.4502852592617309	0.3025567086980316	T	T	T
0.4084640723233326	0.4489917664503614	0.3126142306459861	T	T	T
0.0692499976183629	0.6228266882627356	0.0737905109607396	T	T	T
0.0854975000317679	0.4917906819405341	0.0597966895317272	T	T	T
0.1086253557958999	0.3600782645353276	0.0545159502918877	T	T	T
0.3117600018155183	0.6255969301441976	0.0946962287110307	T	T	T
0.3284146692902760	0.4949977521690530	0.0568987176104559	T	T	T
0.3050851986375539	0.3620290528690819	0.0588508998566825	T	T	T
0.5123962076533508	0.5310530448551394	0.2996229503433859	T	T	T
0.5106839732204214	0.3651937647956165	0.2852061656165314	T	T	T
0.4405952547378820	0.7506317588753236	0.6447091582604768	T	T	T
0.1930211902812457	0.7487431232739785	0.6526798183690997	T	T	T
0.2726245210041224	0.7490233519579023	0.0572026365455872	T	T	T
0.1086365791876089	0.7487157933869050	0.0541016604814074	T	T	T

Structure files (CONTCAR) involved in this work:

0.0620542316863058	0.2495835903647947	0.1363131471405822	T	T	T
0.3042439793620121	0.2462824649236078	0.1514092999743522	T	T	T
0.2261609543285960	0.2514653852471818	0.5561340186345413	T	T	T
0.3897466256615503	0.2505135911499963	0.5538438227706926	T	T	T
0.5589000143376245	0.2512000031490278	0.3612225544328318	T	T	T
0.8041360692248466	0.2455254991053509	0.3520453795555786	T	T	T
0.7260692955161797	0.2499978801873026	0.9522118786703007	T	T	T
0.8897402614461732	0.2492233058576476	0.9500590382985830	T	T	T
0.9375083818157314	0.7484423371797679	0.8618221986248886	T	T	T
0.6874365701059889	0.7581783233991279	0.8612303031069926	T	T	T
0.7724409154125501	0.7502343625464328	0.4777677073533037	T	T	T
0.6043335450091509	0.7487065207809493	0.4544798528851697	T	T	T
0.9097646408235573	0.4439601218575611	0.6312376801720386	T	T	T
0.0386310366762199	0.5446036561546420	0.4842195783258568	T	T	T
0.9896155927877752	0.5648094421481733	0.5898694006353806	T	T	T
0.9510509131298578	0.5544387676650500	0.4702331983763666	T	T	T
0.8762460356754310	0.3905673693527887	0.4306719601641103	T	T	T
0.0272761808175690	0.4371997750484004	0.5746479740127364	T	T	T
0.9731002535231079	0.4314428500742826	0.4684585914979207	T	T	T
0.9900656355548544	0.5353390866154932	0.5203488743873619	T	T	T
0.9837800085135762	0.4594622323159588	0.5375419437114796	T	T	T

Figure 4(c) Route(a)-Ga ④

Si Al O Ga H C

1.0000000000000000

20.0219999999999985 0.0000000000000000 0.0000000000000000

0.0000000000000000 19.8990000000000009 0.0000000000000000

0.0000000000000000 0.0000000000000000 13.3829999999999991

93 3 192 1 6 2

Selective dynamics

Direct

0.4233754552401745	0.0559188833859226	0.6470688963268294	T	T	T
0.3023043764319880	0.0257348237795250	0.7882484572747196	T	T	T
0.2804791905242153	0.0598444399869762	0.0110742001979099	T	T	T
0.1209814195685623	0.0630159341671400	0.0115752024260815	T	T	T
0.0690905611814972	0.0288714362300672	0.7997111338311951	T	T	T
0.1775191454211257	0.0542820778067316	0.6498564079290892	T	T	T
0.4203033874588910	0.8266853754097827	0.6699342471845307	T	T	T
0.3029854917257669	0.8675799282342257	0.8097277427810764	T	T	T
0.2683138025216684	0.8280517719252274	0.0307165242056061	T	T	T
0.1134259592202187	0.8259028771640198	0.0183140479516718	T	T	T
0.0642304279513622	0.8705736833871340	0.8040586835352581	T	T	T
0.1803822421194850	0.8274941439324165	0.6726605577792620	T	T	T
0.0753984909467947	0.9428519098167233	0.1489156576664497	T	T	T
0.1966379313840322	0.9726132296690105	0.2922998182174525	T	T	T
0.2176284906497217	0.9361074274713986	0.5124461318481863	T	T	T
0.3771043185133074	0.9329769370512518	0.5144498771544012	T	T	T
0.4310055091227346	0.9698635567250523	0.3048021831118815	T	T	T
0.3216253579929385	0.9451103655244422	0.1544596494131283	T	T	T
0.0794921723379130	0.1720930842078626	0.1649795892640471	T	T	T
0.1965929778267101	0.1297680949883071	0.3080640699492306	T	T	T
0.2321039796862052	0.1724226443682726	0.5253103147986240	T	T	T
0.3867272743943166	0.1733190517954755	0.5128645641625380	T	T	T

Structure files (CONTCAR) involved in this work:

0.4365211506677518	0.1276412284807248	0.3024987053826457	T	T	T
0.3190329424185293	0.1666432059561929	0.1704066087109365	T	T	T
0.5832677547288992	0.5524927402330205	0.3541769404295156	T	T	T
0.6937600659891136	0.5290496321624691	0.1906599577844350	T	T	T
0.7177997017878573	0.5663800346385678	0.9773019132377984	T	T	T
0.8750420799925551	0.5670798465829499	0.9897755185115609	T	T	T
0.9335407588046847	0.5273213117433487	0.1884747688460842	T	T	T
0.5766822545005242	0.3296587279840154	0.3355628310292064	T	T	T
0.6985798512791350	0.3755107972421532	0.2017220609243090	T	T	T
0.7331373851469342	0.3276094651957192	0.9879793801614091	T	T	T
0.8853296710845796	0.3259322439187237	0.9893829859979942	T	T	T
0.9366037810956390	0.3717388587255209	0.1941658950783307	T	T	T
0.9313070491427483	0.4439715278678672	0.8679227461621329	T	T	T
0.7861233810755603	0.4360042892230661	0.5012313303114950	T	T	T
0.6269056335522455	0.4284895202792164	0.4959706846396306	T	T	T
0.5682953331571011	0.4692797475041224	0.7068616595208445	T	T	T
0.6729524618757562	0.4390377159497298	0.8557397372508455	T	T	T
0.9200255618036690	0.6743187981620635	0.8344004556499702	T	T	T
0.8034160339600176	0.6368715802705420	0.6934498226295412	T	T	T
0.7718432556759478	0.6712510261174836	0.4735964917039636	T	T	T
0.6163031954234313	0.6706825320909545	0.4883134352604991	T	T	T
0.5674351593908102	0.6276600489075090	0.7049625628299281	T	T	T
0.6848935028271291	0.6811690510086560	0.8246333510370085	T	T	T
0.5758651719486226	0.9431728753647803	0.3630312684259820	T	T	T
0.6948317737618488	0.9741777429195181	0.2194153394347550	T	T	T
0.7186689614807579	0.9420209979470739	0.9980761752567529	T	T	T
0.8782539401544786	0.9345258477018807	0.9947160032703082	T	T	T
0.9307573881384986	0.9710515979167345	0.2043159852302183	T	T	T
0.8204298674073986	0.9476196560468488	0.3553382902414383	T	T	T
0.5800890619668143	0.1744164026343229	0.3335783223332650	T	T	T
0.6962693590381717	0.1295744377822186	0.1958964846690774	T	T	T
0.7323155977417758	0.1719527454841218	0.9755731595106892	T	T	T
0.8868535771176852	0.1735786427850434	0.9896586704650338	T	T	T
0.9343949384789492	0.1287025366835093	0.2016213700325452	T	T	T
0.8174262459136519	0.1683842973334474	0.3323682910649667	T	T	T
0.9246649419768793	0.0566801273055209	0.8600890318713734	T	T	T
0.8044821668031100	0.0293690299845897	0.7185117042244542	T	T	T
0.7809296338253090	0.0639747468404285	0.4962711945408386	T	T	T
0.6212346669299219	0.0679233086547113	0.4927712929797404	T	T	T
0.5686805613582475	0.0311797320632393	0.7012245051595275	T	T	T
0.6782840623267682	0.0560231894361461	0.8536830858504399	T	T	T
0.9198037054554070	0.8271559106442521	0.8395593116316333	T	T	T
0.8038122378330286	0.8729587870806318	0.7004780504095723	T	T	T
0.7676044494647323	0.8308718622339497	0.4819326329973513	T	T	T
0.6131119075629005	0.8250873554308904	0.4942122045869031	T	T	T
0.5633137941491878	0.8745075650537506	0.7010845071398643	T	T	T
0.6794072068824490	0.8373738676834245	0.8359204132196623	T	T	T
0.4236544281769097	0.4451277918812778	0.6435085849208217	T	T	T
0.3036473961300641	0.4735089658734393	0.7903438017665203	T	T	T
0.2886263647814983	0.4339401842924597	0.0100905443226449	T	T	T
0.1318745964700781	0.4330281607216010	0.0100627805312979	T	T	T
0.0773233367893265	0.4725174061128243	0.8040109030170237	T	T	T
0.1806347270093385	0.4481658974185212	0.6484351041119418	T	T	T

Structure files (CONTCAR) involved in this work:

0.4252590565887022	0.6719261653430583	0.6657572146623287	T	T	T
0.3019329755111785	0.6302999984268350	0.8008511880495188	T	T	T
0.2709500191946427	0.6721286345222836	0.0203079533827596	T	T	T
0.1170428130789558	0.6730162781786805	0.0127276210889164	T	T	T
0.0666617253608284	0.6296073424595725	0.8038313344254667	T	T	T
0.1788235884920734	0.6691383466972919	0.6642756912899116	T	T	T
0.0801925248521764	0.5537588139333725	0.1411830536651537	T	T	T
0.2025520844784594	0.5275695669512140	0.2832816992083529	T	T	T
0.2217271262836146	0.5659642520337748	0.5070636734940049	T	T	T
0.3811934340462202	0.5685639959169504	0.5094932276001020	T	T	T
0.4313029946984139	0.5268081798985933	0.3021402362928911	T	T	T
0.3301740879158466	0.5529167987214224	0.1434882361469345	T	T	T
0.0835311284043029	0.3268078746404094	0.1590421800367156	T	T	T
0.1982735366142903	0.3689930395350376	0.3056454974055848	T	T	T
0.2323857873889839	0.3291518421592333	0.5271651406036041	T	T	T
0.3865172048190512	0.3266080453187114	0.5161886597001966	T	T	T
0.4319139208583542	0.3707648789075095	0.3015483835486869	T	T	T
0.3195089300479928	0.3248046745243449	0.1675970804605836	T	T	T
0.8220388328160932	0.3295559393379897	0.3266157047692337	T	T	T
0.8012500214488870	0.4742185101276279	0.7286042513444821	T	T	T
0.8112032836784367	0.5556757253070503	0.3397464010018678	T	T	T
0.3580928414882244	0.0612319981274314	0.7183499266347697	T	T	T
0.2999510405975266	0.0655100878989897	0.8939588223555781	T	T	T
0.2004384123785954	0.0501344278777742	0.0261004670687897	T	T	T
0.1018797501688502	0.0680751766005314	0.8943394648037244	T	T	T
0.1028664790070011	0.0556340204622506	0.6969245308652512	T	T	T
0.2293768391545230	0.0301701702730845	0.7359993887745025	T	T	T
0.3590622554064508	0.8255560575347295	0.7492136552454652	T	T	T
0.3045780684400582	0.8426368890283480	0.9246969677220090	T	T	T
0.1905498619577579	0.8518913233485026	0.0229651871417959	T	T	T
0.0864271576359242	0.8307417036499151	0.9045509565804514	T	T	T
0.1033090437176143	0.8383248012916267	0.7084915129402789	T	T	T
0.2294643582711771	0.8536557972830415	0.7617716674853703	T	T	T
0.3210250257497068	0.9470756438297082	0.8044618442150782	T	T	T
0.0838324890625255	0.9492509684756650	0.8147358718457752	T	T	T
0.4314897761302720	0.1251948178636638	0.5838639547344213	T	T	T
0.4173728253923221	0.9935902778724449	0.5689194730718450	T	T	T
0.3965583428996716	0.8618928588459458	0.5661951091063274	T	T	T
0.1950126165290151	0.1294238516357786	0.6115341982930270	T	T	T
0.1793197223271109	0.0017085912003238	0.5568774972538308	T	T	T
0.1941936356965492	0.8681128646093285	0.5695384391069034	T	T	T
0.9897750014643779	0.0441208444415355	0.7904810739530308	T	T	T
0.9841171071619772	0.8635263951962897	0.7877497806032545	T	T	T
0.1411429718417222	0.9399493632714935	0.2191918295419882	T	T	T
0.1983672631714447	0.9291696207232800	0.3951009433322648	T	T	T
0.2975509225578459	0.9469333271240874	0.5266938574541994	T	T	T
0.3977034158308593	0.9288072370998418	0.3975269116885019	T	T	T
0.3964075542480033	0.9466207436921474	0.2006891828566436	T	T	T
0.2696662034985467	0.9702947426228778	0.2400073232781340	T	T	T
0.1416494221307306	0.1694406602114346	0.2421441185143483	T	T	T
0.1949579667159636	0.1625117674895672	0.4187204013062912	T	T	T
0.3093404086110761	0.1477238890795860	0.5154169780601975	T	T	T
0.4140300477004169	0.1718518581354400	0.3989262006389982	T	T	T

Structure files (CONTCAR) involved in this work:

0.3961049584311168	0.1540950173637487	0.2043559866741187	T	T	T
0.2703919713018931	0.1386194852139267	0.2588622949269463	T	T	T
0.1775920513122780	0.0505578475336578	0.3150306818705573	T	T	T
0.4183726128949884	0.0495267326935972	0.3241829984856759	T	T	T
0.0673686397041091	0.8711051178324689	0.0919235411283460	T	T	T
0.0809375097953536	0.0015462373998013	0.0644783204337392	T	T	T
0.0990614388541412	0.1335722313385735	0.0623218257559435	T	T	T
0.3048666111700377	0.8688796874197207	0.1199015567493835	T	T	T
0.3181539124052795	0.9947296236912938	0.0580167361699334	T	T	T
0.3043822359560425	0.1284040781577912	0.0657411490824896	T	T	T
0.5100448243695797	0.9539584702028180	0.2941362135304708	T	T	T
0.5161965787141719	0.1362575266589631	0.2831663732657314	T	T	T
0.6383324190794393	0.5601654746085580	0.2670489930883488	T	T	T
0.6883167185088788	0.5742111058962887	0.0891603251422315	T	T	T
0.7973294834384835	0.5461217669554014	0.9811452646524267	T	T	T
0.8982823967824496	0.5751041651637679	0.1067935524914391	T	T	T
0.9008084343913291	0.5459274637298922	0.3016927066157703	T	T	T
0.7681645174296364	0.5343210270908428	0.2345922028228237	T	T	T
0.6372982342101816	0.3376565208014500	0.2578658120622721	T	T	T
0.7163035526934372	0.3282379469385188	0.1059101496065397	T	T	T
0.8100418927701398	0.3543724599796000	0.9703006286695052	T	T	T
0.9036357502156305	0.3249546476203830	0.1073662061955831	T	T	T
0.9049125331714090	0.3502067433416658	0.2993748108503059	T	T	T
0.7627347645942566	0.3799403424239000	0.2734843894376692	T	T	T
0.6751534924539034	0.4504037636537565	0.1658737243346962	T	T	T
0.9184340399642398	0.4497248729908058	0.1646663293947276	T	T	T
0.5734654117728631	0.6235712064896585	0.4123145336996726	T	T	T
0.6083003472248854	0.4958761760223837	0.4339325307456186	T	T	T
0.5943932695820480	0.3630847389180467	0.4432715107485062	T	T	T
0.8055384318559824	0.6374501479944568	0.3777486685880097	T	T	T
0.8068492410834458	0.5003028594968361	0.4391890153646183	T	T	T
0.8275909208967246	0.3667121216545973	0.4545091985694489	T	T	T
0.0121285704425868	0.5425870231366231	0.2063990476198783	T	T	T
0.0176479451701510	0.3670059443957190	0.1965404529001696	T	T	T
0.8718197368029552	0.4346192363722586	0.7858591635297431	T	T	T
0.8197460876317245	0.4354085930698496	0.6119794600625132	T	T	T
0.7079323993699154	0.4178704628388581	0.5005887215268656	T	T	T
0.5981869943980419	0.4326878113520541	0.6082394208277666	T	T	T
0.5983676547286818	0.4352149283297218	0.8069523845538817	T	T	T
0.7287592985490940	0.4391569169054509	0.7700808323065801	T	T	T
0.8645807281251677	0.6772042178950088	0.7473044496723212	T	T	T
0.8121267660537247	0.6485544365441350	0.5742395635058649	T	T	T
0.6938894204360672	0.6470805003940652	0.4865667771617079	T	T	T
0.5863161830171606	0.6636102904874845	0.6002282378523233	T	T	T
0.6077641066585426	0.6631379471006730	0.7962562894216024	T	T	T
0.7317994444579308	0.6697154065256594	0.7267024477581506	T	T	T
0.8071672963561407	0.5594593407353440	0.7258533255720535	T	T	T
0.5871534742339610	0.5486518926122981	0.7006853250995865	T	T	T
0.9382911546049623	0.3743746219470226	0.9309426640480061	T	T	T
0.9205055324226319	0.5074290613780708	0.9411287752357715	T	T	T
0.8913910795024860	0.6371177642629370	0.9340068950725230	T	T	T
0.6806839264496927	0.3738548918123609	0.9281232459807870	T	T	T
0.6766628601167931	0.5077744800316140	0.9213680596591304	T	T	T

Structure files (CONTCAR) involved in this work:

0.7104527648107125	0.6370921634288942	0.9188348265785113	T	T	T
0.4878889246728282	0.4599340576842708	0.7126894396148742	T	T	T
0.4873669689311320	0.6364661344325455	0.7240766765852757	T	T	T
0.6411493097001176	0.9376196731653890	0.2918442511819773	T	T	T
0.6979624677338928	0.9337401425811400	0.1143148914163855	T	T	T
0.7990437979686092	0.9499052123957145	0.9849575866585742	T	T	T
0.9001183159159233	0.9288284903304059	0.1109577424935547	T	T	T
0.8950900168185165	0.9484797947972747	0.3077395007436063	T	T	T
0.7684240511126533	0.9730610315314557	0.2701097866389136	T	T	T
0.6422031572655271	0.1745772137274571	0.2561557849794497	T	T	T
0.6969242759160378	0.1561268499627244	0.0816740523385647	T	T	T
0.8100824883399618	0.1472962588134616	0.9809085986716090	T	T	T
0.9104524173038748	0.1725649719620209	0.1054982101611592	T	T	T
0.8952990562825947	0.1536134183007688	0.3010540110436800	T	T	T
0.7701090551944719	0.1352586690715717	0.2454693935820902	T	T	T
0.6722059540823930	0.0514785735313553	0.1998987590901383	T	T	T
0.9183790299383766	0.0500941154713324	0.1803385288761225	T	T	T
0.5668709474098913	0.8733664977211152	0.4247942785174861	T	T	T
0.5815558857184002	0.0056788226502709	0.4410785091005510	T	T	T
0.6014903105523084	0.1377835392695973	0.4375004069165560	T	T	T
0.8027687053111473	0.8718887092344130	0.3911384333730609	T	T	T
0.8184728810525842	0.9982767854064190	0.4506454081118590	T	T	T
0.8037630390758481	0.1321826167766509	0.4399154459959430	T	T	T
0.0100810602022868	0.9558257194936743	0.2176861768812368	T	T	T
0.0144150353075582	0.1388437051596968	0.2182071222538774	T	T	T
0.8593505477928169	0.0655630592332147	0.7896353225597897	T	T	T
0.8015085181159765	0.0699184398469419	0.6133801110615726	T	T	T
0.7007610368674889	0.0536103400540799	0.4835915072667937	T	T	T
0.5996550281253368	0.0748726147742033	0.6093780674550171	T	T	T
0.6038818606835336	0.0518152814746060	0.8061098422538995	T	T	T
0.7310252827083363	0.0307968102901433	0.7694577525454281	T	T	T
0.8576323196863789	0.8287245319747217	0.7623752645972419	T	T	T
0.8052583099768552	0.8481140645356363	0.5859341473007770	T	T	T
0.6894733730876227	0.8531663334746696	0.4905304081736864	T	T	T
0.5863069812432594	0.8268297434116773	0.6087813296039796	T	T	T
0.6026319878722411	0.8515306736024811	0.8016387137268224	T	T	T
0.7294332940950689	0.8636277700565622	0.7477921230471285	T	T	T
0.8262879161605495	0.9514356955575042	0.7040096064829137	T	T	T
0.5811510475154303	0.9522511530852588	0.6753981994277345	T	T	T
0.9351645009003576	0.1259896414484686	0.9227691955219544	T	T	T
0.9181756353047795	0.9948410550058485	0.9387482797310975	T	T	T
0.8981579516382899	0.8635500571811578	0.9431464333120309	T	T	T
0.6939166052382950	0.1329425920715821	0.8859740339680711	T	T	T
0.6827802672593012	0.0087015157077891	0.9525937377302043	T	T	T
0.6937723613754263	0.8754772090969059	0.9402752360878752	T	T	T
0.4894465583641686	0.0461422316094611	0.7153746736435397	T	T	T
0.4832512396734270	0.8665748012026783	0.7191998673012499	T	T	T
0.3581373943275969	0.4429719335765672	0.7141440280581065	T	T	T
0.3037058271437296	0.4282915138533991	0.8913660492321142	T	T	T
0.2098543284832077	0.4508416900297177	0.0293711975409696	T	T	T
0.1156477292883007	0.4306938204309018	0.8912662192256501	T	T	T
0.1052247923478041	0.4524645916206319	0.6939049971170720	T	T	T
0.2307050005013268	0.4701750217676198	0.7377759278900400	T	T	T

Structure files (CONTCAR) involved in this work:

0.3586545073315527	0.6657005483545089	0.7336461488948371	T	T	T
0.3002191365112715	0.6686434983647782	0.9074835525701339	T	T	T
0.1936618995368525	0.6457767099627275	0.0206831170667124	T	T	T
0.0932406167520784	0.6744882540371253	0.8969236111013303	T	T	T
0.1022133581947013	0.6562038979978441	0.7017057698290887	T	T	T
0.2293980440367269	0.6366297961570148	0.7465451881631977	T	T	T
0.3195651684370824	0.5513760557388850	0.8182301164690368	T	T	T
0.0873497744669887	0.5519837957620305	0.8256837120199297	T	T	T
0.4328822768943926	0.3732170703794017	0.5874578836600652	T	T	T
0.4167984902643195	0.5029969224601433	0.5582706919531919	T	T	T
0.4119525306925739	0.6364139238042544	0.5580812221126897	T	T	T
0.1930961184042503	0.3714568119601261	0.6125455369467507	T	T	T
0.1877987584391748	0.4982146851898854	0.5530279686435128	T	T	T
0.1886465160101184	0.6327247151987456	0.5564449916392240	T	T	T
-0.0013982082554725	0.4531553598058161	0.8017593177934638	T	T	T
0.9861605766133731	0.6351538887827780	0.7924928678055306	T	T	T
0.1425666157395253	0.5605257314708570	0.2174470112616979	T	T	T
0.2069044304759278	0.5683437906791141	0.3880580529313398	T	T	T
0.3012620346633068	0.5646253393358933	0.5307591012527545	T	T	T
0.3960808742830802	0.5701520922104419	0.3907959714744897	T	T	T
0.4030643813409803	0.5563090981056860	0.1967066880612069	T	T	T
0.2731553168735213	0.5335542478945634	0.2255212785190685	T	T	T
0.1389314387912018	0.3303806734922710	0.2471283792969890	T	T	T
0.1973931235185233	0.3417481899328372	0.4194368422699254	T	T	T
0.3097391886573490	0.3539522454130770	0.5229202499101756	T	T	T
0.4105344444065875	0.3294171247466805	0.4009522612281867	T	T	T
0.3958378459433538	0.3371165353117442	0.2046164754703471	T	T	T
0.2699540073213260	0.3543385028262100	0.2537432995137802	T	T	T
0.1838554581904798	0.4494263125993737	0.3046818144001940	T	T	T
0.4083767292947856	0.4485630047306678	0.3135528933064975	T	T	T
0.0703141500510840	0.6227046747692560	0.0781200085831244	T	T	T
0.0874434453981757	0.4910379889174341	0.0642808619325684	T	T	T
0.1131368080156585	0.3603118139769829	0.0571590813868342	T	T	T
0.3147381220946989	0.6257844080570560	0.0947986740620454	T	T	T
0.3321624550333084	0.4949833836514438	0.0576163495191782	T	T	T
0.3071185515179803	0.3625325633024739	0.0615080270038230	T	T	T
0.5117953977175038	0.5317824487028650	0.3056745295175233	T	T	T
0.5119253029701573	0.3664585496661804	0.2862313111698323	T	T	T
0.4416172371894832	0.7501746232970942	0.6444283410167529	T	T	T
0.1936253153035311	0.7484970814210795	0.6503426462176426	T	T	T
0.2740235037396607	0.7490586234620810	0.0591955848549112	T	T	T
0.1097755619307768	0.7484681920655749	0.0567649728677244	T	T	T
0.0642502634121667	0.2496313188327715	0.1353594730313394	T	T	T
0.3050972018614039	0.2457258683857590	0.1509617635327591	T	T	T
0.2277109517765138	0.2507142053255775	0.5578519482129334	T	T	T
0.3913903990936953	0.2496380148505219	0.5551275179332966	T	T	T
0.5598458143985547	0.2514052208411421	0.3577683794660837	T	T	T
0.8033880712920902	0.2469543930564599	0.3424224864834924	T	T	T
0.7282709926001354	0.2509234061296516	0.9477264736738736	T	T	T
0.8927698651348343	0.2499668696630114	0.9464906912222113	T	T	T
0.9398997848488171	0.7502622907762423	0.8664737814380113	T	T	T
0.6902718855643009	0.7587089432519948	0.8589687673889783	T	T	T
0.7739833335284501	0.7520438067778193	0.4592339343999455	T	T	T

Structure files (CONTCAR) involved in this work:

0.6087089108777536	0.7485717697404314	0.4530507175416873	T	T	T
0.8979104097077634	0.3641828656165896	0.6689280534371547	T	T	T
0.9898185871909232	0.4452671921304635	0.5114912211104929	T	T	T
0.8759978106164104	0.3731312342770146	0.4607388901153291	T	T	T
0.0455326955844913	0.4622007671852408	0.4035015847361970	T	T	T
0.0282372726623665	0.5850856819426277	0.4268035846418410	T	T	T
0.9710780276067859	0.5679348480104462	0.5336698535781118	T	T	T
0.9329397644553119	0.5399012981155518	0.3579469402869651	T	T	T
0.0127144275083091	0.4822509702624301	0.4615762971263430	T	T	T
0.0028488583428787	0.5482361762341980	0.4740525947941050	T	T	T

Figure 5(a) TS-CH₄ as same as Figure 1(b) Zn/ZSM-5**Figure 5(a) TS-CH₃OH same as Figure2(a) Zn-TS****Figure 5(a) TS1**

Si Al O Zn H C

1.0000000000000000

20.0219999999999985 0.0000000000000000 0.0000000000000000

0.0000000000000000 19.8990000000000009 0.0000000000000000

0.0000000000000000 0.0000000000000000 13.3829999999999991

93 3 193 2 6 2

Selective dynamics

Direct

0.4225003085793865	0.0600992539153168	0.6482480892415603	T	T	T
0.3052234000808174	0.0318617301749768	0.7923177212648842	T	T	T
0.2823962487775691	0.0559898295783903	0.0169692775398607	T	T	T
0.1233194367681815	0.0617434370857240	0.0116264443982596	T	T	T
0.0680697809753092	0.0314230718087522	0.8004854049413136	T	T	T
0.1805132415858145	0.0646656784412318	0.6648750647205428	T	T	T
0.4184979538818891	0.8271562054321522	0.6681597510384893	T	T	T
0.3010515985221630	0.8728197526340694	0.8007323388259501	T	T	T
0.2668740936231799	0.8302173361434048	0.0199554450760280	T	T	T
0.1111903460194948	0.8266357628049246	0.0120380129700209	T	T	T
0.0661857303552324	0.8748260700443700	0.7977828043990636	T	T	T
0.1793729199949756	0.8288177071608418	0.6644588067926064	T	T	T
0.0757946447720131	0.9404128223574572	0.1486150606819648	T	T	T
0.1948623581285154	0.9696033633962229	0.2900382526604084	T	T	T
0.2166034664276687	0.9436295981577667	0.5158739889572226	T	T	T
0.3768729332266922	0.9356465672407813	0.5134440264758253	T	T	T
0.4335364261687226	0.9682264935600542	0.3012598688456335	T	T	T
0.3204187737885001	0.9351962855556211	0.1641670740135122	T	T	T
0.0825080472933802	0.1715414639132183	0.1662344636581930	T	T	T
0.1979499245803660	0.1281727331031023	0.3018590886904763	T	T	T
0.2318408857830310	0.1689960132587705	0.5188156607121259	T	T	T
0.3873222655502395	0.1736040083761564	0.5083305380559621	T	T	T
0.4351201185514113	0.1267083665183049	0.2947769961541933	T	T	T
0.3182760662639728	0.1721086828134661	0.1666285278922516	T	T	T
0.5781073730113745	0.5552999097980570	0.3564053993752709	T	T	T
0.6905720869602942	0.5270269747312829	0.2031483908363591	T	T	T
0.7158617826345808	0.5684974375963702	0.9866198319934922	T	T	T
0.8746680025873748	0.5739118146894706	0.9859530003628777	T	T	T
0.8112151746104955	0.5496334516295005	0.3469031289349229	T	T	T
0.5728644028017306	0.3288163250483832	0.3324357174294441	T	T	T
0.6928294922058479	0.3730883966733608	0.1927118865816631	T	T	T
0.7308241145651904	0.3277268361279480	0.9799314107244086	T	T	T

Structure files (CONTCAR) involved in this work:

0.8856778213509027	0.3252689825080975	0.9929550559428425	T	T	T
0.9433295118576704	0.3728750434698566	0.1892217471295737	T	T	T
0.9196997683932384	0.4456491196231830	0.8619767289459944	T	T	T
0.8007537872602200	0.4735606113995415	0.7207021560673306	T	T	T
0.7780500425013721	0.4365985731038134	0.4973788195015674	T	T	T
0.6203728261096373	0.4278868339664612	0.4908604950846288	T	T	T
0.5690917425543894	0.4690589193301102	0.7028016224556308	T	T	T
0.6765500975844218	0.4479594544350702	0.8561943108392135	T	T	T
0.9205401471204022	0.6791327838386702	0.8292187810643132	T	T	T
0.7700657689814595	0.6687384465881329	0.4659341750141146	T	T	T
0.6147344375750368	0.6728775227382974	0.4886737236949408	T	T	T
0.5607814941143185	0.6274837004528229	0.6985661915475343	T	T	T
0.6721463897602614	0.6739080975678625	0.8281183306558946	T	T	T
0.5782178821647062	0.9450563440673926	0.3582586351370979	T	T	T
0.6986498021130870	0.9740017353286569	0.2148124234489774	T	T	T
0.7195326283373248	0.9379077360767359	0.9928514533966700	T	T	T
0.8795722737866162	0.9342728603218213	0.9948298500444014	T	T	T
0.9311315475014766	0.9708959941824531	0.2048930697149773	T	T	T
0.8224925447255167	0.9463834703001834	0.3549437255936396	T	T	T
0.5777383386045278	0.1736952488028259	0.3292473121498065	T	T	T
0.6979713846580062	0.1323496307193979	0.1934975097764536	T	T	T
0.7319752227124019	0.1715823347427640	0.9720640972117168	T	T	T
0.8866457086982349	0.1733239500978696	0.9824503570266001	T	T	T
0.9355697084439583	0.1289962138181423	0.1966922671582536	T	T	T
0.8203813881398123	0.1742295038558651	0.3305275168618994	T	T	T
0.9231016184124504	0.0541566943979294	0.8554965325047843	T	T	T
0.8017667950945488	0.0263251574708775	0.7089984316792373	T	T	T
0.7810998827147746	0.0662332882037809	0.4913203539847232	T	T	T
0.6207620471392987	0.0698336970643759	0.4899065894707618	T	T	T
0.5679061917084867	0.0321445551462358	0.6988471611611682	T	T	T
0.6784294201899987	0.0538990917843219	0.8491733176414011	T	T	T
0.9237641645255258	0.8313947616503616	0.8368263408465403	T	T	T
0.8026327617289364	0.8689920387241294	0.6953786411009080	T	T	T
0.7703285667544847	0.8262473978195557	0.4782187233032194	T	T	T
0.6153085519411625	0.8264775712644835	0.4900262932168726	T	T	T
0.5636549163382102	0.8748750615334737	0.6975870682866622	T	T	T
0.6782692438597080	0.8328733799767497	0.8329047294766776	T	T	T
0.4228412945942480	0.4416203176261957	0.6465281882820406	T	T	T
0.3040946387283668	0.4691459666906730	0.7889110496378331	T	T	T
0.2790838450295285	0.4453481630919409	0.0160007755644995	T	T	T
0.1208630004146055	0.4379750872456933	0.0163989188087949	T	T	T
0.0634142052272172	0.4691138482835439	0.8017677788692932	T	T	T
0.1765226972679108	0.4356218859728145	0.6628388997055250	T	T	T
0.4152146693697955	0.6733271227076597	0.6662363075244252	T	T	T
0.3004902103233393	0.6277113228767986	0.8007802246201057	T	T	T
0.2665731560618761	0.6687870308760405	0.0194078266982961	T	T	T
0.1112920318649209	0.6726348128152940	0.0077737282750128	T	T	T
0.0621817385022820	0.6280767948556141	0.7930966965706855	T	T	T
0.1793601294768343	0.6716995517453777	0.6642609583959048	T	T	T
0.0775837203190435	0.5599221836646059	0.1494713167896971	T	T	T
0.1959247320032131	0.5287496954554045	0.2900535946597456	T	T	T
0.2140647002429592	0.5555763207527626	0.5164318669036841	T	T	T
0.3730357589733518	0.5648728111456068	0.5149214516901575	T	T	T

Structure files (CONTCAR) involved in this work:

0.4297001969227658	0.5310389779563993	0.3045837316751754	T	T	T
0.3210492570168634	0.5634209652514475	0.1628404287767759	T	T	T
0.0866289449777005	0.3236605866710620	0.1622399703733751	T	T	T
0.1988517989898576	0.3706530447125555	0.3005247323087547	T	T	T
0.2300922578592510	0.3303696417479842	0.5189305115869418	T	T	T
0.3850541196281351	0.3277693090335491	0.5066376336033337	T	T	T
0.4305452703999331	0.3740051542821559	0.2931894591329027	T	T	T
0.3170874825683740	0.3295765524143391	0.1634160424843382	T	T	T
0.9223830164699600	0.5278927804610137	0.1935605075674268	T	T	T
0.8212545199821506	0.3359932119487802	0.3263233015137013	T	T	T
0.7984000468423413	0.6364709353515043	0.6964335139443324	T	T	T
0.0102214696645661	0.5577003489321420	0.2274587101809490	T	T	T
0.3587535955378632	0.0704705911831570	0.7217541226707661	T	T	T
0.3169198136508887	0.0546188482291726	0.9072372555471647	T	T	T
0.2024684223999783	0.0454857534726561	0.0062887553145413	T	T	T
0.0926136667592954	0.0701265363643773	0.9006280796984774	T	T	T
0.1037333129616573	0.0649857438444568	0.7035643810972123	T	T	T
0.2295038288253726	0.0516577434634072	0.7600607639754956	T	T	T
0.3598931503746173	0.8278479015795323	0.7519352900152017	T	T	T
0.3009300633348477	0.8605691769780065	0.9200091085996446	T	T	T
0.1883968613862242	0.8512533983764961	0.0225922665316682	T	T	T
0.0879275896101154	0.8328480258152667	0.8967206282961997	T	T	T
0.1026523114340563	0.8411637578775332	0.7009689826285991	T	T	T
0.2288450549704376	0.8509263490984742	0.7554573988817432	T	T	T
0.3159940441345553	0.9514063611152047	0.7771811711332235	T	T	T
0.0897256453178833	0.9526190726736317	0.8090624764899974	T	T	T
0.4328400648254326	0.1275975572258370	0.5815123826217833	T	T	T
0.4121515377079289	0.9964756126671506	0.5740568005368983	T	T	T
0.3926348408643272	0.8644767880067051	0.5675098782635535	T	T	T
0.1967713738568642	0.1378950907835399	0.6174422590813214	T	T	T
0.1895147252796173	0.0057041010279052	0.5825182784760012	T	T	T
0.1946834667016559	0.8721249636723341	0.5643965054060863	T	T	T
0.9880463922583771	0.0393056166620961	0.7862392439534542	T	T	T
0.9856188657748897	0.8717584060732229	0.7842176193862240	T	T	T
0.1401640418573833	0.9312895658740075	0.2212148978740471	T	T	T
0.1833200229205374	0.9488062627953180	0.4056809792401385	T	T	T
0.2971228678096369	0.9486140663943375	0.5084667560165139	T	T	T
0.4073218584244950	0.9314550541261707	0.4019401011664493	T	T	T
0.3966239958727780	0.9350831209102859	0.2050375238182506	T	T	T
0.2700307211762789	0.9478955968255656	0.2578654957063435	T	T	T
0.1391120587214601	0.1729880507163365	0.2529623958815107	T	T	T
0.1948505036575602	0.1375330410287449	0.4217355357050792	T	T	T
0.3102112638032970	0.1479511253129337	0.5152265642104034	T	T	T
0.4132954191612483	0.1680846027646254	0.3941510680454833	T	T	T
0.3954989810315360	0.1581197961640448	0.1990206463591286	T	T	T
0.2706672489214894	0.1527554660253397	0.2614356902605797	T	T	T
0.1854631531899614	0.0499712493093854	0.2725659999533950	T	T	T
0.4156078843984859	0.0479451975066793	0.3078622948978314	T	T	T
0.0646840623147484	0.8713373933088914	0.0856106822781129	T	T	T
0.0855608418280922	0.0010204117351131	0.0690110539620552	T	T	T
0.1106176735685208	0.1317505219476114	0.0695768283940602	T	T	T
0.3049696608971846	0.8620139851164553	0.1156158022527555	T	T	T
0.3124579358009576	0.9944444165415062	0.0819524263627812	T	T	T

Structure files (CONTCAR) involved in this work:

0.2987069054648780	0.1277653177968524	0.0692081372240948	T	T	T
0.5131185561594556	0.9560662415131019	0.2877440201768932	T	T	T
0.5151866897915731	0.1339458287138127	0.2776897795056465	T	T	T
0.6364643712186530	0.5640676137605792	0.2741821451589002	T	T	T
0.7013620663446668	0.5739917430998831	0.1056703384743848	T	T	T
0.7952927660036633	0.5617718089439721	0.9630457999022641	T	T	T
0.8902011169137192	0.5794146473208099	0.1033726477186983	T	T	T
0.8858104588935930	0.5323231282939996	0.3110263400384004	T	T	T
0.7603989907170656	0.5218666258591156	0.2639873007937707	T	T	T
0.6382297030790178	0.3355916315316200	0.2633392871053125	T	T	T
0.6905672386786111	0.3358831873510296	0.0841486096055467	T	T	T
0.8084203265070958	0.3508157668353012	0.9948097922342714	T	T	T
0.9145375687106413	0.3202367538941583	0.1064662378170198	T	T	T
0.9052294701081546	0.3593186671383143	0.2957536820232585	T	T	T
0.7655477186533587	0.3695553222816169	0.2422398778418778	T	T	T
0.6680130591704367	0.4509899366921505	0.1758253281326432	T	T	T
0.9334483690400165	0.4481665959117625	0.1506432825077669	T	T	T
0.5694697962191185	0.6256654492282339	0.4165034273744441	T	T	T
0.5952567293809443	0.4963437925708811	0.4366030953463135	T	T	T
0.5843804737588610	0.3628786557183743	0.4419818749941974	T	T	T
0.8010315495733394	0.6296966651155349	0.3691562390820269	T	T	T
0.7953459102484943	0.5137843969471393	0.4573393725443499	T	T	T
0.8276399638783628	0.3851545076097462	0.4392976902984284	T	T	T
0.0223785041613935	0.3598729204500559	0.2112734327819657	T	T	T
0.8538744981043197	0.4355843733221743	0.7920237801306799	T	T	T
0.7955121809922377	0.4332612933230340	0.6151420813115053	T	T	T
0.7007475410123537	0.4198061237837456	0.4745462138196620	T	T	T
0.6031835646971269	0.4298354587879210	0.6089154972758620	T	T	T
0.6026036626727070	0.4440642538389851	0.8067585242662569	T	T	T
0.7275334747477409	0.4755359483253354	0.7705543006201193	T	T	T
0.8592249324928226	0.6826981720209331	0.7534272590956158	T	T	T
0.8144825479546481	0.6452216681274981	0.5638424737966324	T	T	T
0.6924945533265620	0.6475192474450673	0.4852631457846644	T	T	T
0.5865131448442503	0.6689833368767757	0.6015203274543509	T	T	T
0.5937872211221036	0.6602178617729427	0.7982181601427742	T	T	T
0.7186072451325365	0.6484897083167533	0.7372843077288164	T	T	T
0.8257415192308575	0.5502826850446028	0.6963925245743707	T	T	T
0.5812082604220847	0.5489465755242620	0.6863201636556057	T	T	T
0.9300285633465889	0.3775018556877888	0.9272303635578172	T	T	T
0.9141282398550558	0.5108315729867055	0.9337971854747089	T	T	T
0.9005185140793263	0.6428588557516862	0.9338070506661968	T	T	T
0.6973527310589674	0.3734779800050756	0.8930010278486311	T	T	T
0.6773285816668646	0.5010421503503918	0.9480478007808452	T	T	T
0.6870119724871423	0.6351868327528486	0.9329694694803058	T	T	T
0.4901357320833050	0.4515075423217637	0.7117031104029417	T	T	T
0.4798669873812973	0.6325333795209596	0.7069320396367470	T	T	T
0.6438224148644199	0.9400981083207587	0.2880956553587223	T	T	T
0.6988258087258371	0.9333889622578829	0.1097218757546329	T	T	T
0.7999549131240687	0.9453066548869630	0.9797601732080513	T	T	T
0.8984692310776815	0.9292432402226531	0.1123844109395619	T	T	T
0.8977731036246981	0.9480728760875224	0.3100083057533036	T	T	T
0.7719065369202706	0.9675576278983792	0.2654881766421455	T	T	T
0.6405601436350197	0.1733151111585637	0.2533301820958122	T	T	T

Structure files (CONTCAR) involved in this work:

0.6961587360087216	0.1577528862455117	0.0786347402259065	T	T	T
0.8095903411784414	0.1471203444950638	0.9783769055064638	T	T	T
0.9136473961922774	0.1687387012957302	0.0961874723598673	T	T	T
0.8970415732449943	0.1589368943157885	0.2934492377395752	T	T	T
0.7708341453811075	0.1459091511146741	0.2422951928433809	T	T	T
0.6804755152533868	0.0525492342707787	0.1974493699085534	T	T	T
0.9181043861244907	0.0499355625734501	0.1831689899046128	T	T	T
0.5702018696713590	0.8749281817830689	0.4196753689621453	T	T	T
0.5826436233816399	0.0066943820387812	0.4378097611370063	T	T	T
0.5983137658039897	0.1390106028303552	0.4349769027537814	T	T	T
0.8084118397270523	0.8705794799430748	0.3944663051177144	T	T	T
0.8161634135451724	0.9985840162822339	0.4474662813610002	T	T	T
0.8067964320362967	0.1325993463002852	0.4336664737211062	T	T	T
0.0103401489612420	0.9548005343531637	0.2160641659106352	T	T	T
0.0157810688953928	0.1373976415069010	0.2125444561854818	T	T	T
0.8575039131042123	0.0552454078552299	0.7851219415617978	T	T	T
0.8013945872024046	0.0722509164795907	0.6086682154314006	T	T	T
0.7005818283146483	0.0583514045646510	0.4789395106392458	T	T	T
0.5992373254409422	0.0754246371958519	0.6066906765990476	T	T	T
0.6033027252983760	0.0518557626099195	0.8038231116651354	T	T	T
0.7288514450465299	0.0294125341929337	0.7614082949478195	T	T	T
0.8597957607684964	0.8352723330809835	0.7636800367824934	T	T	T
0.8054828667325946	0.8326837882471383	0.5869157282098810	T	T	T
0.6929573803555289	0.8510031025139826	0.4857262612256708	T	T	T
0.5888715272492310	0.8290049010290079	0.6044932975468832	T	T	T
0.6026102765584391	0.8526818135882549	0.7987401562761534	T	T	T
0.7295341592211303	0.8578601965468485	0.7455862162760875	T	T	T
0.8176780045117951	0.9485802101950724	0.6809283548823409	T	T	T
0.5787738212882160	0.9531380949138353	0.6722259758954124	T	T	T
0.9319175410490155	0.1271178574584042	0.9087201581609867	T	T	T
0.9181331210320359	0.9971158146529641	0.9425091557636068	T	T	T
0.9041981122627457	0.8645402887287541	0.9439255741323299	T	T	T
0.6945653402911059	0.1301292526115164	0.8840778861596822	T	T	T
0.6836925764142880	0.0037543827345614	0.9447355764766923	T	T	T
0.6949725825179831	0.8696179470600246	0.9382149218017287	T	T	T
0.4890591976356546	0.0482251097244603	0.7145315558675390	T	T	T
0.4839956728195452	0.8639015272265124	0.7144937671788358	T	T	T
0.3597250356964506	0.4307667404998827	0.7216254526034719	T	T	T
0.3105804203005333	0.4456051319184548	0.9044268591251954	T	T	T
0.1989305980885720	0.4605626752218406	0.0138580647430041	T	T	T
0.0901092759753214	0.4363855290289860	0.9054075264895544	T	T	T
0.1014081417271538	0.4338638597270839	0.7081461523126008	T	T	T
0.2290089334196203	0.4504809959722559	0.7526361997154091	T	T	T
0.3584427097908711	0.6742494250489909	0.7529934640898185	T	T	T
0.3015017375504334	0.6379444683925216	0.9204998444528680	T	T	T
0.1880967991478831	0.6470886205100820	0.0183768423190468	T	T	T
0.0865043585828303	0.6671202873782172	0.8935250605195970	T	T	T
0.1021796987018181	0.6591348250514836	0.6976195085163542	T	T	T
0.2276990152326404	0.6490082518465188	0.7565106249872038	T	T	T
0.3160689068091008	0.5494903807265751	0.7751191948317022	T	T	T
0.0804508540867254	0.5489206894034725	0.8036025813917296	T	T	T
0.4316054161646112	0.3758376504190858	0.5755164747634930	T	T	T
0.4131300673525312	0.5070928203816546	0.5754948453179689	T	T	T

Structure files (CONTCAR) involved in this work:

0.3841079266836434	0.6375879505407968	0.5671329436293149	T	T	T
0.1920008407692296	0.3623832050546480	0.6146528610155408	T	T	T
0.1805426383115353	0.4946495829622310	0.5790595302743906	T	T	T
0.1955379171711129	0.6280893112402953	0.5643510839107134	T	T	T
0.9841725244721929	0.4551934415254772	0.7888689413241028	T	T	T
0.9827526128590870	0.6380208499476361	0.7764331772207146	T	T	T
0.1425292755804483	0.5691299663915664	0.2197839136550958	T	T	T
0.1831614378890437	0.5531652448998826	0.4038401646763787	T	T	T
0.2942497410652303	0.5452748486578720	0.5131246367905288	T	T	T
0.4014472178517476	0.5700787043343239	0.4021736995803483	T	T	T
0.3969013168165832	0.5648868640341067	0.2052122221559407	T	T	T
0.2711824857889528	0.5473929945933490	0.2565570577319551	T	T	T
0.1451221202699993	0.3226303739400690	0.2461119579186670	T	T	T
0.1940646999530073	0.3602648782469449	0.4198184192517246	T	T	T
0.3080143886035600	0.3531904610699915	0.5186081263911159	T	T	T
0.4070305510893265	0.3307213739449801	0.3901068580738803	T	T	T
0.3944194181765203	0.3454950708480710	0.1924966775865586	T	T	T
0.2730411004804372	0.3512789375519387	0.2611482239121565	T	T	T
0.1816310629772907	0.4490191554073212	0.2749859584077403	T	T	T
0.4092122690305184	0.4520022931366357	0.3111498776901842	T	T	T
0.0656108598457650	0.6251169704992687	0.0802240033430859	T	T	T
0.0787226506872149	0.4918286672011313	0.0850439493946001	T	T	T
0.1130211536811632	0.3636709745495889	0.0637414660379608	T	T	T
0.3027534576745153	0.6365374922536718	0.1166553307690085	T	T	T
0.3146462820905951	0.5049013137538060	0.0791504312757399	T	T	T
0.2934792171165823	0.3724452374600587	0.0662086620382354	T	T	T
0.5098054845430592	0.5383197975128623	0.2970150322180880	T	T	T
0.5104942726918663	0.3665568538261562	0.2774921596473919	T	T	T
0.4356323469839726	0.7499122376092306	0.6388634629917727	T	T	T
0.1908028286620616	0.7501664573342902	0.6368099518406948	T	T	T
0.2746011068276159	0.7493512651330263	0.0229616252761962	T	T	T
0.1039341658190646	0.7489276458593955	0.0473385391743526	T	T	T
0.0680063441243593	0.2478208172445761	0.1295098692439466	T	T	T
0.3077166455522016	0.2506379679986446	0.1373071724934615	T	T	T
0.2232917015000827	0.2497094682176348	0.5218348659098565	T	T	T
0.3925123410607846	0.2510168757447972	0.5454650039698564	T	T	T
0.5551748976347465	0.2504328559527926	0.3515657582423457	T	T	T
0.8099386215460441	0.2524563298213219	0.3509422802296769	T	T	T
0.7271199208201464	0.2503401512867550	0.9426272152416643	T	T	T
0.8911828478232372	0.2506926140240272	0.9439383912974075	T	T	T
0.9467041070737795	0.7545620389620551	0.8565726143833953	T	T	T
0.6839177758869938	0.7531211897984926	0.8506686807256564	T	T	T
0.7756667659415682	0.7482367562583903	0.4438273471311224	T	T	T
0.6094689230657816	0.7498309178958730	0.4492898347890085	T	T	T
0.9356290212875614	0.5033028871561115	0.5103766188448233	T	T	T
0.9277333553020213	0.4163642773504437	0.4222211777514082	T	T	T
0.8760528422318926	0.5623023612484229	0.5638063329493627	T	T	T
0.9900299505045339	0.4716706522102708	0.5083183701097128	T	T	T
0.0614133502916240	0.4419539440204030	0.4080838380173202	T	T	T
0.0489651971991859	0.3835141356614213	0.5096675959641767	T	T	T
-0.0031038933883626	0.5725369962818779	0.3811246369727465	T	T	T
0.9774241336627753	0.6442918246694955	0.3037411551603378	T	T	T
0.0632682439788116	0.6214914083272302	0.3256883488445550	T	T	T

Structure files (CONTCAR) involved in this work:

0.0257906493507005 0.4225902884910110 0.4634815352393614 T T T
0.0122833326119669 0.6026711437531874 0.3165072797333707 T T T

Figure 5(a) TS2

Si Al O Zn H C

1.0000000000000000

20.0219999999999985 0.0000000000000000 0.0000000000000000

0.0000000000000000 19.8990000000000009 0.0000000000000000

0.0000000000000000 0.0000000000000000 13.3829999999999991

93 3 193 2 6 2

Selective dynamics

Direct

0.4232624577637601 0.0612423545797371 0.6470390086939215 T T T

0.3053677306395476 0.0320172323904512 0.7897810078803401 T T T

0.2833816660765149 0.0552305805138127 0.0153179824918334 T T T

0.1243149176965803 0.0620737676083339 0.0111924219254794 T T T

0.0684146553371393 0.0316194202613569 0.8003643535437838 T T T

0.1802919333569585 0.0659336304274008 0.6640156088028099 T T T

0.4178868320322678 0.8281484285172988 0.6662987531111892 T T T

0.3003685473097897 0.8733215211097856 0.7979567895839997 T T T

0.2671886454918623 0.8309612374894593 0.0174457696972213 T T T

0.1112290754722212 0.8263262311484847 0.0112733154312302 T T T

0.0666081179760916 0.8749941294536838 0.7968386480149473 T T T

0.1788663387577776 0.8288714112231355 0.6616519953495988 T T T

0.0761543188785243 0.9406608808054230 0.1478302598679732 T T T

0.1954294768230365 0.9698454396191378 0.2886160463900917 T T T

0.2166484415025970 0.9449063088474411 0.5150391909264491 T T T

0.3767645914002322 0.9373997641664601 0.5122581399589450 T T T

0.4338661726797366 0.9691849453852510 0.2999631502495325 T T T

0.3209697730077672 0.9346408922718710 0.1634452157365570 T T T

0.0830056105190606 0.1720027242757798 0.1648574050456108 T T T

0.1989326352386614 0.1283410657922492 0.2987834095621793 T T T

0.2315599291935477 0.1698331708084067 0.5165042932135190 T T T

0.3877024878746696 0.1748939414350912 0.5074837533360506 T T T

0.4351989876715072 0.1278352036406231 0.2931611121066049 T T T

0.3191472102537409 0.1726198758943357 0.1625896783762767 T T T

0.5766331839434615 0.5557934839601452 0.3537030480324269 T T T

0.6905270877601758 0.5278397087322878 0.2014090080639011 T T T

0.7133852080001848 0.5695576245205333 0.9847013213514466 T T T

0.8718219174388073 0.5741515218648381 0.9878781230636230 T T T

0.8107319430497476 0.5507071392388868 0.3479931115496900 T T T

0.5723922534220054 0.3303852171544561 0.3332749952620143 T T T

0.6946220317498066 0.3733073695667222 0.1955143093485553 T T T

0.7297015830976282 0.3272205719754903 0.9816014183759922 T T T

0.8844819640185474 0.3254826723304556 0.9899012980423393 T T T

0.9412596633988050 0.3733962578206892 0.1853275992558461 T T T

0.9179238712676526 0.4467261898145334 0.8612643712912508 T T T

0.7966315158151518 0.4734074110463238 0.7223439643760432 T T T

0.7772624546395184 0.4375293496144085 0.4970213893357810 T T T

0.6197567994825658 0.4299072839866565 0.4906764595418398 T T T

0.5674386785375531 0.4703704054467457 0.7034691657530893 T T T

0.6724619568309601 0.4467468535625888 0.8589102007694298 T T T

0.9197545805450772 0.6787311824944017 0.8322699632783102 T T T

0.7691089305458518 0.6704803166631652 0.4651511330346763 T T T

Structure files (CONTCAR) involved in this work:

0.6135434877790451	0.6732757042063729	0.4846756804328072	T	T	T
0.5587484382477214	0.6291468881675537	0.6967658644946804	T	T	T
0.6679246245298471	0.6762421486119295	0.8286162308093165	T	T	T
0.5785042678321088	0.9461817841403779	0.3586555843574630	T	T	T
0.6995698563869502	0.9748544886529995	0.2172526984990707	T	T	T
0.7197162736090993	0.9386292984661961	0.9943153773619433	T	T	T
0.8798425285311142	0.9343496086522899	0.9956060585876609	T	T	T
0.9313659076515804	0.9715338646319778	0.2053858794329461	T	T	T
0.8237788571582714	0.9474673856528819	0.3572240661057099	T	T	T
0.5777845031661110	0.1751275590914911	0.3298763974295525	T	T	T
0.6989467095240532	0.1335813726415893	0.1961027557457242	T	T	T
0.7317823374786964	0.1712925886961807	0.9729111929701418	T	T	T
0.8863267176788652	0.1734578960405449	0.9813253992842991	T	T	T
0.9357035306438922	0.1297645430913420	0.1959556764949801	T	T	T
0.8220975541555889	0.1765245572124540	0.3325045400564508	T	T	T
0.9233786553307375	0.0540637181542519	0.8559307529710501	T	T	T
0.8017539545159884	0.0266550629202569	0.7092972942351261	T	T	T
0.7822998184880311	0.0681666099872883	0.4919402608564575	T	T	T
0.6218407308301186	0.0712366788918003	0.4897676144383053	T	T	T
0.5687221267505294	0.0323547740060961	0.6981945256094122	T	T	T
0.6784086265077113	0.0541380557874581	0.8499709793945062	T	T	T
0.9240844600267387	0.8316254604697132	0.8375340962290475	T	T	T
0.8018508282611385	0.8694751173613562	0.6974398331212524	T	T	T
0.7699468695009661	0.8273155385086750	0.4796592123102428	T	T	T
0.6148680397581797	0.8272321738046408	0.4896287488509975	T	T	T
0.5635130482474952	0.8751953149800323	0.6968564186112679	T	T	T
0.6769421245969144	0.8341852364489343	0.8354778798219709	T	T	T
0.4219665495120341	0.4435036871398211	0.6407250981828437	T	T	T
0.3026236115730088	0.4698047531369881	0.7823743609350435	T	T	T
0.2795991946528520	0.4451774389512443	0.0087678847114001	T	T	T
0.1213586472434161	0.4375798149028135	0.0115013914271522	T	T	T
0.0620294627940440	0.4696577319931597	0.7994204480872267	T	T	T
0.1741761871088300	0.4362929839269870	0.6581230211283534	T	T	T
0.4133402590703926	0.6745804875130902	0.6604853714593469	T	T	T
0.2984102052976588	0.6282770640657694	0.7948226293206180	T	T	T
0.2666658622387953	0.6697308070570550	0.0143627429610162	T	T	T
0.1107311899353070	0.6721865257590673	0.0061494998221247	T	T	T
0.0614351151523578	0.6285547404571821	0.7918242912748158	T	T	T
0.1767080450585187	0.6717292484272266	0.6595264988189303	T	T	T
0.0738714004323716	0.5589420152859184	0.1483377768907454	T	T	T
0.1954022425494042	0.5301444719711891	0.2834488852317951	T	T	T
0.2130202443461058	0.5558026873794915	0.5123933402438600	T	T	T
0.3717756348352719	0.5660906490547783	0.5102647911037210	T	T	T
0.4277957343125088	0.5305709135367643	0.3004471014634635	T	T	T
0.3209910729981049	0.5638145154256360	0.1559950912545542	T	T	T
0.0863151413637448	0.3245496508365936	0.1567957877472560	T	T	T
0.1987865948094282	0.3717657563687940	0.2949381399442110	T	T	T
0.2289935620399121	0.3310621566895203	0.5145528279699776	T	T	T
0.3845763275169538	0.3284276631577079	0.5033501994461294	T	T	T
0.4296745455510497	0.3736858481697009	0.2900128804049139	T	T	T
0.3174838539555607	0.3296549740578428	0.1574684931094463	T	T	T
0.9239223790276738	0.5285997132889806	0.1943400077966926	T	T	T
0.8246731126111133	0.3379408308793552	0.3288624354231041	T	T	T

Structure files (CONTCAR) involved in this work:

0.7948518105799995	0.6385216996924489	0.7005791748863308	T	T	T
0.0083965595779113	0.5537775199585865	0.2220000377869455	T	T	T
0.3597367143023121	0.0710102782136716	0.7211097936387755	T	T	T
0.3178391977555739	0.0517914168502533	0.9056770613826014	T	T	T
0.2033591220051613	0.0454770640111037	0.0048971912672263	T	T	T
0.0930591369200256	0.0701522799669243	0.9005029038005932	T	T	T
0.1037280799533181	0.0659114707380813	0.7036903302125710	T	T	T
0.2300955281128493	0.0543445358157590	0.7587493231302578	T	T	T
0.3600878938919853	0.8283545787379277	0.7513327719725326	T	T	T
0.2997553526139855	0.8636240355561862	0.9177795492948101	T	T	T
0.1884882439185973	0.8507446554361965	0.0228861328897772	T	T	T
0.0889287422846793	0.8331051461213488	0.8954448487628343	T	T	T
0.1024660275022787	0.8419141405208185	0.6990645601050564	T	T	T
0.2288198230699892	0.8491275793877188	0.7529887877949298	T	T	T
0.3141467191226231	0.9516377977144472	0.7705688216501247	T	T	T
0.0901767461947412	0.9528132058928933	0.8079628245703594	T	T	T
0.4332948339937135	0.1287958714425082	0.5804247578189242	T	T	T
0.4128424966264409	0.9978495314071514	0.5725337009613384	T	T	T
0.3917211740481991	0.8662291659315209	0.5665950275527784	T	T	T
0.1956197360341579	0.1387949847514108	0.6145514989335975	T	T	T
0.1891828362601993	0.0060537205260998	0.5831346120656744	T	T	T
0.1952037146890049	0.8728639411545519	0.5625224185649785	T	T	T
0.9882815950085360	0.0388523518685603	0.7868592211626548	T	T	T
0.9859627760141126	0.8713215907800268	0.7839717395543504	T	T	T
0.1402460508394172	0.9312786791689629	0.2209508801618310	T	T	T
0.1834061498275138	0.9509645366512409	0.4049100092113360	T	T	T
0.2971083322775304	0.9507981258979757	0.5073310525643178	T	T	T
0.4073609756394985	0.9329933262832396	0.4008984862888941	T	T	T
0.3972376429016846	0.9348784078843905	0.2043976196631197	T	T	T
0.2702979040861879	0.9464435684892404	0.2571765925066332	T	T	T
0.1391371880028570	0.1732069075983767	0.2524236077283176	T	T	T
0.1970951515536401	0.1363904374203993	0.4188869598292332	T	T	T
0.3103620297724420	0.1503954913181499	0.5164320604566440	T	T	T
0.4125625456759579	0.1683535581696749	0.3928788834810051	T	T	T
0.3961494605126721	0.1595057957832304	0.1970706268529803	T	T	T
0.2709102728874347	0.1539554762590588	0.2569575846278979	T	T	T
0.1871966652647270	0.0501419643880192	0.2684706163418455	T	T	T
0.4157997229672510	0.0489193999013757	0.3046977587161585	T	T	T
0.0649147097566509	0.8718789306709405	0.0841455210869571	T	T	T
0.0864314752648652	0.0017368335027785	0.0692207581197975	T	T	T
0.1122259380510600	0.1323430166938301	0.0687124870230929	T	T	T
0.3059755104906531	0.8618211215534357	0.1133318414463789	T	T	T
0.3128753976874349	0.9945040236896306	0.0823593538838821	T	T	T
0.3006819849279125	0.1274237765547646	0.0655453974931422	T	T	T
0.5136587897533071	0.9575778237120932	0.2877975304332987	T	T	T
0.5153393572086723	0.1357700235552760	0.2774113769029588	T	T	T
0.6345534734095833	0.5634543603449816	0.2705643831774971	T	T	T
0.7014428165072228	0.5750411988524123	0.1044146338353786	T	T	T
0.7926468827274110	0.5653306065676850	0.9580164474059197	T	T	T
0.8834704107273335	0.5775462621246591	0.1065325469117901	T	T	T
0.8859230327881430	0.5280248396187853	0.3169492195047432	T	T	T
0.7598869939963884	0.5254640467431483	0.2645457764977010	T	T	T
0.6384843960642494	0.3380418528850665	0.2660495934459290	T	T	T

Structure files (CONTCAR) involved in this work:

0.6929136346429647	0.3337451724085226	0.0888130661347730	T	T	T
0.8073128462604652	0.3517383034994634	0.9896327309500138	T	T	T
0.9123990597493824	0.3199482234041163	0.1035300956428578	T	T	T
0.9074098177827693	0.3591787210043269	0.2942811023798516	T	T	T
0.7666915839450242	0.3704841452666212	0.2465918160077397	T	T	T
0.6708037959154460	0.4511589491374880	0.1741999725037558	T	T	T
0.9266758455054863	0.4482235448391401	0.1486091331588821	T	T	T
0.5680112533450783	0.6271707765535024	0.4113360089121638	T	T	T
0.5952791914627598	0.4985107135046369	0.4359376487727648	T	T	T
0.5825982579713204	0.3652324219891890	0.4427850206874800	T	T	T
0.8049538499033394	0.6309897055442818	0.3718134235488508	T	T	T
0.7931624351998119	0.5166942493952887	0.4598282140332750	T	T	T
0.8306365778312704	0.3917119420760908	0.4373092068888608	T	T	T
0.0214163628009967	0.3623688446077277	0.2000658303893457	T	T	T
0.8525181626220439	0.4367698882410756	0.7901563573460055	T	T	T
0.7927128539018727	0.4343961008303699	0.6153999197026200	T	T	T
0.7001728897398245	0.4206636111022534	0.4727286394450062	T	T	T
0.6035806712817648	0.4332257829461005	0.6090892172225494	T	T	T
0.5988506150329335	0.4435426162158110	0.8080833012326916	T	T	T
0.7238994475002195	0.4720676869727063	0.7724637530125754	T	T	T
0.8573504531674923	0.6817192932744611	0.7580311065076495	T	T	T
0.8106443806577259	0.6477172131056373	0.5667481357661227	T	T	T
0.6914792822766358	0.6479023231298910	0.4782367299906656	T	T	T
0.5862839904681066	0.6673069631282655	0.5977282276948533	T	T	T
0.5897391373711883	0.6654781350154413	0.7953135441039799	T	T	T
0.7146665924377029	0.6515709061674099	0.7375926809504341	T	T	T
0.8185432173052427	0.5512674372240105	0.6993708401564793	T	T	T
0.5800751035170405	0.5505318257305025	0.6918740922235763	T	T	T
0.9291552385416578	0.3776716536860800	0.9239285167992235	T	T	T
0.9109224183449255	0.5108764858027116	0.9345653817769285	T	T	T
0.9011279015328216	0.6427014939372598	0.9377409037780031	T	T	T
0.6917077066217525	0.3725968683107984	0.8983809942876884	T	T	T
0.6750239088264437	0.5013276736430585	0.9486702229858448	T	T	T
0.6810007236895171	0.6348930825644820	0.9317458128378326	T	T	T
0.4883963771227256	0.4526749648554230	0.7081764385300853	T	T	T
0.4777426798526276	0.6335574073078075	0.7016513143161014	T	T	T
0.6441910551435069	0.9402255177766800	0.2888413531474889	T	T	T
0.7000953571989300	0.9350858306118087	0.1115395861927746	T	T	T
0.8001263397585464	0.9440039984471634	0.9789244750018566	T	T	T
0.8978131551952208	0.9298455852621781	0.1135180645918149	T	T	T
0.8987356749597502	0.9486624866286409	0.3111177239519746	T	T	T
0.7725870462103307	0.9674644665782407	0.2681125698102624	T	T	T
0.6408965090333391	0.1747405859528979	0.2544425839841978	T	T	T
0.6973738794026979	0.1573423863320360	0.0804494209761529	T	T	T
0.8094209943507737	0.1466714835388834	0.9768884269793290	T	T	T
0.9130754188158571	0.1689323254911693	0.0952180945623021	T	T	T
0.8980629586393544	0.1605874881583788	0.2928780519923275	T	T	T
0.7713560673797097	0.1486263174643969	0.2453096853048318	T	T	T
0.6819087456901992	0.0537004586172802	0.2020036973699816	T	T	T
0.9179459500816732	0.0505764109788210	0.1841032885311205	T	T	T
0.5695177472145820	0.8763232265276256	0.4206883260203028	T	T	T
0.5840108647740601	0.0078558578985902	0.4378658325736423	T	T	T
0.5977523186696730	0.1402239767987721	0.4357975760913962	T	T	T

Structure files (CONTCAR) involved in this work:

0.8100718189083830	0.8720828148504154	0.3988875746242214	T	T	T
0.8175630746122113	0.0004729104170156	0.4486228418659960	T	T	T
0.8093933729151493	0.1343651127879752	0.4354954387135438	T	T	T
0.0105770027722107	0.9552035510065605	0.2150353199771685	T	T	T
0.0160872738489447	0.1376339426532996	0.2101278005274488	T	T	T
0.8579471076046119	0.0545875209768250	0.7852904643898068	T	T	T
0.8013407449063783	0.0733684633030875	0.6098355321568001	T	T	T
0.7017983671324383	0.0612169231718331	0.4772965828920014	T	T	T
0.6014060553427050	0.0756924888755818	0.6071424333988853	T	T	T
0.6034517711604912	0.0508439938539359	0.8041858781910372	T	T	T
0.7291312992348944	0.0300282916001859	0.7624484397832558	T	T	T
0.8597363076626700	0.8363941526471663	0.7650485099529646	T	T	T
0.8029985829335408	0.8315039165030055	0.5900304247869892	T	T	T
0.6924947759204941	0.8518912835903916	0.4844173831058850	T	T	T
0.5895542144626744	0.8287263794081035	0.6047490481855903	T	T	T
0.6017032115855407	0.8535662998353245	0.7989095722257995	T	T	T
0.7293155506452319	0.8590399942353918	0.7496569023308789	T	T	T
0.8167085693495950	0.9488295346609171	0.6798909238464105	T	T	T
0.5787413880717656	0.9533225690057013	0.6707187440994835	T	T	T
0.9321101405079628	0.1273415748375758	0.9081271129869215	T	T	T
0.9179738041926667	0.9976677300315668	0.9438187548536194	T	T	T
0.9057446803523470	0.8649883274104413	0.9449648018355136	T	T	T
0.6932672761862206	0.1305365887759630	0.8852124798103477	T	T	T
0.6845322177375999	0.0047202461135370	0.9461453998714473	T	T	T
0.6925160581918056	0.8708381247883948	0.9411208631424784	T	T	T
0.4900517732563526	0.0494801251145669	0.7127852321472881	T	T	T
0.4838097074343042	0.8641661955960891	0.7124529648220379	T	T	T
0.3575719962160338	0.4321288894262834	0.7129986263941290	T	T	T
0.3113383522227777	0.4455280573427025	0.8971853603553914	T	T	T
0.1995493083308329	0.4591298764335109	0.0039861682775876	T	T	T
0.0882645271964559	0.4348656434527634	0.9013184401506922	T	T	T
0.0986558540709735	0.4352704708693181	0.7033073778274769	T	T	T
0.2270201324555772	0.4513561289428357	0.7474558283604008	T	T	T
0.3556867029330687	0.6751421167804740	0.7458226691284207	T	T	T
0.2999669744192903	0.6387197991009677	0.9142665543532931	T	T	T
0.1882424528592971	0.6484511097994756	0.0169120356376149	T	T	T
0.0876616579505441	0.6680985781708094	0.8903857538332849	T	T	T
0.0996132387585962	0.6587592116376990	0.6937500636556294	T	T	T
0.2252693184905776	0.6488205885963758	0.7512476411419171	T	T	T
0.3144395273734689	0.5501735120896234	0.7691208525227416	T	T	T
0.0797517269653112	0.5492454643738279	0.8021757680227443	T	T	T
0.4313929222010102	0.3782503589675735	0.5689695600403185	T	T	T
0.4140332021527785	0.5096281619484248	0.5704318051021904	T	T	T
0.3833563043320258	0.6394829578082775	0.5600774503037379	T	T	T
0.1897923889019102	0.3632162037043986	0.6094839030758359	T	T	T
0.1775067346309502	0.4951355903495993	0.5736875471804586	T	T	T
0.1926432143604900	0.6282235014546449	0.5592381045762855	T	T	T
0.9818964033554164	0.4577974226339934	0.7861972188901513	T	T	T
0.9815435052658491	0.6379017448011951	0.7777658052268671	T	T	T
0.1402043124393580	0.5701152417936970	0.2171970817118613	T	T	T
0.1846906432336412	0.5531492900614734	0.3986793148327859	T	T	T
0.2932140053960919	0.5454078172266249	0.5139097403224825	T	T	T
0.3974452514249533	0.5703513257627925	0.3960039586129202	T	T	T

Structure files (CONTCAR) involved in this work:

0.3967395725659397	0.5635075691269271	0.1992960258440530	T	T	T
0.2703620784360106	0.5495207466288405	0.2491726622221576	T	T	T
0.1428695468080897	0.3245807968168196	0.2439006741532380	T	T	T
0.1951084405289580	0.3622976396710066	0.4146772265090659	T	T	T
0.3072815797814455	0.3525531483823988	0.5172241814773425	T	T	T
0.4049262023035112	0.3302462497949998	0.3860794184719745	T	T	T
0.3946424869262170	0.3451523014351943	0.1885344116397834	T	T	T
0.2721734462723620	0.3508399930504253	0.2540805094136170	T	T	T
0.1828778833706630	0.4500512553657007	0.2681232062631415	T	T	T
0.4076582045889409	0.4515145740052730	0.3078395983289166	T	T	T
0.0647210512696567	0.6235407658043438	0.0752026002781351	T	T	T
0.0813851842223620	0.4916005952116659	0.0805753341494697	T	T	T
0.1153363394000975	0.3627024291079253	0.0583774339733387	T	T	T
0.3049702346982064	0.6373996199885544	0.1097386456322083	T	T	T
0.3138013971044668	0.5054585949898343	0.0721672308886536	T	T	T
0.2952809676649207	0.3727685596145797	0.0598171258337050	T	T	T
0.5080708979975287	0.5376006776888632	0.2962156128758838	T	T	T
0.5099316251778759	0.3669139688907743	0.2767103247337355	T	T	T
0.4344118831582999	0.7511754295430112	0.6346503585197113	T	T	T
0.1882995959498498	0.7502054666753754	0.6321289613492728	T	T	T
0.2760136548920262	0.7502291889891100	0.0168878383046704	T	T	T
0.1026879356993154	0.7486629132397075	0.0458281620649102	T	T	T
0.0680539733836258	0.2479848366626241	0.1274907159388083	T	T	T
0.3084513228240334	0.2507194761510446	0.1309709582108438	T	T	T
0.2209444411092404	0.2504192794895287	0.5166290939751647	T	T	T
0.3943348161169494	0.2523568322486156	0.5438944439551051	T	T	T
0.5553489055337421	0.2518829775678034	0.3527350402514549	T	T	T
0.8124536920675247	0.2545736756265995	0.3550854918556934	T	T	T
0.7264958826930670	0.2500374199619348	0.9436509494168160	T	T	T
0.8901491772454811	0.2506418784218479	0.9416443378087335	T	T	T
0.9459274405808951	0.7544829116771568	0.8573386711810258	T	T	T
0.6822361848886805	0.7544910862909975	0.8545615003836808	T	T	T
0.7752882554227787	0.7496292693383595	0.4429250833969456	T	T	T
0.6086902327050434	0.7507959763514007	0.4479406671712456	T	T	T
0.9315729495529658	0.5024113684819647	0.5358082155577073	T	T	T
0.9301307220365523	0.4383610701329047	0.4024760476605755	T	T	T
0.8634086768867593	0.5627569978245579	0.5645368559936788	T	T	T
0.9501331129156104	0.4821103664570533	0.5962085744783105	T	T	T
0.0585490269694393	0.4616958949371616	0.4584317651346430	T	T	T
0.0571889199594647	0.4478829775093656	0.3241054413200871	T	T	T
0.0065219733684082	0.5574754614130353	0.4331462124185469	T	T	T
0.9846385383626585	0.6272633028430066	0.3474822633815345	T	T	T
0.0739674399691336	0.6018674699904609	0.3617376119948425	T	T	T
0.0273085850516384	0.4533664304823577	0.3919583974391491	T	T	T
0.0213322553073541	0.5906153524982790	0.3720181159461578	T	T	T

Figure 5(a) TS3

Si Al O Zn H C

1.0000000000000000

20.0219999999999985 0.0000000000000000 0.0000000000000000

0.0000000000000000 19.8990000000000009 0.0000000000000000

0.0000000000000000 0.0000000000000000 13.3829999999999991

93 3 193 2 6 2

Selective dynamics

Structure files (CONTCAR) involved in this work:

Direct

0.4233115791869735	0.0617351788562071	0.6475202793983041	T	T	T
0.3057835439584447	0.0299762259786978	0.7918530919736082	T	T	T
0.2830296001324792	0.0559082199256675	0.0157835266992746	T	T	T
0.1243706940189675	0.0595418826448359	0.0127300647708643	T	T	T
0.0676164395829531	0.0318183142819365	0.8013555733227066	T	T	T
0.1802398345857099	0.0644532835821345	0.6658391028877637	T	T	T
0.4181835611990478	0.8282975905130985	0.6680270344868476	T	T	T
0.3021822287273064	0.8705999509709187	0.8034543571937590	T	T	T
0.2664092736135607	0.8319017839309045	0.0229730269451626	T	T	T
0.1121394929221043	0.8266479522402574	0.0114112060639530	T	T	T
0.0657160974662915	0.8749858349737935	0.7969863584740515	T	T	T
0.1806730822324464	0.8282809373022414	0.6668864960570128	T	T	T
0.0766521093977478	0.9384843658165509	0.1502323585223521	T	T	T
0.1944234468237094	0.9704147246971481	0.2927669645347228	T	T	T
0.2170731500268721	0.9442881763460618	0.5178757272748977	T	T	T
0.3766662148706851	0.9384111538523472	0.5139627542662938	T	T	T
0.4335897079970237	0.9686870812349369	0.3027985461596956	T	T	T
0.3205625015291697	0.9377093879838762	0.1659521262036303	T	T	T
0.0834163955939679	0.1710083612552056	0.1657088196690079	T	T	T
0.1967317480389086	0.1291455931677207	0.3039861976057963	T	T	T
0.2319373277069003	0.1705376424525265	0.5214542935247262	T	T	T
0.3870871358862655	0.1754740492182650	0.5084759652191169	T	T	T
0.4347030015472241	0.1271392762740519	0.2951617122348026	T	T	T
0.3170715604938946	0.1710683707691455	0.1666776823146277	T	T	T
0.5758993746695522	0.5561552707366307	0.3528138847204621	T	T	T
0.6923097788267309	0.5257708644038103	0.2038380877883573	T	T	T
0.7129862895497980	0.5676992633025129	0.9858570774343444	T	T	T
0.8711640799816442	0.5728972691724077	0.9849483974224091	T	T	T
0.8133646896279534	0.5508497234329603	0.3464629229615606	T	T	T
0.5749219112561992	0.3279949910228573	0.3333267297049206	T	T	T
0.6961648406721559	0.3713234738662257	0.1956565965377456	T	T	T
0.7297167274845500	0.3269490094571242	0.9818659440010205	T	T	T
0.8845123123782168	0.3261902319575468	0.9935744272149464	T	T	T
0.9439290849788491	0.3742390754895621	0.1887083429019744	T	T	T
0.9187878652277381	0.4452960575080466	0.8599664054846361	T	T	T
0.7969778252896644	0.4721253956894607	0.7223639195244383	T	T	T
0.7749121274758851	0.4370233746880171	0.4959296200636731	T	T	T
0.6166474965183546	0.4305371811238587	0.4897147943027175	T	T	T
0.5663124663517165	0.4700364235957379	0.7033780819561674	T	T	T
0.6721477394809452	0.4461455228422071	0.8587533941387984	T	T	T
0.9184125577495980	0.6793695443228724	0.8305529847024280	T	T	T
0.7694780856863194	0.6689824031722016	0.4659275220740136	T	T	T
0.6140782068842836	0.6724809202428024	0.4862622907453479	T	T	T
0.5588165966938226	0.6289638898113766	0.6985003509936165	T	T	T
0.6692010232213829	0.6745994627174760	0.8298095336992927	T	T	T
0.5785601401401804	0.9447566086245706	0.3594983026754027	T	T	T
0.6994958335811654	0.9735601898678603	0.2169688773906196	T	T	T
0.7197761811066813	0.9378202623478497	0.9943730042379091	T	T	T
0.8799186892957406	0.9349977270033974	0.9960035711359579	T	T	T
0.9316394443863599	0.9702615073291043	0.2058411812981290	T	T	T
0.8235685245034717	0.9466932243288709	0.3577171237326024	T	T	T
0.5776318347699106	0.1730824807383272	0.3307048468829815	T	T	T

Structure files (CONTCAR) involved in this work:

0.6992060143646066	0.1321523290077300	0.1965766239545222	T	T	T
0.7321134699948295	0.1711551097453262	0.9744317696520568	T	T	T
0.8865564178816081	0.1737119920550163	0.9832771483777666	T	T	T
0.9366859408020887	0.1281839701227898	0.1965538462047697	T	T	T
0.8228502775315237	0.1744366377241559	0.3323277294134405	T	T	T
0.9227046534483578	0.0548392124185151	0.8565812277472987	T	T	T
0.8009599625634753	0.0263575116129837	0.7102639403302684	T	T	T
0.7822456468612244	0.0673977145294896	0.4926247267315583	T	T	T
0.6218595388369278	0.0695058517077875	0.4911154451388523	T	T	T
0.5686799824598500	0.0322838338337059	0.7000662335274888	T	T	T
0.6780303044928641	0.0539062337001786	0.8515204249991927	T	T	T
0.9236631705199890	0.8318238006371288	0.8376724630703065	T	T	T
0.8013557881184912	0.8690543454370522	0.6977062379203148	T	T	T
0.7702088991815150	0.8264850100895978	0.4804321588244190	T	T	T
0.6151800898677638	0.8265469213497140	0.4908370445409526	T	T	T
0.5634649059339997	0.8748477225407273	0.6986172169749205	T	T	T
0.6771421713224161	0.8327050172258044	0.8354584116357153	T	T	T
0.4221695053347688	0.4455092850376474	0.6357429100934718	T	T	T
0.3007082986657700	0.4713461757411438	0.7782003448369859	T	T	T
0.2807588376695165	0.4386285910155854	0.0009207346769693	T	T	T
0.1215829601805197	0.4352973547798824	0.0048632365694527	T	T	T
0.0634852082510591	0.4716560436010473	0.7934235119269542	T	T	T
0.1738530581464092	0.4434180150759490	0.6452566655101311	T	T	T
0.4166478843772186	0.6747612067888339	0.6503239425648141	T	T	T
0.2982940597467801	0.6300387032959792	0.7886647613359561	T	T	T
0.2686500702410544	0.6725900402198087	0.0074579390547046	T	T	T
0.1144817824113267	0.6726703386596766	0.9966812722664156	T	T	T
0.0604416365680403	0.6308125204745698	0.7867918646605138	T	T	T
0.1762346636448516	0.6706090611652050	0.6551861325055646	T	T	T
0.0765011676854313	0.5584564022672864	0.1376578732898646	T	T	T
0.1984812747555558	0.5289826213907511	0.2745675693642781	T	T	T
0.2178852036960319	0.5614171469422542	0.5036693333079068	T	T	T
0.3767797290980195	0.5677322444859191	0.5019142672357066	T	T	T
0.4288379753198449	0.5289894853432295	0.2905040538467495	T	T	T
0.3242948868075018	0.5577874776749809	0.1376781131192598	T	T	T
0.0860176012357954	0.3231987426166905	0.1515201597664224	T	T	T
0.1994777379566234	0.3709709595080326	0.2914529757524946	T	T	T
0.2292327817705345	0.3310661516575711	0.5120920505572187	T	T	T
0.3844474782785793	0.3292598806433964	0.4997246936873629	T	T	T
0.4336214627214179	0.3710229042204888	0.2861139251311278	T	T	T
0.3191664778870256	0.3287792877765002	0.1578681860469056	T	T	T
0.9249423728149817	0.5300374362307282	0.1917382398657660	T	T	T
0.8250065833548527	0.3366599301877177	0.3283691821322217	T	T	T
0.7955702628224941	0.6365598347445096	0.6990179629796811	T	T	T
0.0099528034650048	0.5583103236236252	0.2107143370194941	T	T	T
0.3590795519479004	0.0685481521500856	0.7208897942724137	T	T	T
0.3175840547139683	0.0541586245941853	0.9061640433100789	T	T	T
0.2034118645677767	0.0429323452440648	0.0048887352585863	T	T	T
0.0919933073623111	0.0689032427586780	0.9029444331368093	T	T	T
0.1038213844531474	0.0667364895493748	0.7060616102013489	T	T	T
0.2299457360542261	0.0490957232648471	0.7593921724761739	T	T	T
0.3606410924695488	0.8253376037796727	0.7535012168620574	T	T	T
0.3036200315987554	0.8583262773139594	0.9228232565922724	T	T	T

Structure files (CONTCAR) involved in this work:

0.1884225964349547	0.8548080718711714	0.0188634614769052	T	T	T
0.0859839643028187	0.8346068885679319	0.8978189053700997	T	T	T
0.1036813686421485	0.8411610147216197	0.7016027888290265	T	T	T
0.2295606437004734	0.8479869653173437	0.7599674916038535	T	T	T
0.3165231622593981	0.9492653977815028	0.7786245707683259	T	T	T
0.0888522148171171	0.9528918451092648	0.8067172167307854	T	T	T
0.4323717125926964	0.1308345032299569	0.5840025417284049	T	T	T
0.4145338704226684	0.9995278617713198	0.5702467205220786	T	T	T
0.3900994193226924	0.8679681391204368	0.5709523403413311	T	T	T
0.1977210875808040	0.1375661831200110	0.6193162316318477	T	T	T
0.1865241564540317	0.0057595690254330	0.5824274797442872	T	T	T
0.1987280898842577	0.8724713094953067	0.5686458382652841	T	T	T
0.9875682978595788	0.0396643419652712	0.7873339169242716	T	T	T
0.9853504678810703	0.8702900782093963	0.7815655531176432	T	T	T
0.1410147485741099	0.9308838240818148	0.2232094427940147	T	T	T
0.1840362458066593	0.9463571823931116	0.4073154365450772	T	T	T
0.2972798328210854	0.9538375053785852	0.5104150817538595	T	T	T
0.4065410232511470	0.9311125415386061	0.4024016612410189	T	T	T
0.3969204073468615	0.9358799235298227	0.2061967758045490	T	T	T
0.2704390363304739	0.9529258504002213	0.2591358046384644	T	T	T
0.1391088258322924	0.1750225938546283	0.2536773061142024	T	T	T
0.1943734805823369	0.1414907794462366	0.4232592713809376	T	T	T
0.3101908681072502	0.1492827833039929	0.5155293569126403	T	T	T
0.4132964610292255	0.1687418837127172	0.3945076244175597	T	T	T
0.3943970927265210	0.1572947096891222	0.1991039228741829	T	T	T
0.2699324973024805	0.1502453096127113	0.2612702578853617	T	T	T
0.1815354864550915	0.0506589799601980	0.2792268040539808	T	T	T
0.4158614684020667	0.0483870336379251	0.3101193509788732	T	T	T
0.0659424692629255	0.8683308292994592	0.0895208686913326	T	T	T
0.0868400414339594	-0.0016455025559296	0.0694107057203566	T	T	T
0.1135684076197562	0.1292402386700160	0.0722822322410506	T	T	T
0.3028783356358786	0.8648187200098261	0.1190295235002327	T	T	T
0.3148731442953982	0.9960623525099905	0.0821243530865601	T	T	T
0.2976178537179696	0.1281859683052507	0.0676550267755125	T	T	T
0.5132797314461872	0.9569912665024425	0.2899329556798118	T	T	T
0.5146495267455830	0.1352509458841656	0.2771410168812850	T	T	T
0.6377641027376634	0.5613339061303985	0.2757368656466546	T	T	T
0.7016099935535655	0.5725158818446948	0.1058319843877193	T	T	T
0.7919260452504967	0.5620829253183580	0.9572491954888792	T	T	T
0.8830251408659895	0.5766610364051953	0.1033733637450198	T	T	T
0.8897134903353032	0.5320984341835081	0.3153924486930849	T	T	T
0.7632052523311251	0.5230562761134572	0.2633418417451769	T	T	T
0.6427387130538563	0.3347899438572083	0.2696361350394528	T	T	T
0.6913692179164977	0.3332447692455633	0.0879373045140666	T	T	T
0.8071512255909986	0.3519778905044088	0.9923364064232896	T	T	T
0.9124737735114148	0.3214675167263310	0.1078101954425251	T	T	T
0.9093545843678746	0.3620617586351338	0.2992382634519256	T	T	T
0.7700036703380738	0.3681756096645418	0.2408758520371238	T	T	T
0.6712967417832507	0.4491819306252633	0.1781545182160174	T	T	T
0.9314133195742694	0.4489426875532777	0.1503799825677228	T	T	T
0.5686470678078935	0.6271479854735225	0.4117016403429496	T	T	T
0.5873393976738459	0.4971841834601849	0.4352927608342544	T	T	T
0.5827221877396564	0.3638489563296479	0.4425236159084210	T	T	T

Structure files (CONTCAR) involved in this work:

0.8033038495024553	0.6306075172138943	0.3700657730459729	T	T	T
0.7973373072799551	0.5147025349415629	0.4576261982137098	T	T	T
0.8239352755606362	0.3860200889039080	0.4390899684754306	T	T	T
0.0234708415963929	0.3599510490212564	0.2050738558077340	T	T	T
0.8538247037850725	0.4342723649370920	0.7876145892788460	T	T	T
0.7898101811041548	0.4345547732331137	0.6146942156335395	T	T	T
0.6970604750158289	0.4266423058995004	0.4702191984011320	T	T	T
0.6016012209794488	0.4328652873908151	0.6084306347317373	T	T	T
0.5988415470884185	0.4423081167899136	0.8067842856160965	T	T	T
0.7248730805028462	0.4722378152604430	0.7745058215401511	T	T	T
0.8560857417550943	0.6827807869205309	0.7563982554074434	T	T	T
0.8118666032675770	0.6443308741042091	0.5655883863833568	T	T	T
0.6918059415619481	0.6466867616347655	0.4811479677457049	T	T	T
0.5860399124835971	0.6667628890225575	0.5989689724658509	T	T	T
0.5908604081306971	0.6642900114201391	0.7968971809678798	T	T	T
0.7156289399143893	0.6486979213637234	0.7390977749225336	T	T	T
0.8210987549601363	0.5495848354928929	0.6999452683812218	T	T	T
0.5792884898651484	0.5501539424199858	0.6929723778286121	T	T	T
0.9292748511839335	0.3776302407742183	0.9263059076818250	T	T	T
0.9112293735868952	0.5104641440161212	0.9311198146688674	T	T	T
0.8995757199965998	0.6416541123220871	0.9346375443514879	T	T	T
0.6922280353092427	0.3720284341306891	0.8977127874152857	T	T	T
0.6732376773951205	0.5003405743347744	0.9492007218706680	T	T	T
0.6817294826753317	0.6339774543220935	0.9339036183092608	T	T	T
0.4869208413632919	0.4531809818809213	0.7075024350772515	T	T	T
0.4777805530030263	0.6351817243461905	0.7044450827734366	T	T	T
0.6437841340504852	0.9395468867642512	0.2886243131659402	T	T	T
0.7004086806865609	0.9333313163893310	0.1116546045554062	T	T	T
0.8001490450274336	0.9441454460613696	0.9789007660108425	T	T	T
0.8976268014342089	0.9290793417953593	0.1138978993783632	T	T	T
0.8985123537823244	0.9482163412630414	0.3115622387940927	T	T	T
0.7722666709597987	0.9665714790731982	0.2687352048227158	T	T	T
0.6410886778247142	0.1722661207982722	0.2560784296315703	T	T	T
0.6972710135281474	0.1577942386527677	0.0818189348449838	T	T	T
0.8097324706033345	0.1467092642045105	0.9798462734663244	T	T	T
0.9142197146178608	0.1683394687652442	0.0965848303690042	T	T	T
0.8988237616702579	0.1574463384596183	0.2941226597150686	T	T	T
0.7717496471365013	0.1463562894188522	0.2457640917123087	T	T	T
0.6821316533339226	0.0522571376905828	0.1999079525617172	T	T	T
0.9192418643592775	0.0491732109131874	0.1828517250618046	T	T	T
0.5697676340111414	0.8743640719549994	0.4199991584530866	T	T	T
0.5846704659118476	0.0053293321598338	0.4405049477373597	T	T	T
0.5965614363197957	0.1377280392927742	0.4365562306794736	T	T	T
0.8099600743270380	0.8711482360208026	0.3989465353285215	T	T	T
0.8174619827881006	0.9996822678999995	0.4492200642934845	T	T	T
0.8094837330982176	0.1336737733433360	0.4363594966090953	T	T	T
0.0107125338372163	0.9534028347781832	0.2164237794194646	T	T	T
0.0168929835069621	0.1363348353900659	0.2116195829057991	T	T	T
0.8571004353339738	0.0543276099467519	0.7863395519837003	T	T	T
0.8008642382797967	0.0728463750303070	0.6106002703416596	T	T	T
0.7018140658755969	0.0606087932046702	0.4775820081289848	T	T	T
0.6018154701713969	0.0747487905600605	0.6084829077225338	T	T	T
0.6029317522616926	0.0516646892145261	0.8060955671717238	T	T	T

Structure files (CONTCAR) involved in this work:

0.7283219506683840	0.0299162451424554	0.7633334413717411	T	T	T
0.8586170406048628	0.8364910069928825	0.7668569949902694	T	T	T
0.8040916345460970	0.8314388992802095	0.5901604535234988	T	T	T
0.6927992339359610	0.8513486655031902	0.4860320870178391	T	T	T
0.5888798932810203	0.8290970803934117	0.6053475978893116	T	T	T
0.6014928959324665	0.8515248596063013	0.8000085528928992	T	T	T
0.7284438917914305	0.8576408456335409	0.7482252104773666	T	T	T
0.8157146702845578	0.9485538193700048	0.6808536309601723	T	T	T
0.5791977323140464	0.9531088615878801	0.6743658021751591	T	T	T
0.9314006235012526	0.1285162338206443	0.9075674908246313	T	T	T
0.9177048593939602	0.9990761353354290	0.9455474421603879	T	T	T
0.9068592805775678	0.8663569977639403	0.9447074893737869	T	T	T
0.6938549448178282	0.1300199799722089	0.8869990701070335	T	T	T
0.6839412639542507	0.0039485859760743	0.9471734162938661	T	T	T
0.6932284300435849	0.8700369373629822	0.9404539782454990	T	T	T
0.4899912378396752	0.0497969627686518	0.7134994775111195	T	T	T
0.4836092851484612	0.8649421528387904	0.7146157608920003	T	T	T
0.3554397008415320	0.4380598469272106	0.7039347167267982	T	T	T
0.3031171614057870	0.4326240306000322	0.8848142331505310	T	T	T
0.2008203699970734	0.4530546597617781	0.0111623778823935	T	T	T
0.0965804891599416	0.4353770165344274	0.8899019494781726	T	T	T
0.0982499677184906	0.4437883280816243	0.6910251070451399	T	T	T
0.2258077131066494	0.4632157932792022	0.7333714311457803	T	T	T
0.3506910791150129	0.6704904401620213	0.7198056129329127	T	T	T
0.3039595828954527	0.6602239750945620	0.9003208118041628	T	T	T
0.1915368196265820	0.6463304705229855	0.0019761116018279	T	T	T
0.0884284318532185	0.6729413690011924	0.8821319935627396	T	T	T
0.0984281117934492	0.6576750702401022	0.6863182210219921	T	T	T
0.2230596323438223	0.6406664812313921	0.7446832096524092	T	T	T
0.3170317637706623	0.5507502731325149	0.7914870232606418	T	T	T
0.0769126971819772	0.5516907903847220	0.8030400654416839	T	T	T
0.4305831631089754	0.3787584239980260	0.5669205517434008	T	T	T
0.4185154381342462	0.5105069009578532	0.5618975632718543	T	T	T
0.3988986713317458	0.6413700196061660	0.5423310015960884	T	T	T
0.1903795394935784	0.3689617205262738	0.6026324162649312	T	T	T
0.1786486419277180	0.4984315583197937	0.5550217086493431	T	T	T
0.1921900899017797	0.6322015005496766	0.5504126828109865	T	T	T
0.9836873260855822	0.4551485061693637	0.7861132977243794	T	T	T
0.9805512923775150	0.6403088989275619	0.7740199328338130	T	T	T
0.1414425889081559	0.5678394278357605	0.2097467297369351	T	T	T
0.1993298306680182	0.5616894215596741	0.3856236560304749	T	T	T
0.2976426614176261	0.5533810442072291	0.5215882036291747	T	T	T
0.3927656292021190	0.5666259693754611	0.3836951913405366	T	T	T
0.3985032492345166	0.5583496224025729	0.1865624307344174	T	T	T
0.2712701895000048	0.5388389008399544	0.2252616275685724	T	T	T
0.1486277070492193	0.3247140653012379	0.2282732199459871	T	T	T
0.1930262990470957	0.3517489189942194	0.4082527217563756	T	T	T
0.3070634255060972	0.3547139828037602	0.5078918689886395	T	T	T
0.4085994214699343	0.3297485563871548	0.3841125008862794	T	T	T
0.3972581709202682	0.3410774230675278	0.1866509984967264	T	T	T
0.2750663854561063	0.3572293144060227	0.2517802597181812	T	T	T
0.1793452670560418	0.4497534000193264	0.2777875823829791	T	T	T
0.4131897333968251	0.4493142021607862	0.3003660835804257	T	T	T

Structure files (CONTCAR) involved in this work:

0.0689331165496533	0.6227124591610044	0.0641401292126903	T	T	T
0.0807767078342528	0.4904693728295315	0.0714474332172543	T	T	T
0.1068939724647744	0.3607437291213904	0.0480610951382269	T	T	T
0.3084803097927107	0.6318212302333885	0.0936097141955433	T	T	T
0.3207685861013886	0.5016869522598743	0.0496857389855503	T	T	T
0.2996838342397737	0.3685932515149611	0.0560863932289220	T	T	T
0.5084721539272676	0.5423797243948093	0.2895575740953580	T	T	T
0.5137690014058797	0.3634266087099595	0.2720979147639803	T	T	T
0.4367527092391466	0.7526144254972332	0.6326826284317134	T	T	T
0.1904111081509134	0.7497976688502554	0.6372988643668911	T	T	T
0.2718182548880060	0.7513402611344906	0.0348233884114668	T	T	T
0.1090383591117502	0.7478377126228767	0.0424979329755329	T	T	T
0.0673884922166732	0.2461290779759516	0.1253033982137677	T	T	T
0.3055858150205426	0.2496007629229660	0.1391706895238803	T	T	T
0.2237259440057439	0.2511305321174123	0.5298050005672202	T	T	T
0.3914767856766974	0.2535089015462182	0.5429415820640079	T	T	T
0.5567242419298342	0.2500654299472945	0.3543306792703330	T	T	T
0.8145880118911447	0.2528815223984325	0.3516655402276992	T	T	T
0.7273099146259551	0.2497308495632746	0.9439171931639936	T	T	T
0.8903279220939057	0.2512994665071486	0.9458005692948296	T	T	T
0.9444702625264635	0.7546170602578554	0.8588883079797267	T	T	T
0.6834534962410397	0.7531011960383732	0.8547997707084998	T	T	T
0.7753400377023681	0.7484871232868602	0.4452391249632101	T	T	T
0.6096005832839007	0.7500105962511355	0.4499485981369513	T	T	T
0.9319692788698597	0.4892487800372943	0.5380741503893846	T	T	T
0.9284546513997407	0.4354223734143994	0.4088055562328175	T	T	T
0.8666193481924142	0.5573940878321378	0.5649108730465936	T	T	T
0.9477958662441698	0.4653676518931819	0.5978666469937618	T	T	T
0.0041008302775825	0.5682413716565515	0.5020054160187867	T	T	T
0.0829394490635949	0.5404413347596019	0.4452137652504223	T	T	T
-0.0016485074470396	0.6653400459146501	0.3828560593147028	T	T	T
0.0200487444391998	0.5900668949499648	0.2940117223646410	T	T	T
0.0837173595288142	0.6440202157552830	0.3387248211538163	T	T	T
0.0420555272378687	0.5766442428850332	0.4454632469709736	T	T	T
0.0374426151603917	0.6272187752923173	0.3749075558945767	T	T	T

Figure 5(b) TS-CH₄ as same as Figure 1(b) Cu/ZSM-5

Figure 5(b) TS-CH₃OH same as Figure2(a) Cu-TS

Figure 5(b) TS1

Si O Al Cu C H

1.0000000000000000

20.0219993591000005 0.0000000000000000 0.0000000000000000

0.0000000000000000 19.8990001678000006 0.0000000000000000

0.0000000000000000 0.0000000000000000 13.3830003737999998

93 195 3 3 2 7

Selective dynamics

Direct

0.4226311016224522 0.0541802826078710 0.6385584247170132 T T T

0.3021480273312168 0.0258756063751446 0.7826360248758295 T T T

0.2807237044895391 0.0631905339876982 0.0029982449275573 T T T

0.1214054383156660 0.0643332109844787 0.0037784892224472 T T T

0.0714545152629520 0.0284839098864306 0.7935921276577753 T T T

0.1785207696890262 0.0523475231199903 0.6421924573684912 T T T

0.4219609844778284 0.8262977354969985 0.6633561322454496 T T T

Structure files (CONTCAR) involved in this work:

0.3022621885773933	0.8683572711288637	0.8024570006137099	T	T	T
0.2676284210233001	0.8278614608801227	0.0237013721972781	T	T	T
0.1127993045859565	0.8253749933750092	0.0149934956391739	T	T	T
0.0654970732998899	0.8725679095753252	0.8031304920305686	T	T	T
0.1782902475923510	0.8276484685253196	0.6672566862106970	T	T	T
0.0768752744282730	0.9443442777118967	0.1425039677701425	T	T	T
0.1983544509214099	0.9722370115453444	0.2867819111284722	T	T	T
0.2177985409071885	0.9328395623191731	0.5061487319426926	T	T	T
0.3771968499027761	0.9299074243619767	0.5076480477063700	T	T	T
0.4287314657080386	0.9692873486717581	0.2986290537852215	T	T	T
0.3220513149412110	0.9473080729278639	0.1449172216412763	T	T	T
0.0782561409423423	0.1690460494548817	0.1610080618628199	T	T	T
0.1966098376330154	0.1288676410049484	0.3041083087226510	T	T	T
0.2321596469361479	0.1723863893007468	0.5202881943171047	T	T	T
0.3865299003168087	0.1730047902681746	0.5068086610708870	T	T	T
0.4341193462853229	0.1264652507595620	0.2968923101584648	T	T	T
0.3179015050937309	0.1680210364982090	0.1647137074996979	T	T	T
0.5768142189565449	0.5563777626408499	0.3562988815950495	T	T	T
0.6958197502109240	0.5288789057837129	0.2169091532034599	T	T	T
0.7153133864193467	0.5495155165575978	0.9860389659335564	T	T	T
0.8736658122081872	0.5683210207933951	1.0003064563943229	T	T	T
0.9295689192746428	0.5212706316639826	0.2064020440460026	T	T	T
0.8188652041638727	0.5604187765014830	0.3475741540888135	T	T	T
0.5796152029116231	0.3244160421584716	0.3304156359956119	T	T	T
0.7032594852529341	0.3710268140585239	0.2117323989546318	T	T	T
0.7304093112119688	0.3273180810839910	0.9914184921954712	T	T	T
0.8877608150997021	0.3277524094327345	0.9957986856667659	T	T	T
0.9361457013521147	0.3649996882954157	0.2065551178531163	T	T	T
0.8251616181916026	0.3279602579214609	0.3485838610256972	T	T	T
0.9238004802609818	0.4487215863539804	0.8650140765699075	T	T	T
0.8024234453387717	0.4668900448465766	0.7227364544645836	T	T	T
0.7801604250767480	0.4409794629892955	0.4980010990815799	T	T	T
0.6201608299264157	0.4291719143379224	0.4920165604625563	T	T	T
0.5625442289466658	0.4640869646778917	0.7019707638892370	T	T	T
0.6763356104427350	0.4281625111285701	0.8402674598553599	T	T	T
0.7954081714848423	0.6252580299953087	0.7148245358300458	T	T	T
0.6143594593173317	0.6701068337419781	0.4908461698204207	T	T	T
0.5600335354674955	0.6217719233720072	0.7002501975887845	T	T	T
0.6686946618763848	0.6666864395809724	0.8342227568203511	T	T	T
0.5751783567695196	0.9395644976022816	0.3523030189705378	T	T	T
0.6931074951299355	0.9707839834798363	0.2089936762119380	T	T	T
0.7187504553043198	0.9526915735820977	0.9857862305252401	T	T	T
0.8761342847488620	0.9458139382484451	0.9834632707025708	T	T	T
0.9330299649424264	0.9684417602168113	0.1936334327335640	T	T	T
0.8174945174626331	0.9307592478563189	0.3263566260180424	T	T	T
0.5800970815708777	0.1702072605410465	0.3202760728857947	T	T	T
0.7020256892426520	0.1271850382702915	0.2008554870863906	T	T	T
0.7346712436031786	0.1677831378694418	0.9814666664602864	T	T	T
0.8921429001618687	0.1769549559548413	0.9752297888173214	T	T	T
0.9334398785895837	0.1260973146821104	0.1941230969808692	T	T	T
0.8227130588751459	0.1732859478732017	0.3382974960800522	T	T	T
0.9254549692698559	0.0629946720162520	0.8405454293975310	T	T	T
0.8055417731783858	0.0295405690687623	0.7035214321769532	T	T	T

Structure files (CONTCAR) involved in this work:

0.7839000077872593	0.0527034109802529	0.4764275448807501	T	T	T
0.6238499702983306	0.0652492464240362	0.4810301253826025	T	T	T
0.5674859332271527	0.0338187713888487	0.6910659375793525	T	T	T
0.6815146421639829	0.0672511850299721	0.8276606450535817	T	T	T
0.9168578666895636	0.8340965455697845	0.8300871423636863	T	T	T
0.8010991473550335	0.8725855671554198	0.6987761993250208	T	T	T
0.7688425987238777	0.8323925653508314	0.4836666377221541	T	T	T
0.6130758642316131	0.8251183479959664	0.4901410848436281	T	T	T
0.5658224266967075	0.8756497423023897	0.7024386025371367	T	T	T
0.4189317288027828	0.4436358468944153	0.6469982372798863	T	T	T
0.2982574463754017	0.4726146736758528	0.7886938871451484	T	T	T
0.2801312846841573	0.4345253332392900	0.0106206509937724	T	T	T
0.1215139088703213	0.4318244363462467	0.0104479634917733	T	T	T
0.0699671520759511	0.4696844083180119	0.8008187625396895	T	T	T
0.1752812109408080	0.4458075216583210	0.6482998445863833	T	T	T
0.4176654473851784	0.6710515909988976	0.6623044495049825	T	T	T
0.2993900492576167	0.6294990453895479	0.8032558405763618	T	T	T
0.2679312514788260	0.6714543522667612	0.0252289886362300	T	T	T
0.1141036854443178	0.6715954972152751	0.0143215848826885	T	T	T
0.0626786542775743	0.6277558525426428	0.8029813587010431	T	T	T
0.1765133117055920	0.6688562795766336	0.6664838301120276	T	T	T
0.0738533524967571	0.5534997176547560	0.1428609021979738	T	T	T
0.1959531741774908	0.5260153684806249	0.2846597681443860	T	T	T
0.2147068050060873	0.5627458002575781	0.5073892886006764	T	T	T
0.3743441076556394	0.5654363792585720	0.5097844579181624	T	T	T
0.4297483790399723	0.5266419549490615	0.3003410347111184	T	T	T
0.3229393251502388	0.5531070427035891	0.1471211961586729	T	T	T
0.0802493708190259	0.3234120834006855	0.1633936682276206	T	T	T
0.1975206287824558	0.3676390486186943	0.3036052185161281	T	T	T
0.2320436057888530	0.3284061771190416	0.5230972189397602	T	T	T
0.3868994983959038	0.3258595846341402	0.5114311136219903	T	T	T
0.4362422681440757	0.3690340602867703	0.2986247304015884	T	T	T
0.3195171959548253	0.3268787170997413	0.1683242097324889	T	T	T
0.3571948013527874	0.0592239450726773	0.7093325780725291	T	T	T
0.3002940049828974	0.0689380319849369	0.8857913730863560	T	T	T
0.2008546373496774	0.0515810251947907	0.0173840384064318	T	T	T
0.1014264605157186	0.0712366668069523	0.8870073163640384	T	T	T
0.1038760839540902	0.0531373444051457	0.6889143063521701	T	T	T
0.2294339225100179	0.0286600062884504	0.7297492558201950	T	T	T
0.3592580239438666	0.8290931370593562	0.7401833684159688	T	T	T
0.3015616219723544	0.8384833468907470	0.9150364813861562	T	T	T
0.1896730039261304	0.8514673250135439	0.0202056871200859	T	T	T
0.0874124532998750	0.8293532126440863	0.9006109318806075	T	T	T
0.1017019317063292	0.8402722308660141	0.7050411714545942	T	T	T
0.2292298449014841	0.8571311048480224	0.7516190296976388	T	T	T
0.3202070030170189	0.9479565077173346	0.8060906619335043	T	T	T
0.0893215412109761	0.9501826404028156	0.8156772260759632	T	T	T
0.4313418602384392	0.1233935668112680	0.5753279993458992	T	T	T
0.4169823993391365	0.9916660799541003	0.5605450527469076	T	T	T
0.4004290792350443	0.8590839213805250	0.5565162858217748	T	T	T
0.1951676183386570	0.1277495049744649	0.6045472673904341	T	T	T
0.1811090285461483	0.9998127651176685	0.5492712759046777	T	T	T
0.1902271516276554	0.8655091149673098	0.5609660658023737	T	T	T

Structure files (CONTCAR) involved in this work:

0.9919597673614512	0.0409818900782474	0.7807760844479353	T	T	T
0.9849665094219046	0.8719986157597146	0.7933147983885267	T	T	T
0.1425554909208555	0.9411439342256400	0.2124571012298659	T	T	T
0.2011241096118882	0.9267720164045435	0.3875760712057724	T	T	T
0.2975884903512191	0.9408132549424604	0.5252391698492668	T	T	T
0.3940649422496316	0.9273134694270909	0.3891891753360684	T	T	T
0.3965028569884907	0.9478397120076000	0.1920957238922800	T	T	T
0.2702693029345959	0.9713080950830214	0.2314211391363434	T	T	T
0.1397542146285770	0.1658104806168144	0.2386738139968709	T	T	T
0.1955596762846064	0.1640941577562765	0.4129375696829890	T	T	T
0.3092698172320795	0.1474437283586399	0.5098484012286266	T	T	T
0.4127949532949438	0.1724143834867280	0.3920826421477754	T	T	T
0.3948102216485133	0.1531163929513137	0.1978746402390184	T	T	T
0.2693268154371765	0.1380994734331253	0.2517561562721204	T	T	T
0.1795060181350661	0.0493993716130494	0.3147737887585139	T	T	T
0.4154314381765681	0.0487057966299834	0.3202337134845146	T	T	T
0.0668324429522784	0.8717502984518426	0.0879328464554503	T	T	T
0.0820959023119248	0.0019228593236942	0.0563248449545298	T	T	T
0.0992089034458488	0.1342030204014887	0.0561743666970355	T	T	T
0.3059761853761817	0.8715658472818122	0.1078459847470096	T	T	T
0.3192581437687724	0.9988596711960730	0.0507866019612141	T	T	T
0.3027078759733797	0.1324871367502327	0.0579066388345477	T	T	T
0.5075380572710055	0.9528076243391780	0.2890141552452042	T	T	T
0.5139810939716853	0.1324613079099498	0.2775960611053055	T	T	T
0.6369923950217197	0.5680174212849329	0.2756642063804325	T	T	T
0.6861358606275185	0.5437995468288775	0.0978922229588447	T	T	T
0.7956410795864785	0.5491396502125521	0.9828590135728577	T	T	T
0.8925902881350072	0.5626500751551226	0.1175822148677653	T	T	T
0.8948039174683797	0.5420949661688170	0.3112021637315905	T	T	T
0.7693091084073819	0.5555496615979928	0.2499397908410717	T	T	T
0.6427371256649469	0.3259403591382057	0.2545368882569299	T	T	T
0.7038253128971252	0.3639811743521920	0.0917234714369501	T	T	T
0.8091593111700250	0.3456354110989909	0.9799094941153541	T	T	T
0.9067131384501685	0.3214216780461465	0.1137798615048217	T	T	T
0.9013757527599522	0.3409448009490328	0.3099761436887413	T	T	T
0.7743364724121418	0.3464774789412946	0.2572261452995881	T	T	T
0.6901525500900048	0.4491344987470762	0.2410831793354888	T	T	T
0.9180453950873814	0.4428106779501313	0.1828566816496185	T	T	T
0.5647456866556336	0.6236938095273665	0.4215750464533276	T	T	T
0.5940885801099965	0.4935090645819937	0.4291472648504847	T	T	T
0.6001040050435145	0.3600204077984072	0.4350026085669956	T	T	T
0.8192473501051426	0.6372529342790250	0.3875875686279298	T	T	T
0.7951086789283208	0.5071863819134572	0.4311498867978968	T	T	T
0.8107488941887093	0.3740347499509265	0.4457003287010045	T	T	T
0.0077291589176422	0.5424525161340356	0.2118153759643515	T	T	T
0.0164933017484396	0.3585406474705453	0.2179550816577789	T	T	T
0.8607069216097279	0.4339017628520310	0.7922822120338725	T	T	T
0.8160515637928937	0.4496707669247342	0.6059531365702857	T	T	T
0.7001048008457501	0.4328756447593720	0.5088453274351509	T	T	T
0.5839061629488707	0.4263183927920828	0.5998281961402743	T	T	T
0.6010687333627110	0.4299295349433255	0.7961966687179318	T	T	T
0.7304479629566830	0.4333988323592988	0.7506846577053622	T	T	T
0.8432472226396833	0.6686215388938224	0.7852256123104084	T	T	T

Structure files (CONTCAR) involved in this work:

0.8071380691166196	0.6323025094783203	0.5979735055076314	T	T	T
0.6898387587019374	0.6455589576630044	0.4781065102951606	T	T	T
0.5881400124098309	0.6639282530249738	0.6066552815139226	T	T	T
0.5919754020952031	0.6524935212689058	0.8043438201680507	T	T	T
0.7173548158768267	0.6477659890223214	0.7442873295468954	T	T	T
0.8004699958680273	0.5459806770190642	0.7479011598677033	T	T	T
0.5820803373375802	0.5432720951330535	0.6935616607616137	T	T	T
0.9317484539244327	0.3865177984069267	0.9436103273876907	T	T	T
0.9166645696669153	0.5184444255916015	0.9296571991597854	T	T	T
0.8919691115063839	0.6476006040333807	0.9759226010362699	T	T	T
0.6876760992515470	0.3578968910987074	0.8991475912284195	T	T	T
0.6844098143649191	0.4922142333157291	0.9159893688284607	T	T	T
0.6883252122258164	0.6240479007580055	0.9409214949990072	T	T	T
0.4828466444815656	0.4549813749555249	0.7199878742059798	T	T	T
0.4794481533551193	0.6280631014725665	0.7094322928148703	T	T	T
0.6363812557984865	0.9321721293028513	0.2728297720580175	T	T	T
0.6781448504929455	0.9625967902511875	0.0897778770418041	T	T	T
0.7981009847907816	0.9632823940091432	0.0086611658800307	T	T	T
0.9146790819054526	0.9324378243691527	0.0879629995675359	T	T	T
0.8935898370612037	0.9311735364818791	0.2836114796275371	T	T	T
0.7659828580771624	0.9374045536379936	0.2314465570442471	T	T	T
0.6357351794137918	0.1693777162008262	0.2313274592987146	T	T	T
0.7115040457884146	0.1267971973666037	0.0806330449337721	T	T	T
0.8138849674447085	0.1563704844018084	0.9615364769014967	T	T	T
0.9130709592211423	0.1629340478510944	0.0904055788770938	T	T	T
0.8961390036951911	0.1613054668751248	0.2885675734612393	T	T	T
0.7673646014881236	0.1613782197514050	0.2510157901744515	T	T	T
0.6937597509094622	0.0500329158340931	0.2396764068366121	T	T	T
0.9118287076551430	0.0473143590643989	0.1889542404844768	T	T	T
0.5660939003788412	0.8717909369819626	0.4182062075135774	T	T	T
0.5873736192478606	0.0027932640934236	0.4263459535660816	T	T	T
0.6096683334268239	0.1340906610025125	0.4195232489812604	T	T	T
0.8060913815507353	0.8600858103351126	0.3824363612884873	T	T	T
0.8070201252889706	0.9941277053939350	0.4003152206490512	T	T	T
0.8102062023904141	0.1243032324610897	0.4330150238961262	T	T	T
0.0125823483185885	0.9591568132981927	0.2133517113106692	T	T	T
0.0137338742224577	0.1319273167192177	0.2104118391334691	T	T	T
0.8637901446833796	0.0698859272405937	0.7632717328626774	T	T	T
0.8175433829871899	0.0404070891496359	0.5849861874281594	T	T	T
0.7034650565029574	0.0522609932264496	0.4876689300966154	T	T	T
0.5925939689835512	0.0737532021308392	0.5918854461752407	T	T	T
0.6054120984940301	0.0660072815233535	0.7874799390522996	T	T	T
0.7333234359741133	0.0614404744328128	0.7345333752323869	T	T	T
0.8682634985082066	0.8319840545892561	0.7330416677011884	T	T	T
0.7983101267717687	0.8754215198060333	0.5776528939317461	T	T	T
0.6893906981968276	0.8506173236329861	0.4737202377039150	T	T	T
0.5916165065667318	0.8319827129387681	0.6067062740521847	T	T	T
0.6003985017552025	0.8518145434948183	0.8049937074875160	T	T	T
0.7364604471740365	0.8378649427021034	0.7471750450657302	T	T	T
0.8082634621738740	0.9511134740499683	0.7368054333997446	T	T	T
0.5837402492559325	0.9544450388590212	0.6794393565623413	T	T	T
0.9374631764806862	0.1342527704288989	0.8972929361914050	T	T	T
0.9105682032684479	0.0081430709645224	0.9274701273017880	T	T	T

Structure files (CONTCAR) involved in this work:

0.8785802016997067	0.8777264238533163	0.9179547602950264	T	T	T
0.6933341476628163	0.1372529171348120	0.8876659497114193	T	T	T
0.6915463433162291	0.0024567087547267	0.9011649923507444	T	T	T
0.7113210244727302	0.8731306709120400	0.9506750267632695	T	T	T
0.4880084430837757	0.0452555265408132	0.7086342889882977	T	T	T
0.4846635033516182	0.8666517839800885	0.7111573657704718	T	T	T
0.3523833473037685	0.4377602653300834	0.7151896663173319	T	T	T
0.2955623089202485	0.4297271582483517	0.8919528085576314	T	T	T
0.2004777906288938	0.4444878565342124	0.0312270448566711	T	T	T
0.1057491740579593	0.4289067579522922	0.8920997905400487	T	T	T
0.1004803681405452	0.4432389951554272	0.6952005662566028	T	T	T
0.2254920609259985	0.4715320322254912	0.7357728112175361	T	T	T
0.3558065301732725	0.6692466642860235	0.7402711765499778	T	T	T
0.2980019042464935	0.6619689729134877	0.9139621383308868	T	T	T
0.1905912927997889	0.6456598034304756	0.0288298691033218	T	T	T
0.0940931089061436	0.6689805142999661	0.8979894046365696	T	T	T
0.0998134193130223	0.6567907989658978	0.7024855594315339	T	T	T
0.2267438668869562	0.6379972377458567	0.7508126666835113	T	T	T
0.3188123776867767	0.5502376059950849	0.8108712190418313	T	T	T
0.0841597417061231	0.5490475061698199	0.8166899583929081	T	T	T
0.4296104274998541	0.3739784103614358	0.5854129619979198	T	T	T
0.4141440106716244	0.5056483555847729	0.5677596046906283	T	T	T
0.3946531249739477	0.6379599744283732	0.5565010925095376	T	T	T
0.1959737746910650	0.3713019699315937	0.6104969183632795	T	T	T
0.1766061040393265	0.4978682141747520	0.5546313881073998	T	T	T
0.1897731645788273	0.6318717517206351	0.5597255454867968	T	T	T
0.9905089874265748	0.4539216461985159	0.7977323599014824	T	T	T
0.9834964021568255	0.6366864493897033	0.7990825565321102	T	T	T
0.1384262764031033	0.5587921655168717	0.2147000445010400	T	T	T
0.1964877015211112	0.5668652826667772	0.3894445457790255	T	T	T
0.2946959514271417	0.5525914642365729	0.5232532814686272	T	T	T
0.3949366952342718	0.5663267966238666	0.3928135981090347	T	T	T
0.3970499923975598	0.5519210076791741	0.1959221789972727	T	T	T
0.2684447341375699	0.5332162753770224	0.2321282691065868	T	T	T
0.1434413072631897	0.3257904139505601	0.2386257077932593	T	T	T
0.1942195280108381	0.3402326913362045	0.4172598393952696	T	T	T
0.3096291770161427	0.3517801654538928	0.5111100467860576	T	T	T
0.4165345102910264	0.3278443137240848	0.3988736515211975	T	T	T
0.3967925685689547	0.3381269188237049	0.2026059619742496	T	T	T
0.2717158719335327	0.3561462361624396	0.2570331591533205	T	T	T
0.1788934340471728	0.4470661665785913	0.3019850503890235	T	T	T
0.4154824582797254	0.4468989030070120	0.3151667409706692	T	T	T
0.0651130376876617	0.6243139773177551	0.0824813280530065	T	T	T
0.0795072408610780	0.4926384644619547	0.0625636374218750	T	T	T
0.0982836784023033	0.3609407923620505	0.0591513352600883	T	T	T
0.3105464933410387	0.6284477043970639	0.1054563743398631	T	T	T
0.3194208326819818	0.4992437771343076	0.0558245195928629	T	T	T
0.3052932374009822	0.3655604223734902	0.0635051386595265	T	T	T
0.5092471433809116	0.5404738371975280	0.2936215103903664	T	T	T
0.5161891376532803	0.3623170970360442	0.2787601703715475	T	T	T
0.4406034098859677	0.7479937113766977	0.6432692867057899	T	T	T
0.1915426682621633	0.7482209180806728	0.6503837763170461	T	T	T
0.2725800797277270	0.7497864758683684	0.0569585853883417	T	T	T

Structure files (CONTCAR) involved in this work:

0.1059411938469920	0.7483870886558311	0.0546391731698889	T	T	T
0.0607439944865286	0.2466870405272140	0.1367159937872575	T	T	T
0.3050123090796916	0.2477895246786605	0.1507526721912733	T	T	T
0.2279505659065605	0.2500983250923187	0.5554628593042492	T	T	T
0.3920094449832986	0.2488752846342146	0.5509906479625059	T	T	T
0.5609387036395541	0.2465548780659060	0.3511483891625833	T	T	T
0.8169382729018583	0.2497296699890785	0.3798144244156415	T	T	T
0.7182427125986734	0.2469613338213669	0.9959393218997402	T	T	T
0.9039491726539022	0.2552664180507048	0.9461715350693100	T	T	T
0.9322376678423734	0.7621547208474005	0.8787655332000334	T	T	T
0.6776957623595392	0.7418749539110946	0.8844067717821426	T	T	T
0.6029578036060924	0.7477388142820792	0.4559911839367946	T	T	T
0.7731387617592818	0.6719843903642028	0.0975093449251201	T	T	T
0.6955663943918200	0.7770631873198749	0.1002255917178084	T	T	T
0.8323189497923301	0.7947410082054088	0.1227354350726040	T	T	T
0.7834919962792782	0.7545652874717858	0.4929031712936767	T	T	T
0.9162664163212276	0.6787640199252516	0.8502560977917946	T	T	T
0.6793691775053542	0.8286538498904809	0.8417428881910649	T	T	T
0.7732139037986466	0.6690135494055717	0.4925506375717413	T	T	T
0.7031894464501273	0.7054774844414868	0.0207502096216358	T	T	T
0.7647754935029816	0.8258282521576992	0.0525029608825674	T	T	T
0.8655077963045035	0.7171145861616274	0.0743219488416688	T	T	T
0.9501015733151610	0.7384495799558162	0.1583542029914379	T	T	T
0.8814888648107910	0.6983924730555230	0.2742977922315623	T	T	T
0.9583080291300577	0.7706344104054977	0.0919615121382871	T	T	T
0.9544536238063741	0.7726530024546446	0.2221682034775207	T	T	T
0.9818463912299931	0.6937553611419609	0.1580194613894829	T	T	T
0.8446055159892615	0.7384645733718416	0.2783582186917166	T	T	T
0.9217626348625844	0.6976962951630814	0.3288564410164812	T	T	T
0.8728071301798629	0.6529135431723474	0.2317673617711675	T	T	T
0.7622870185327647	0.6854175783594068	0.1662589083523199	T	T	T

Figure 5(b) TS2

Si O Al Cu C H

1.0000000000000000

20.0219993591000005 0.0000000000000000 0.0000000000000000

0.0000000000000000 19.8990001678000006 0.0000000000000000

0.0000000000000000 0.0000000000000000 13.3830003737999998

93 195 3 3 2 7

Selective dynamics

Direct

0.4217442876854557	0.0523567619909481	0.6423833314398182	T	T	T
0.2998257362404169	0.0251891985912590	0.7856680666757074	T	T	T
0.2782187212404535	0.0623173009586991	0.0057652678959148	T	T	T
0.1186052852680110	0.0629698674104559	0.0078475420723274	T	T	T
0.0645206963533640	0.0204452556278119	0.7984919595055017	T	T	T
0.1731953399780983	0.0493091076700447	0.6469719352249322	T	T	T
0.4186847730463799	0.8257341170925362	0.6616976086237089	T	T	T
0.3017489660455637	0.8676807688420777	0.8052634198487634	T	T	T
0.2670756850256709	0.8260619041220595	0.0252345740755661	T	T	T
0.1130288016110348	0.8238368197122270	0.0146768101974235	T	T	T
0.0649909589736060	0.8604550561178952	0.7980682304335522	T	T	T
0.1828424735987716	0.8246308185253139	0.6659660171110207	T	T	T
0.0753322467480384	0.9417973606680036	0.1457609177474704	T	T	T

Structure files (CONTCAR) involved in this work:

0.1963085175754195	0.9707188869372797	0.2866618072323698	T	T	T
0.2172715672418035	0.9328357217221181	0.5077956730032668	T	T	T
0.3756345585042593	0.9301573219192019	0.5086812810339643	T	T	T
0.4269467656543999	0.9697124857868923	0.2987378226698664	T	T	T
0.3203960216289585	0.9456791449636927	0.1458493485601179	T	T	T
0.0785836072332163	0.1710156537608754	0.1601863095857629	T	T	T
0.1952707057508057	0.1277722658842204	0.3033610904851240	T	T	T
0.2269022074281441	0.1690568008945963	0.5235175019266586	T	T	T
0.3817480616546224	0.1704805438810184	0.5107465745148325	T	T	T
0.4311864671530558	0.1267843326031149	0.2996055552626263	T	T	T
0.3165574979220903	0.1679126442036534	0.1672250198372582	T	T	T
0.5751438714401339	0.5571909602493127	0.3531017476837023	T	T	T
0.6914339019649365	0.5292755970781401	0.2116245784532267	T	T	T
0.7143902551107031	0.5466489441135938	0.9849273937666493	T	T	T
0.8721854050970257	0.5626641122099794	0.9915426121448938	T	T	T
0.9304315329916930	0.5280634351773196	0.1996342257678649	T	T	T
0.8152692029120576	0.5640537940514899	0.3344804239827885	T	T	T
0.5788821696126242	0.3253179376428332	0.3285465265873893	T	T	T
0.6989890520384122	0.3724800311504453	0.2081281675604239	T	T	T
0.7309982203104949	0.3294367459643893	0.9881354251011882	T	T	T
0.8869072862139485	0.3282429671657702	0.9919123993340442	T	T	T
0.9341747518771070	0.3710724014066800	0.2026687313128876	T	T	T
0.8226955207229949	0.3325163874179020	0.3465848543214229	T	T	T
0.9236473584262515	0.4442717789220475	0.8551564886488899	T	T	T
0.8027007282567837	0.4697367584789012	0.7173227380806124	T	T	T
0.7806752156074478	0.4458004798087081	0.4917863664334322	T	T	T
0.6211864632797287	0.4315426029978786	0.4884929895684658	T	T	T
0.5625520241711749	0.4627461735496170	0.6985054956798453	T	T	T
0.6768013755573241	0.4283445762682319	0.8348574649697830	T	T	T
0.7928714563307425	0.6236749105943523	0.6979741150528328	T	T	T
0.6047509653937401	0.6720199092448784	0.4866662238215964	T	T	T
0.5601524542865013	0.6210178197075639	0.7011887942122956	T	T	T
0.6715522531970129	0.6660496489709635	0.8343087526019193	T	T	T
0.5730920351630184	0.9430740560964026	0.3525239658133283	T	T	T
0.6935500899174230	0.9749193975178938	0.2121708944090888	T	T	T
0.7133879325057296	0.9503068046604212	0.9860610167561643	T	T	T
0.8758263144178747	0.9445532469060790	0.9837978703689433	T	T	T
0.9324370495022618	0.9697160454402387	0.2001342699186968	T	T	T
0.8153387988306845	0.9298811507273759	0.3297589999993404	T	T	T
0.5774953895654616	0.1715277490724013	0.3273530895436569	T	T	T
0.7007043777585376	0.1306841499511576	0.2027320376037735	T	T	T
0.7329474370109663	0.1688576811676433	0.9837192094267372	T	T	T
0.8900412908867936	0.1750832426939037	0.9805903172193614	T	T	T
0.9352260609276264	0.1281426622078360	0.2004435740138583	T	T	T
0.8213080970860153	0.1778209567836352	0.3349936787255903	T	T	T
0.9175019265347584	0.0640129123491743	0.8426096129413496	T	T	T
0.8041825562571965	0.0339841286112074	0.6990704154941745	T	T	T
0.7817105699981568	0.0553787292095891	0.4722028829466979	T	T	T
0.6217725133227233	0.0663391155352487	0.4851116434755511	T	T	T
0.5675015740872853	0.0322351117217455	0.6970206460940362	T	T	T
0.6832951673505979	0.0689145801939973	0.8283150826111784	T	T	T
0.9149512798301099	0.8291914866262949	0.8292126812421982	T	T	T
0.7949712356756421	0.8764886028467640	0.7034539213262884	T	T	T

Structure files (CONTCAR) involved in this work:

0.7653501386765171	0.8283893605115833	0.4870571877493720	T	T	T
0.6073861020106917	0.8242075167109348	0.4873603621737490	T	T	T
0.5618719705774550	0.8740128449553319	0.7017128870701914	T	T	T
0.4194917469517752	0.4415527031761601	0.6442522138940989	T	T	T
0.3001471559317995	0.4707849070590943	0.7879520612351835	T	T	T
0.2797068001403156	0.4338004328059831	0.0088098741558071	T	T	T
0.1204606042129157	0.4328752503015717	0.0082220731608761	T	T	T
0.0689123947408485	0.4711710462196163	0.7975589471045988	T	T	T
0.1769710883033709	0.4450657716314375	0.6480403392406294	T	T	T
0.4185443198978669	0.6705179795962896	0.6647294062679671	T	T	T
0.3018459056435900	0.6272801585113874	0.8060924483238366	T	T	T
0.2672748321450246	0.6692685047019582	0.0263551951946712	T	T	T
0.1131362194799836	0.6713423230234020	0.0141160899973419	T	T	T
0.0640613758538431	0.6299867337112122	0.7997434758039154	T	T	T
0.1816560167921943	0.6671789241447329	0.6676715135163517	T	T	T
0.0746684529579186	0.5540841865882373	0.1437782031671797	T	T	T
0.1960218690522801	0.5246357341018050	0.2856817359481743	T	T	T
0.2181484997188237	0.5611240579486771	0.5064540401720224	T	T	T
0.3777435272899161	0.5647342093313849	0.5087995977764438	T	T	T
0.4303482241473441	0.5252254537733971	0.2990938664861899	T	T	T
0.3217940437964978	0.5505554453046909	0.1481146589557628	T	T	T
0.0782517558470436	0.3254339374660423	0.1620060097329642	T	T	T
0.1948301218047314	0.3671681385120044	0.3053220298058105	T	T	T
0.2290474568312942	0.3256816577922902	0.5238609209123944	T	T	T
0.3842168882638042	0.3232392102748992	0.5106521518922719	T	T	T
0.4340218320120729	0.3682301825781639	0.2996816993623432	T	T	T
0.3169010994186912	0.3268023115830078	0.1695505644027532	T	T	T
0.3562610266861139	0.0570770449829627	0.7133143794543747	T	T	T
0.2971005733298019	0.0688195642895772	0.8883296803888844	T	T	T
0.1982187296203063	0.0509964454181929	0.0208189459784741	T	T	T
0.0975216642676875	0.0614150986924258	0.8911762327271133	T	T	T
0.0985251703726089	0.0465578468053500	0.6953556975150675	T	T	T
0.2270489807384232	0.0283678817043129	0.7323614374775900	T	T	T
0.3579474946391569	0.8284324970474455	0.7417974131195039	T	T	T
0.3014642841729918	0.8365213566660912	0.9168952232227138	T	T	T
0.1894778778440060	0.8510401448348861	0.0208318224262588	T	T	T
0.0893595697808111	0.8230042385104395	0.8991563309735480	T	T	T
0.1054786116952646	0.8341514369958297	0.7006707246432430	T	T	T
0.2289021520010619	0.8571821085301158	0.7537511961351278	T	T	T
0.3182509554200840	0.9475104882634716	0.8105976257538524	T	T	T
0.0764859291453533	0.9404783908469472	0.8136888980446140	T	T	T
0.4281548074155336	0.1213218949353846	0.5778243287478425	T	T	T
0.4175583293897635	0.9890161267208962	0.5653578332989770	T	T	T
0.3937790101938898	0.8571232304545957	0.5554627885284672	T	T	T
0.1871604865887976	0.1248862726301664	0.6063715313496899	T	T	T
0.1764021531773318	0.9959802625470174	0.5549689552784286	T	T	T
0.1952609058968365	0.8625793714637274	0.5600657172854833	T	T	T
0.9843988361423751	0.0328353204882322	0.7935070634313826	T	T	T
0.9873853423738657	0.8411792295417696	0.7788325202340601	T	T	T
0.1411683270161654	0.9355975772184563	0.2149059408173768	T	T	T
0.1994781735176706	0.9279954501815029	0.3897503293050239	T	T	T
0.2965894283764517	0.9460621367545187	0.5246492460683874	T	T	T
0.3940703868328757	0.9277674041968617	0.3907477761268378	T	T	T

Structure files (CONTCAR) involved in this work:

0.3948422892563790	0.9468845319686203	0.1928191581280772	T	T	T
0.2684674422823570	0.9693473827583206	0.2322716176597144	T	T	T
0.1419903402609198	0.1677600957173663	0.2347698252154664	T	T	T
0.1923540429777247	0.1592010228719906	0.4147121364451701	T	T	T
0.3045239938182476	0.1445568072801632	0.5178218144137503	T	T	T
0.4062397436656137	0.1702013620243302	0.3952136732411299	T	T	T
0.3939881385050352	0.1545349315003084	0.1993424160486958	T	T	T
0.2694832920639839	0.1372714489025459	0.2558492966359130	T	T	T
0.1757035349862888	0.0484535839020682	0.3079211961118822	T	T	T
0.4120746077010287	0.0487669994652904	0.3193724576181283	T	T	T
0.0657632029908563	0.8724066893327099	0.0825038886691329	T	T	T
0.0790393431937287	0.0039070524208346	0.0673641602780114	T	T	T
0.0965225455653602	0.1349466821391520	0.0543397419219572	T	T	T
0.3054006723872049	0.8695487168264434	0.1096101473829383	T	T	T
0.3165425255560473	0.9971567065996398	0.0516111909357921	T	T	T
0.3007399966945303	0.1311124987986202	0.0614484799960538	T	T	T
0.5060671289489517	0.9556649648900070	0.2878146446489624	T	T	T
0.5114159405173078	0.1336918118026321	0.2845384021553825	T	T	T
0.6367248947540894	0.5711168295287821	0.2756141598653606	T	T	T
0.6788002459651754	0.5451178743410452	0.0929570302012251	T	T	T
0.7944556480780536	0.5389434668700320	0.9928038306168098	T	T	T
0.9027631723517094	0.5693517951793303	0.1027210530650463	T	T	T
0.8928513591517225	0.5526502566985380	0.2993465979043866	T	T	T
0.7677577779875721	0.5505071587092857	0.2356324970478617	T	T	T
0.6393423202576956	0.3243362312502387	0.2475234304862096	T	T	T
0.7029901664578823	0.3654588367608060	0.0879759943829840	T	T	T
0.8092397433462311	0.3496709112032063	0.9765153161231176	T	T	T
0.9063020152032776	0.3266005738335119	0.1096280838083503	T	T	T
0.8979971496292501	0.3466694246369200	0.3049268699667722	T	T	T
0.7699226434298616	0.3514079949564607	0.2578606918881017	T	T	T
0.6804464427843301	0.4497461947140998	0.2355849266372236	T	T	T
0.9168278384620550	0.4489473810796829	0.1782337693374806	T	T	T
0.5566681698939384	0.6230685953249907	0.4187233751307625	T	T	T
0.5929203481198729	0.4954535606096512	0.4275015544617921	T	T	T
0.6038330468470513	0.3623201107062167	0.4296058835477752	T	T	T
0.8061358923124807	0.6390179361326260	0.3728126245472725	T	T	T
0.7970347281869569	0.5062237436852985	0.4158716943578431	T	T	T
0.8097339039255684	0.3755393959762486	0.4468670276442379	T	T	T
0.0096626785415116	0.5427883133400249	0.2141384218327411	T	T	T
0.0143966071204964	0.3616767877938307	0.2146082054672548	T	T	T
0.8599878295752714	0.4317508164124382	0.7829622626576932	T	T	T
0.8161159269753976	0.4573397347568609	0.5995749558876396	T	T	T
0.7006144326448223	0.4385914132139878	0.5058538685382484	T	T	T
0.5841258116248470	0.4260267682639671	0.5956576804790936	T	T	T
0.6014426171296922	0.4280810398300124	0.7917402696937101	T	T	T
0.7302917708070068	0.4368910536624608	0.7449493515709358	T	T	T
0.8488578856849968	0.6738565549305818	0.7397488373306776	T	T	T
0.7902644024650897	0.6174237834192111	0.5802912325464047	T	T	T
0.6805162151293068	0.6541592794328969	0.4663895204697659	T	T	T
0.5845169813567919	0.6630251793915385	0.6051297362362141	T	T	T
0.5951894345957692	0.6501581555349175	0.8042164050125368	T	T	T
0.7198688207854714	0.6505814944418173	0.7427772853367992	T	T	T
0.8037957224242855	0.5485678129253103	0.7491570523212013	T	T	T

Structure files (CONTCAR) involved in this work:

0.5808417686835686	0.5423045398332342	0.6921145562321300	T	T	T
0.9333899802622730	0.3804048952381529	0.9300370643106081	T	T	T
0.9150277240591342	0.5112390514151766	0.9241928895977081	T	T	T
0.8809509273231617	0.6374546101846941	0.9402679650121524	T	T	T
0.6893993248717534	0.3581748059541313	0.8935101596763274	T	T	T
0.6825847082584459	0.4920763996834812	0.9114362864052954	T	T	T
0.6962060713633547	0.6230740083805317	0.9378959624307832	T	T	T
0.4832262956378242	0.4517598492412748	0.7177090207373020	T	T	T
0.4799127960523891	0.6289800095834267	0.7157098208705895	T	T	T
0.6345655045065933	0.9378834584283957	0.2729960725539670	T	T	T
0.6808535513887702	0.9716760387045479	0.0917788281373172	T	T	T
0.7948060457886457	0.9321683478655050	0.0064949500984377	T	T	T
0.9135484148178230	0.9422456348214866	0.0893126076066103	T	T	T
0.8907299047993353	0.9286368968058085	0.2838690692199251	T	T	T
0.7638047953126054	0.9361610920666532	0.2342844841234685	T	T	T
0.6341583119795519	0.1693662450566109	0.2401012110012854	T	T	T
0.7035842272947145	0.1304643615868703	0.0816472164221998	T	T	T
0.8120577478950817	0.1522462702613287	0.9716333374576394	T	T	T
0.9150106379639407	0.1605978391100198	0.0935248015096039	T	T	T
0.8963244972858141	0.1664931985664767	0.2903735227820352	T	T	T
0.7678971296273738	0.1669481104378197	0.2441268075449322	T	T	T
0.6980943091876931	0.0536050097288978	0.2442170273950814	T	T	T
0.9146430051148877	0.0490570583152626	0.2049086445591324	T	T	T
0.5641524693599692	0.8749187787583713	0.4166358084619627	T	T	T
0.5837657441486500	0.0053470738285167	0.4289034888600571	T	T	T
0.6052850278540517	0.1365833682656604	0.4287214384839281	T	T	T
0.8038093564151488	0.8607783563935428	0.3894011984211175	T	T	T
0.8066782040063946	0.9956706213612598	0.3993358196427682	T	T	T
0.8060019989695498	0.1270099956154730	0.4267679988256151	T	T	T
0.0110174558863117	0.9533835621898999	0.2182872819182053	T	T	T
0.0155267899516339	0.1345615161281574	0.2152522993590367	T	T	T
0.8624770938883292	0.0762325931950204	0.7561769723713362	T	T	T
0.8157617382474178	0.0449806059902803	0.5807868154846325	T	T	T
0.7014133574847479	0.0528992710092317	0.4839680011856149	T	T	T
0.5946637258341746	0.0718670607195426	0.5987592157331841	T	T	T
0.6058509649883413	0.0624027432016517	0.7951739431770083	T	T	T
0.7314895437917702	0.0645881602410446	0.7309250439182040	T	T	T
0.8609081643643420	0.8346554373105884	0.7407579560297171	T	T	T
0.7886387035769390	0.8737989696642895	0.5830469119738662	T	T	T
0.6855836661237720	0.8415151271165001	0.4687256768855545	T	T	T
0.5892058647038454	0.8335994216483813	0.6045333210709125	T	T	T
0.5919004740130577	0.8432582611580037	0.8032117876540582	T	T	T
0.7310204124334082	0.8478995310886940	0.7609342568243603	T	T	T
0.8089004838348720	0.9557081177589563	0.7328978349317435	T	T	T
0.5833898043504517	0.9528039012445993	0.6873159583423800	T	T	T
0.9349309827616749	0.1335753148657748	0.9001178778538252	T	T	T
0.8849165224403008	0.0151698422919757	0.9281305050978627	T	T	T
0.9026294515947003	0.8837431701375993	0.9167812571218681	T	T	T
0.6935852866254283	0.1395105526093965	0.8869505948014430	T	T	T
0.7035044060619646	0.0063786730001706	0.9026062522813664	T	T	T
0.6891417225505077	0.8743428588136937	0.9587086161644361	T	T	T
0.4879381943500956	0.0454220698929318	0.7117617656571622	T	T	T
0.4804152220214862	0.8694430362296537	0.7050606292764496	T	T	T

Structure files (CONTCAR) involved in this work:

0.3528151536747248	0.4361136486270197	0.7122111875415998	T	T	T
0.2982550181287071	0.4277123233861836	0.8911229807616219	T	T	T
0.1998748734063520	0.4451363323527965	0.0247563995566095	T	T	T
0.1022687110623764	0.4302290396806724	0.8905249242223982	T	T	T
0.1018109414770420	0.4461806862778058	0.6930854338700650	T	T	T
0.2268250679619958	0.4700714882111851	0.7365212351156040	T	T	T
0.3561707374007372	0.6688796639381478	0.7418063356177870	T	T	T
0.3013400752456402	0.6582087703284497	0.9178753524471667	T	T	T
0.1897077843106674	0.6445477947204106	0.0230897597388269	T	T	T
0.0904449515646124	0.6703776081388664	0.8985144808201786	T	T	T
0.1044955632894153	0.6581137003900156	0.7022056333133099	T	T	T
0.2285960332308405	0.6354811989444609	0.7552906931139532	T	T	T
0.3219112212926278	0.5481003379273663	0.8102688925332622	T	T	T
0.0814689250021209	0.5506681448147615	0.8159357489964763	T	T	T
0.4280850882724456	0.3719255291198709	0.5821348966337943	T	T	T
0.4167978272878372	0.5040894701130012	0.5658150705731700	T	T	T
0.3973790408243967	0.6364228035416258	0.5588434374908987	T	T	T
0.1945934883444840	0.3692867034841241	0.6121160980801572	T	T	T
0.1808922993158597	0.4955915185342009	0.5528320415756142	T	T	T
0.1942048431121903	0.6294683433615126	0.5617566183248157	T	T	T
0.9899557053940087	0.4539094057495978	0.7881287521192284	T	T	T
0.9859817063071280	0.6426986815022676	0.7850468573822394	T	T	T
0.1406390613548192	0.5587654526870490	0.2133819941855343	T	T	T
0.1981545522871011	0.5669111759254611	0.3892959647348190	T	T	T
0.2981298566955632	0.5512095832092437	0.5203495005711338	T	T	T
0.3989053320010504	0.5673529997991875	0.3920892454545369	T	T	T
0.3963014389615040	0.5496489354954543	0.1951697938378240	T	T	T
0.2690469337832083	0.5270711028953756	0.2335499772219751	T	T	T
0.1404430156796924	0.3268554894742543	0.2390487651110112	T	T	T
0.1912432441405930	0.3378078506789698	0.4180370402145991	T	T	T
0.3067481173485864	0.3484591634502873	0.5111217535706063	T	T	T
0.4133100340355499	0.3248733983112637	0.3976527540264735	T	T	T
0.3943184461554319	0.3388988612334370	0.2026522952768996	T	T	T
0.2690451791058796	0.3557464681127685	0.2584141230821180	T	T	T
0.1763120175874121	0.4466449548845585	0.3063819665195590	T	T	T
0.4140521019884871	0.4461551609270863	0.3186035708887744	T	T	T
0.0651618039369341	0.6245143422417017	0.0832020028595384	T	T	T
0.0798540389070566	0.4934636659740482	0.0626940684400772	T	T	T
0.0981715932356441	0.3618061434319238	0.0575575564863853	T	T	T
0.3064609132001741	0.6265254927145322	0.1108198532272783	T	T	T
0.3187282877877319	0.4986322142846336	0.0542669747976186	T	T	T
0.3022338284325899	0.3649022882415630	0.0644388050220280	T	T	T
0.5098758959021469	0.5372249714685350	0.2870917346078006	T	T	T
0.5139458142237420	0.3621961927224749	0.2798846971028869	T	T	T
0.4396803654144417	0.7479125566058291	0.6437977767684906	T	T	T
0.1997604316799280	0.7458634940187202	0.6507908800331070	T	T	T
0.2712721529404034	0.7478397116176899	0.0575652713557558	T	T	T
0.1066934648984326	0.7476983469801998	0.0574577698145943	T	T	T
0.0597395472947534	0.2482408331706256	0.1354898319662595	T	T	T
0.3027556028899741	0.2474358277088496	0.1524603494228722	T	T	T
0.2229220050422529	0.2473340498858599	0.5561739378923242	T	T	T
0.3885972460659287	0.2467432006124940	0.5528328234937067	T	T	T
0.5592006082305131	0.2484340747055083	0.3551905488131724	T	T	T

Structure files (CONTCAR) involved in this work:

0.8152312746453426	0.2538461268346686	0.3768461514529560	T	T	T
0.7206609684279798	0.2488613504594916	0.9940993320690932	T	T	T
0.8987814209307926	0.2530233265051584	0.9497266638313072	T	T	T
0.9117932470924165	0.7551800517253338	0.8858587136438791	T	T	T
0.6789908130243947	0.7407098799229351	0.8868749865185326	T	T	T
0.5862810862642901	0.7489385942777594	0.4549134876104381	T	T	T
0.7945631248747936	0.6747257768891749	0.0870562735846030	T	T	T
0.7155162516043122	0.7730430860747973	0.1033163067656266	T	T	T
0.8456687776962620	0.7963191558461461	0.0881123713403851	T	T	T
0.7844347418920514	0.7517481331037636	0.5001709722633666	T	T	T
0.9114335330412154	0.6733923366615505	0.8250425546191558	T	T	T
0.6708449992813488	0.8274124338806602	0.8471434140067847	T	T	T
0.7656193799430113	0.6676276789146008	0.4802944501303854	T	T	T
0.7159362308747659	0.7030998364650599	0.0201198176668942	T	T	T
0.7666507216083063	0.8375075532698307	0.0523732285441809	T	T	T
0.8609641338904461	0.7211450697240301	0.0077295841799279	T	T	T
0.9495140296682490	0.7784504320047732	0.2001355780115003	T	T	T
0.9251611987178142	0.7456735180940763	0.2936402615898401	T	T	T
0.9012036917089551	0.7977402887969154	0.1526710608440151	T	T	T
0.9773100421149271	0.8254252121711394	0.2101180608180713	T	T	T
0.9754457857279488	0.7449957668268216	0.1474214206720088	T	T	T
0.8997705160019357	0.7810010453771824	0.3438807578510057	T	T	T
0.9685516351171560	0.7248480157882662	0.3349965194222179	T	T	T
0.8920161061038192	0.7024435647502097	0.2807379604853075	T	T	T
0.7929571037815425	0.6998352787422869	0.1508915900437103	T	T	T

Figure 5(b) TS3

Si O Al Cu C H

1.0000000000000000

20.0219993591000005 0.0000000000000000 0.0000000000000000

0.0000000000000000 19.8990001678000006 0.0000000000000000

0.0000000000000000 0.0000000000000000 13.3830003737999998

93 195 3 3 2 7

Selective dynamics

Direct

0.4219098596007571	0.0525723017530670	0.6393540218462094	T	T	T
0.3018048977782843	0.0245392309411322	0.7845504374972383	T	T	T
0.2809967259701177	0.0631292758233119	0.0038540886624327	T	T	T
0.1216596027205518	0.0636759788479344	0.0045300613956942	T	T	T
0.0697983855216141	0.0242361810278870	0.7950730227599122	T	T	T
0.1780716659918906	0.0493186472829329	0.6437220795494046	T	T	T
0.4244166996902389	0.8251478514061431	0.6645342533455401	T	T	T
0.3033150535468599	0.8674993159520498	0.8021641924014544	T	T	T
0.2701963898755433	0.8261357461978834	0.0247433436870318	T	T	T
0.1159456342192108	0.8237860482166169	0.0173592392622840	T	T	T
0.0672743720824196	0.8658270690773866	0.8044247801683994	T	T	T
0.1803107050330832	0.8263863452921330	0.6649117593197886	T	T	T
0.0759244018049421	0.9427500797733374	0.1420154761567025	T	T	T
0.1979883246823822	0.9699551746253101	0.2847258757973477	T	T	T
0.2187949554288285	0.9312714630033335	0.5053936543381342	T	T	T
0.3780678978127966	0.9274057675380658	0.5089574148358974	T	T	T
0.4289374904328091	0.9691392169863075	0.3014379830423894	T	T	T
0.3240286075799110	0.9466036051525674	0.1434422641148934	T	T	T
0.0776044618185815	0.1684909746434307	0.1602338161010615	T	T	T

Structure files (CONTCAR) involved in this work:

0.1956294541164078	0.1273878594460514	0.3038454147520583	T	T	T
0.2294346176790060	0.1699815526595083	0.5220348364933872	T	T	T
0.3840943318220475	0.1717108684783326	0.5085919605023357	T	T	T
0.4331937671040965	0.1256400558157792	0.3001649697684217	T	T	T
0.3180125441114230	0.1675037375859302	0.1664094006299106	T	T	T
0.5749782371965385	0.5552172167034136	0.3586120079386400	T	T	T
0.6939257712014509	0.5273131127052371	0.2187408475197445	T	T	T
0.7109318780527338	0.5467934860808750	0.9895502468624549	T	T	T
0.8694159066190420	0.5670863829215752	0.9948242255658831	T	T	T
0.9292608718367007	0.5265471333302711	0.2011993095925993	T	T	T
0.8174087134869356	0.5631078538260866	0.3417981082675633	T	T	T
0.5795592453350793	0.3246346946331987	0.3289320766690025	T	T	T
0.7035260440983787	0.3697656994251445	0.2134358673449045	T	T	T
0.7303752504482606	0.3255728503732934	0.9919403930928785	T	T	T
0.8873535887687236	0.3281104321223491	0.9951421280719857	T	T	T
0.9336140662391981	0.3696502306000082	0.2050547644551643	T	T	T
0.8262007249326021	0.3287697277102968	0.3534891766925431	T	T	T
0.9226179783870904	0.4472152823116147	0.8621776773321020	T	T	T
0.8018112552750571	0.4672290719202196	0.7233948306248248	T	T	T
0.7809166587720417	0.4438807400263273	0.4964636199983832	T	T	T
0.6209987897597526	0.4288362763090763	0.4917425222442169	T	T	T
0.5633181028230502	0.4605911223385857	0.7011893962070594	T	T	T
0.6757708052066314	0.4258069369481856	0.8412329113498098	T	T	T
0.7925175843593313	0.6220962504590817	0.7075863460097518	T	T	T
0.6076858830506127	0.6722378498825956	0.4882158733129276	T	T	T
0.5621515266877110	0.6184670162874589	0.7004759491590419	T	T	T
0.6683622281950620	0.6658891179360249	0.8414575680276922	T	T	T
0.5757470547451570	0.9418701115781385	0.3574566353319974	T	T	T
0.6948664879775140	0.9712157581787418	0.2158005098124479	T	T	T
0.7171095675671133	0.9496077364277220	0.9897367677518921	T	T	T
0.8740807165236935	0.9492948691576182	0.9839698386463090	T	T	T
0.9300423188329915	0.9668182401801579	0.1960545677371634	T	T	T
0.8178544855113052	0.9301533860736854	0.3359312519017228	T	T	T
0.5797599989493131	0.1701017480927170	0.3224888802313867	T	T	T
0.7038914179129225	0.1276670458265073	0.2086120783417202	T	T	T
0.7358252248542122	0.1669526709146975	0.9870675315659813	T	T	T
0.8930685977224481	0.1780429206884831	0.9757102079847969	T	T	T
0.9327687181989289	0.1247267792520070	0.1940814301082255	T	T	T
0.8251880532703739	0.1738458916635958	0.3456393603189116	T	T	T
0.9260570563465396	0.0632340481193457	0.8462438723174815	T	T	T
0.8032472408553216	0.0284198293794329	0.7116729536267491	T	T	T
0.7850417844317358	0.0538841802694455	0.4837897892908442	T	T	T
0.6246408194436163	0.0681188138701106	0.4853836304718896	T	T	T
0.5671143453248757	0.0351254468458113	0.6946340619601334	T	T	T
0.6783677920917532	0.0639753919988577	0.8359621002230443	T	T	T
0.9133506310508248	0.8324749373289840	0.8319050471283319	T	T	T
0.7973756746427639	0.8713465995434385	0.7044164333321157	T	T	T
0.7683559968444231	0.8275496706944842	0.4888222091834689	T	T	T
0.6107690553374513	0.8239486069654754	0.4933619252817583	T	T	T
0.5686456818004266	0.8767191469351818	0.7067802981875428	T	T	T
0.4190333870975754	0.4421579171473747	0.6466683949936839	T	T	T
0.2986695958949135	0.4710235554408165	0.7888176720211346	T	T	T
0.2795665981448379	0.4336448154092221	0.0106814180732639	T	T	T

Structure files (CONTCAR) involved in this work:

0.1210659354695236	0.4313819846819670	0.0102841312095993	T	T	T
0.0691491444379218	0.4707728843651060	0.8011924779387811	T	T	T
0.1750410857866722	0.4452481041067506	0.6484129800765542	T	T	T
0.4194624128410292	0.6696280042968639	0.6652232612492397	T	T	T
0.3017272841098219	0.6278700642790722	0.8058106535756783	T	T	T
0.2698804181060958	0.6698234955815247	0.0289803747622415	T	T	T
0.1161628967880659	0.6710827893364650	0.0171132148290654	T	T	T
0.0658378191213837	0.6301040592355666	0.8043158247185287	T	T	T
0.1801173250019067	0.6679813825458876	0.6662561368988358	T	T	T
0.0742295674941486	0.5531294304131049	0.1429153876678647	T	T	T
0.1958914325839415	0.5245658836856545	0.2850074563061604	T	T	T
0.2159688835644258	0.5612467134777089	0.5067597628569452	T	T	T
0.3753594987355761	0.5650273732869286	0.5110603259821017	T	T	T
0.4299015976736655	0.5248971018489321	0.3030561994961434	T	T	T
0.3233268610372913	0.5506483467984146	0.1486340705802489	T	T	T
0.0781423959377714	0.3235792315101064	0.1624751012309824	T	T	T
0.1954468232609353	0.3664900161063606	0.3044594832141675	T	T	T
0.2293986706476895	0.3265362079196353	0.5241730237575095	T	T	T
0.3844645976295512	0.3239686978752608	0.5124292500979046	T	T	T
0.4344605752786547	0.3684825314366904	0.3022197906239288	T	T	T
0.3186632415314535	0.3267745336283946	0.1694814847192132	T	T	T
0.3562787036711229	0.0571603160590338	0.7098195861913813	T	T	T
0.2996106541015306	0.0691735659816732	0.8862651729092115	T	T	T
0.2010810889288061	0.0510093905513925	0.0187294067871666	T	T	T
0.1016662006517708	0.0669284247957380	0.8872788345240414	T	T	T
0.1031282610501700	0.0462137217738331	0.6897217765881906	T	T	T
0.2289279977071915	0.0259833731100988	0.7315980006546181	T	T	T
0.3618751538769563	0.8295081755511029	0.7417013935876011	T	T	T
0.2991180016291604	0.8346533610801786	0.9126385450472392	T	T	T
0.1922658784918673	0.8503436503047963	0.0293832472198700	T	T	T
0.0958040168131006	0.8252556313020439	0.9004636156644900	T	T	T
0.1039846269468136	0.8377523922773823	0.7043610076814416	T	T	T
0.2315094698299469	0.8580188932014777	0.7468116911923413	T	T	T
0.3205362901483493	0.9471236408864895	0.8109976189893725	T	T	T
0.0827757904727155	0.9452767135351179	0.8186756555321909	T	T	T
0.4293707132888468	0.1216111837793143	0.5755042630236290	T	T	T
0.4172307149399935	0.9894121478748108	0.5623532971580283	T	T	T
0.4021797576969441	0.8566851376882034	0.5570486186549444	T	T	T
0.1928271032895923	0.1256025441185081	0.6075450126688370	T	T	T
0.1827433868690052	0.9984963330126070	0.5488663366974107	T	T	T
0.1892923566770968	0.8638502214501139	0.5577977578627108	T	T	T
0.9905894601684659	0.0394502832672541	0.7830143096171849	T	T	T
0.9877429455968366	0.8540107197471676	0.7964196539098882	T	T	T
0.1397599111092768	0.9377613775893440	0.2153809264743352	T	T	T
0.2029765919235493	0.9260956379422518	0.3866743630867889	T	T	T
0.2983357421710417	0.9374624991412310	0.5271201232646721	T	T	T
0.3939702802327471	0.9256244063603084	0.3901349353598949	T	T	T
0.3974208551009907	0.9489820621318061	0.1938811821768154	T	T	T
0.2687786510196355	0.9674009636328629	0.2267899778156628	T	T	T
0.1389043686449515	0.1648962622727499	0.2384366505895403	T	T	T
0.1929994631837089	0.1596482426502031	0.4147424677871307	T	T	T
0.3068378450703160	0.1459564513223944	0.5119700390589467	T	T	T
0.4101375834719992	0.1721599772608348	0.3937649085774528	T	T	T

Structure files (CONTCAR) involved in this work:

0.3946503618629750	0.1513168417590785	0.1997886403399956	T	T	T
0.2686872739943219	0.1385704705881309	0.2534930773333474	T	T	T
0.1793881547116589	0.0475003753529924	0.3099880842614989	T	T	T
0.4142436831709557	0.0480802336262783	0.3248694300742712	T	T	T
0.0665799877720632	0.8713087772499455	0.0835720496197819	T	T	T
0.0823447670139260	0.0023664649593115	0.0597800691811530	T	T	T
0.0991545870905480	0.1344116786784380	0.0546150548217971	T	T	T
0.3122893876048390	0.8707476014620307	0.1034197852556400	T	T	T
0.3206646139004254	0.9991476523032138	0.0505816269718509	T	T	T
0.3024734769012694	0.1322766398599432	0.0593803214568222	T	T	T
0.5081334588071523	0.9542299758338025	0.2935365721617367	T	T	T
0.5132530536650729	0.1315176862211468	0.2828259802158622	T	T	T
0.6371556025981630	0.5664160399265001	0.2816569878082008	T	T	T
0.6797017593998831	0.5408762382169617	0.1004859445337812	T	T	T
0.7915052367441003	0.5449226816244419	0.9926232379778900	T	T	T
0.8976088731639237	0.5690487468109183	0.1085495022040099	T	T	T
0.8942905826792988	0.5507040757643664	0.3039723035599743	T	T	T
0.7682891617533869	0.5558575251487730	0.2435249179067842	T	T	T
0.6394868028534666	0.3259383087011158	0.2473068649483545	T	T	T
0.7095899041757485	0.3647058741969242	0.0933700574662889	T	T	T
0.8088838186960262	0.3415258640856922	0.9722472527769812	T	T	T
0.9017337900000810	0.3253882631852165	0.1147780703735110	T	T	T
0.9002676538255084	0.3467269257465307	0.3099729739197789	T	T	T
0.7713683299535103	0.3423279145129255	0.2655508439618453	T	T	T
0.6909864896297488	0.4476618262527143	0.2451038683275385	T	T	T
0.9161423076071461	0.4476668193767041	0.1803883313251862	T	T	T
0.5593172026800730	0.6225831643040222	0.4220771866603220	T	T	T
0.5906328467710963	0.4931949707512808	0.4336452979822077	T	T	T
0.6045224373100990	0.3599006130350941	0.4315653689666767	T	T	T
0.8132866365070806	0.6387484684347162	0.3832477189313044	T	T	T
0.7981694223950163	0.5061200715328158	0.4229847067927507	T	T	T
0.8113165701571516	0.3745076148386862	0.4506540316882438	T	T	T
0.0082057385972959	0.5437825946591390	0.2121202964569230	T	T	T
0.0140224960603665	0.3607472353794511	0.2129618782904281	T	T	T
0.8606538804314101	0.4309129704888551	0.7882492572594066	T	T	T
0.8148069764203067	0.4549339548731778	0.6052903634326121	T	T	T
0.7006953291857245	0.4372322930627644	0.5062620532442699	T	T	T
0.5856876304078980	0.4219773695343513	0.5999831940373235	T	T	T
0.6008398820803025	0.4262985562679757	0.7960869943674644	T	T	T
0.7303712682029250	0.4328140690820679	0.7522563592974995	T	T	T
0.8514311854189608	0.6693324631729829	0.7472603368684489	T	T	T
0.7868766740434221	0.6177878276690368	0.5894682449317651	T	T	T
0.6835822685217958	0.6577848417933619	0.4610786098700946	T	T	T
0.5914735701789954	0.6596161871114785	0.6068370840154835	T	T	T
0.5933291658388676	0.6488826840728207	0.8045448987071353	T	T	T
0.7213417695221193	0.6489628205224721	0.7565594010589715	T	T	T
0.8018512750833788	0.5458175287024257	0.7543699514802396	T	T	T
0.5831587203697938	0.5396583949222115	0.6928299716291854	T	T	T
0.9315269614973536	0.3864966892965692	0.9428273831899286	T	T	T
0.9122505434219687	0.5167002878066467	0.9251923306309845	T	T	T
0.8815325591577006	0.6434546958686301	0.9524864022655154	T	T	T
0.6863575367419803	0.3554897789282979	0.9006180833794791	T	T	T
0.6822793251853224	0.4892360569001267	0.9179602739088509	T	T	T

Structure files (CONTCAR) involved in this work:

0.6832112596956571	0.6208375216738309	0.9474714680078281	T	T	T
0.4834821787429086	0.4519181796050291	0.7187575293968754	T	T	T
0.4814405629273702	0.6254135040458846	0.7083903058073806	T	T	T
0.6370413016976364	0.9333445221745442	0.2783988178596461	T	T	T
0.6811946501950300	0.9634777643907658	0.0967563480285340	T	T	T
0.7962348816596305	0.9686477963323741	0.9986645897264987	T	T	T
0.9052156772106441	0.9284616417976526	0.0934149249388611	T	T	T
0.8936630907056119	0.9313104582242290	0.2904491598826517	T	T	T
0.7667783120459205	0.9359377148754522	0.2402977840597897	T	T	T
0.6345709350610380	0.1669156586779980	0.2322256411517696	T	T	T
0.7196135094340727	0.1270708270290590	0.0900418291733806	T	T	T
0.8145138531759262	0.1599494415749299	0.9588113064377499	T	T	T
0.9113283267077290	0.1617591268865686	0.0912728677826588	T	T	T
0.8960348631875189	0.1592245319413749	0.2892329548929298	T	T	T
0.7649413556568280	0.1648004911822031	0.2654429207881554	T	T	T
0.6974962950139828	0.0502518505800419	0.2473438629032831	T	T	T
0.9108189160679715	0.0457802628100473	0.1881503972864323	T	T	T
0.5662427447371513	0.8758702427081749	0.4264602906447771	T	T	T
0.5887710948296082	0.0058424776373741	0.4295458338028454	T	T	T
0.6101119927349830	0.1366981777046229	0.4234023718410652	T	T	T
0.8085721677406290	0.8590377138944862	0.3918483711508673	T	T	T
0.8074001708865398	0.9935286896639837	0.4096549758677091	T	T	T
0.8151693811696099	0.1239874594077779	0.4402520962249087	T	T	T
0.0095468992907077	0.9549355562863846	0.2095648338882646	T	T	T
0.0133015499838233	0.1299373337668303	0.2083676948099502	T	T	T
0.8618280177985268	0.0666113833708020	0.7737835756138510	T	T	T
0.8164303753499558	0.0413517357941916	0.5938201691791981	T	T	T
0.7045361724050540	0.0562916706059220	0.4919252740332232	T	T	T
0.5931514802561951	0.0755829137264387	0.5962429910429686	T	T	T
0.6031026689678854	0.0677899626528703	0.7923625913055697	T	T	T
0.7312000088488922	0.0598782365285013	0.7435685272230502	T	T	T
0.8679305930503777	0.8335660681465803	0.7320948082468600	T	T	T
0.7883456109983789	0.8746467106396351	0.5841001286663626	T	T	T
0.6887575142733440	0.8372806075062184	0.4658962951718647	T	T	T
0.5987862666570681	0.8345127762649683	0.6123733262415659	T	T	T
0.6010859441033737	0.8537300163053514	0.8110544382573927	T	T	T
0.7372360158342830	0.8348104672526987	0.7604007570718517	T	T	T
0.8054233428687391	0.9497049195661660	0.7420511237135858	T	T	T
0.5846411023514353	0.9560371605488711	0.6837053601352387	T	T	T
0.9388041171370451	0.1361498846241930	0.8971922352234293	T	T	T
0.9153036811607987	0.0121272459833991	0.9404434726715645	T	T	T
0.8829025837137913	0.8834570901156839	0.9155558392446009	T	T	T
0.6919203903142206	0.1321323079759283	0.8997433582341792	T	T	T
0.6836669366892776	0.9961885856444643	0.9046900751000342	T	T	T
0.7095298417027994	0.8689665315819441	0.9641652335900819	T	T	T
0.4872519403191584	0.0453125097380324	0.7096524608962231	T	T	T
0.4873907717631477	0.8659019912436001	0.7101942918423825	T	T	T
0.3528072776215967	0.4360411654206348	0.7156379130362120	T	T	T
0.2950569721215249	0.4282233866386734	0.8921191305637898	T	T	T
0.1999559189737002	0.4442796783579827	0.0311502550369721	T	T	T
0.1052693946915873	0.4296584086538925	0.8918469364486431	T	T	T
0.1002256578654859	0.4458463975503144	0.6952525095763079	T	T	T
0.2259942887235029	0.4702548003938740	0.7353791602561206	T	T	T

Structure files (CONTCAR) involved in this work:

0.3593158190287755	0.6683202945550275	0.7463426405753909	T	T	T
0.2986338588069405	0.6585932341745809	0.9174422537627931	T	T	T
0.1922438179995618	0.6451834390845225	0.0347953033572783	T	T	T
0.0991235858690965	0.6693637510697790	0.8995674056439906	T	T	T
0.1037050210113423	0.6565763188662505	0.7033045685120065	T	T	T
0.2300712738615415	0.6373756419348831	0.7507807974625933	T	T	T
0.3200748924007737	0.5483344395306656	0.8113006456817240	T	T	T
0.0816945353818156	0.5502584741357180	0.8192506354478319	T	T	T
0.4282138241642763	0.3729078094901354	0.5836140958441415	T	T	T
0.4148150704548506	0.5050790578937867	0.5689919592845666	T	T	T
0.3934547036900384	0.6373994070880946	0.5602612822094518	T	T	T
0.1930849290736495	0.3697704771452371	0.6112782782092013	T	T	T
0.1777154458719983	0.4964558992220901	0.5538035746263784	T	T	T
0.1918909217763709	0.6304722938586489	0.5597283521173486	T	T	T
0.9900134989478090	0.4538169131315092	0.7967344795202361	T	T	T
0.9879134309857430	0.6453620487807118	0.7981249107167501	T	T	T
0.1391865820456169	0.5579112291064412	0.2141025855514035	T	T	T
0.1968736049300138	0.5661616715440332	0.3891760321929639	T	T	T
0.2957788020606358	0.5505746567869048	0.5217750423197905	T	T	T
0.3972158770531542	0.5675369941458535	0.3944998955506789	T	T	T
0.3971400582876464	0.5475872793723459	0.1975127126632282	T	T	T
0.2686380016886013	0.5299396014774562	0.2329197337379584	T	T	T
0.1402188106118095	0.3258769362302720	0.2398312384473050	T	T	T
0.1922421847516202	0.3383863331371945	0.4177960124411786	T	T	T
0.3070937144108247	0.3497194587299039	0.5134519944806789	T	T	T
0.4131848587632272	0.3245370199159462	0.3991927980814210	T	T	T
0.3954975360286001	0.3404163787833011	0.2038121408410224	T	T	T
0.2694707790765902	0.3545459595118134	0.2575541623800678	T	T	T
0.1775792174622917	0.4461104822782729	0.3039207172289235	T	T	T
0.4139837580943760	0.4459639389319525	0.3237097716012433	T	T	T
0.0655720850188351	0.6238564532593985	0.0821626011987086	T	T	T
0.0789751968736110	0.4917609159476068	0.0633658102689186	T	T	T
0.0983344968562909	0.3598613259173878	0.0579019128348353	T	T	T
0.3120879202260839	0.6269263420983263	0.1097795619618696	T	T	T
0.3191128514584692	0.4983710043597600	0.0553754144852381	T	T	T
0.3039184677508704	0.3646614734469302	0.0642043503204798	T	T	T
0.5093811136845232	0.5374061826425751	0.2923921432928000	T	T	T
0.5144417145278196	0.3627531137370203	0.2830639534907197	T	T	T
0.4426280485217100	0.7465585473742695	0.6465158815093364	T	T	T
0.1951709565105784	0.7472308234215708	0.6490145694784374	T	T	T
0.2758662996213106	0.7483784354639623	0.0591191143769681	T	T	T
0.1069573118221645	0.7475253128720852	0.0589244486037270	T	T	T
0.0589680209302666	0.2462448576450205	0.1379168755971812	T	T	T
0.3061503295233832	0.2473164309216275	0.1521707170490715	T	T	T
0.2244175574906660	0.2480304919785239	0.5556496273856935	T	T	T
0.3895609181812700	0.2473375680412889	0.5537214222171061	T	T	T
0.5608114222126228	0.2469152506085046	0.3504379384386885	T	T	T
0.8245939742109430	0.2504174236120819	0.3871825283432639	T	T	T
0.7159579040749118	0.2455814875867835	0.0005583835442199	T	T	T
0.9086736949091305	0.2558657519132809	0.9498219557709767	T	T	T
0.9136922859476551	0.7593505128372872	0.8879501724852021	T	T	T
0.6735867027158898	0.7403512314047975	0.8911756104318328	T	T	T
0.5859960801442464	0.7492915296538207	0.4628501476611250	T	T	T

Structure files (CONTCAR) involved in this work:

0.7757335694768918	0.6868035833580836	0.0811147113043255	T	T	T
0.6714111388233297	0.7673872489717420	0.1228087677164787	T	T	T
0.8404730676983579	0.8027347203980139	0.1018869364451026	T	T	T
0.7902685763611226	0.7515736586094995	0.5044083346552631	T	T	T
0.9124185867158431	0.6767690381602466	0.8347641298875326	T	T	T
0.6781081377276718	0.8264098220771887	0.8527555039101353	T	T	T
0.7675123719591823	0.6682547904754682	0.4881548559133445	T	T	T
0.6835776896820955	0.6985037099554737	0.0420811193825123	T	T	T
0.7452017955545124	0.8130535985819990	0.0850175338180882	T	T	T
0.8588421242232509	0.7266695824260128	0.0200620812486471	T	T	T
0.9377360442544017	0.7345366452926489	0.2006812210817070	T	T	T
0.9124874119820322	0.7304918737404981	0.2992134426220858	T	T	T
0.9531811473655121	0.7821336378591884	0.1675137965902894	T	T	T
0.8694085240891410	0.8422846189286310	0.0914219105500195	T	T	T
0.9513246972886350	0.6889581154049401	0.1596056903271925	T	T	T
0.9023511444437688	0.7779208996034114	0.3377008292839777	T	T	T
0.9498715158035586	0.6986768992815741	0.3398961554162184	T	T	T
0.8705266556532174	0.6924915488597294	0.3142822939573008	T	T	T
0.7783696492089285	0.6818227859658779	0.1540344410045577	T	T	T

Figure 5(c) TS-CH₄ as same as Figure 1(b) Ga/ZSM-5**Figure 5(c) TS-CH₃OH same as Figure2(a) Ga-TS****Figure 5(c) TS1**

Si Al O Ga H C

1.0000000000000000

20.0219999999999985 0.0000000000000000 0.0000000000000000

0.0000000000000000 19.8990000000000009 0.0000000000000000

0.0000000000000000 0.0000000000000000 13.3829999999999991

93 3 192 1 6 2

Selective dynamics

Direct

0.4214354408638648	0.0565477769545967	0.6487180393426656	T	T	T
0.2999534546199871	0.0254659925053081	0.7879987787539283	T	T	T
0.2800706611375364	0.0589885396873288	0.0120883262750220	T	T	T
0.1206097351425601	0.0618694484186523	0.0129915298191001	T	T	T
0.0670029671651872	0.0282902491003598	0.8008868117536733	T	T	T
0.1749153239277794	0.0549056993835386	0.6504838380980921	T	T	T
0.4185122756715947	0.8270681147352645	0.6680620688685022	T	T	T
0.3012614006808752	0.8671484425669055	0.8082173826143058	T	T	T
0.2674141366441676	0.8268156215676584	0.0292474981309162	T	T	T
0.1123674306270938	0.8246510517940389	0.0186890066982551	T	T	T
0.0607447436185811	0.8687328005883380	0.8045978847520451	T	T	T
0.1778096837439027	0.8275138074199674	0.6728487246527931	T	T	T
0.0746680075380880	0.9414911757105866	0.1499402998030870	T	T	T
0.1960993599480804	0.9717351758816560	0.2920746863441500	T	T	T
0.2154022988366774	0.9370610002382046	0.5137421794220602	T	T	T
0.3746768757484102	0.9342899534513930	0.5153870832382699	T	T	T
0.4290429980315518	0.9698974513370748	0.3047209492926184	T	T	T
0.3209753130820979	0.9433761976323695	0.1538732813988277	T	T	T
0.0783263901393042	0.1714233125866304	0.1649982564128503	T	T	T
0.1960817498778379	0.1292112211939325	0.3071655309450088	T	T	T
0.2308398162548254	0.1718563663422464	0.5256469783124798	T	T	T
0.3854158340489384	0.1734564974546365	0.5144184081553409	T	T	T
0.4358392786647611	0.1282838603405502	0.3032054109994528	T	T	T

Structure files (CONTCAR) involved in this work:

0.3188805412130828	0.1667354717076984	0.1702126733163215	T	T	T
0.5762345882596139	0.5564425384404071	0.3528164358082350	T	T	T
0.6881050904347378	0.5374344475946169	0.1939263210458157	T	T	T
0.7115620880108919	0.5625848915440393	0.9761298003412869	T	T	T
0.8695752355650519	0.5555253503695844	0.9710724846173390	T	T	T
0.9327538474698291	0.5268514640342714	0.1840734779817381	T	T	T
0.5751867540627298	0.3306675387351948	0.3373222210349874	T	T	T
0.7073590813037227	0.3778712777492854	0.2268108677024829	T	T	T
0.7348412380785877	0.3317753624672752	0.0032952772850819	T	T	T
0.8873305129107029	0.3262830286229129	0.9774448070784003	T	T	T
0.9398678063353326	0.3701881002944640	0.1936346023881920	T	T	T
0.9226161342179857	0.4357978057081538	0.8276134294393096	T	T	T
0.7775384879801023	0.4445265877725749	0.4690339318735117	T	T	T
0.6219307584619086	0.4323748178942667	0.4907553002365699	T	T	T
0.5699104767864694	0.4667072424102108	0.7080613763266751	T	T	T
0.6753499514363293	0.4330250002594892	0.8531971202034933	T	T	T
0.9170459330903146	0.6697777491751314	0.8258129903341902	T	T	T
0.7943545927201231	0.6326234697397313	0.7053489428604971	T	T	T
0.7683612741959374	0.6688032944037491	0.4815426840802539	T	T	T
0.6135484320566045	0.6709166615901514	0.4837600155880175	T	T	T
0.5692974064752216	0.6256995124414634	0.7043998361384303	T	T	T
0.6785739755487737	0.6833302785739802	0.8377076820969109	T	T	T
0.5738133239323892	0.9446860246996543	0.3671801598707800	T	T	T
0.6960190393685242	0.9747226593492689	0.2284316897023355	T	T	T
0.7153833496328407	0.9464423314451040	0.0015872974089773	T	T	T
0.8758825924622003	0.9323090842107019	0.9975686788236683	T	T	T
0.9298236328872088	0.9697425314471182	0.2084479020374185	T	T	T
0.8214150274090662	0.9371897494876653	0.3584427182783314	T	T	T
0.5797956625684129	0.1758758480834875	0.3379497105796443	T	T	T
0.7001809466962347	0.1343977499691370	0.2089926356398411	T	T	T
0.7303060631724519	0.1731386937966491	0.9858082405858369	T	T	T
0.8848338348439546	0.1724958924044835	0.9960558683700690	T	T	T
0.9330500802157612	0.1284612640156992	0.2078915836246656	T	T	T
0.8222960758402827	0.1720479836148409	0.3490810721033478	T	T	T
0.9229720956153491	0.0564042752073466	0.8652382939738328	T	T	T
0.8031085734475775	0.0311620772695785	0.7262050433711780	T	T	T
0.7805239722947392	0.0558018886762524	0.4994657722445137	T	T	T
0.6204421822992993	0.0683712339367348	0.4969760641864336	T	T	T
0.5664500916233478	0.0337739695446005	0.7056455494428896	T	T	T
0.6760989193502092	0.0634946733057594	0.8554592682417668	T	T	T
0.9155414413755480	0.8235186756767311	0.8426799587023333	T	T	T
0.7979080002094741	0.8740769310213479	0.7131759906848310	T	T	T
0.7675093453548122	0.8294852149027112	0.4930546418981178	T	T	T
0.6114162433067319	0.8261635665899636	0.4980799210880199	T	T	T
0.5613425220612598	0.8766720196955321	0.7053451871195061	T	T	T
0.6721382409694228	0.8382759229401744	0.8471081179442930	T	T	T
0.4253058511549572	0.4453778321831048	0.6369684509154828	T	T	T
0.3042474614987555	0.4720252308162624	0.7831022843726546	T	T	T
0.2864370231197439	0.4307758922865039	0.0006225007181222	T	T	T
0.1276382894692242	0.4299555837311065	0.0010060724829898	T	T	T
0.0734481140424326	0.4717400099929495	0.7951528512638486	T	T	T
0.1804046520872326	0.4483172014218786	0.6415463981571677	T	T	T
0.4250122523019021	0.6720052674497885	0.6581008503003140	T	T	T

Structure files (CONTCAR) involved in this work:

0.3028630141211268	0.6290878398112404	0.7963567968797838	T	T	T
0.2700741497786302	0.6707424008989911	0.0153346757147117	T	T	T
0.1155868401213081	0.6714256822841504	0.0088441588521610	T	T	T
0.0657426486815368	0.6290827803001682	0.7986294459653334	T	T	T
0.1795811814726471	0.6691892282243510	0.6601992273666190	T	T	T
0.0790034456035669	0.5509841334800949	0.1367438596998019	T	T	T
0.2014529183059860	0.5257041241954401	0.2797747197713498	T	T	T
0.2217206242264725	0.5664691312151060	0.5022896157464051	T	T	T
0.3799205466775719	0.5685593882777152	0.5052206397417844	T	T	T
0.4266758252079097	0.5240230197641340	0.2975688299808698	T	T	T
0.3270795420012435	0.5498723495685259	0.1370648408776041	T	T	T
0.0832923267956231	0.3263163695748812	0.1551441856662417	T	T	T
0.1999072781349843	0.3681031854782092	0.2996187804911589	T	T	T
0.2321767486882661	0.3279806035111293	0.5200096259703624	T	T	T
0.3863027302144413	0.3262618238658168	0.5083887300345399	T	T	T
0.4322335368852913	0.3677205395892305	0.2940439394638455	T	T	T
0.3194262114042140	0.3244992076870203	0.1617997478679682	T	T	T
0.8142237025632709	0.5711425082940882	0.3162948208441899	T	T	T
0.8352633089516264	0.3284237715523345	0.3561650053304485	T	T	T
0.7908357833094631	0.4740221433350443	0.7171652437168899	T	T	T
0.3554029069262082	0.0617187918324999	0.7184185345978015	T	T	T
0.2979694191141740	0.0643524473589768	0.8944082939783194	T	T	T
0.2001273180934160	0.0501792743089980	0.0294069616797217	T	T	T
0.1025923784112305	0.0652388848512484	0.8952270651037260	T	T	T
0.1003418025980297	0.0556193137565835	0.6979912531561165	T	T	T
0.2268797755190043	0.0303622091702759	0.7362804459681329	T	T	T
0.3572018258730051	0.8248907426452390	0.7473710847437433	T	T	T
0.3032922913612594	0.8425033494179963	0.9232472788452528	T	T	T
0.1895425939825779	0.8505787577253630	0.0230339554468581	T	T	T
0.0847717552684898	0.8306619245191935	0.9054484018611907	T	T	T
0.1005816382206946	0.8364725121405002	0.7094636114195377	T	T	T
0.2273274439152825	0.8531196314481373	0.7616848563999674	T	T	T
0.3189896349518798	0.9466756694883119	0.8022653043361052	T	T	T
0.0785556491173105	0.9478875810602260	0.8122902701602839	T	T	T
0.4303639414200682	0.1262084454302121	0.5865615782702039	T	T	T
0.4157766592857596	0.9943857172256558	0.5699859434537609	T	T	T
0.3943038849295895	0.8624811672989697	0.5648224999860031	T	T	T
0.1925742038462719	0.1301609912858000	0.6123638223592426	T	T	T
0.1768446740111993	0.0029425244253650	0.5566978616415031	T	T	T
0.1906618258764325	0.8694729795233619	0.5707178179671980	T	T	T
0.9880496579354885	0.0457544940882438	0.7949265269865737	T	T	T
0.9806644339905523	0.8584094630375855	0.7904090785796081	T	T	T
0.1403132875796018	0.9382706700253161	0.2203647963716222	T	T	T
0.1978155360090716	0.9295335001173427	0.3960105119546301	T	T	T
0.2952049224226312	0.9477797595768422	0.5303372484126724	T	T	T
0.3939322030509754	0.9310021746818190	0.3979825653469947	T	T	T
0.3956473702709469	0.9447456147311196	0.2007076761135945	T	T	T
0.2689241067989721	0.9682794016604956	0.2394219850970515	T	T	T
0.1408925572636260	0.1689708227825911	0.2417732875560704	T	T	T
0.1946234002609921	0.1606760165445040	0.4186762300918782	T	T	T
0.3082281484461520	0.1472345992338511	0.5183780812821019	T	T	T
0.4122162329130025	0.1706300472547508	0.4005207672864625	T	T	T
0.3961800174923467	0.1565136655860035	0.2053206457097246	T	T	T

Structure files (CONTCAR) involved in this work:

0.2700476185886201	0.1385577497930503	0.2584057812834059	T	T	T
0.1773287622630852	0.0499155628183705	0.3127957504162013	T	T	T
0.4171070425676852	0.0499055301605930	0.3204675595931261	T	T	T
0.0667077796857298	0.8693609166096682	0.0936559140432435	T	T	T
0.0807672030437701	0.9999516847039719	0.0652023885748782	T	T	T
0.0978215764572866	0.1326185221355748	0.0622897913702662	T	T	T
0.3043802789649466	0.8671913567995613	0.1186224657192383	T	T	T
0.3176241971750982	0.9933924980654167	0.0578484926655638	T	T	T
0.3057498171004316	0.1271320099052978	0.0661295615066132	T	T	T
0.5081481065229966	0.9535423971873618	0.2974845642026975	T	T	T
0.5159001497173432	0.1372073054540362	0.2881519002738443	T	T	T
0.6283783344990652	0.5672794492396372	0.2633891180992574	T	T	T
0.6693322235340131	0.5552901141539655	0.0783658144769186	T	T	T
0.7909679872874126	0.5484376689182409	0.9952989974862815	T	T	T
0.9143432850550282	0.5514711127258122	0.0710353049589989	T	T	T
0.8956628884183686	0.5667323670357640	0.2713845282209105	T	T	T
0.7572923954984384	0.5730225827569418	0.2208141117440192	T	T	T
0.6417749918794996	0.3392874963214634	0.2712018202354802	T	T	T
0.7251529739163941	0.3398739973785919	0.1222598310446122	T	T	T
0.8109811965045974	0.3543729167970742	0.9734058554977943	T	T	T
0.9200261015803778	0.3362619285259996	0.0863821343596902	T	T	T
0.9087719750501954	0.3327262409710523	0.2887362339734031	T	T	T
0.7692298368371002	0.3722297532451290	0.3032601894206491	T	T	T
0.6886117285341984	0.4557779194330701	0.2063892362354163	T	T	T
0.9146315215273590	0.4475230968189992	0.1909800239089998	T	T	T
0.5642805904610680	0.6267584351034177	0.4129983698354555	T	T	T
0.6030155721901983	0.5016464620783339	0.4340490138643601	T	T	T
0.5818152622629397	0.3693164805791510	0.4441808203742960	T	T	T
0.8178986769287441	0.6420628066429164	0.3954122606762539	T	T	T
0.7958059618327191	0.5031407211333613	0.3951308931276896	T	T	T
0.8375509457114638	0.3824664322806967	0.4715436189508232	T	T	T
0.0129240777943185	0.5376045707425585	0.2026633227666465	T	T	T
0.0216052957487056	0.3692108928740286	0.2006895248940037	T	T	T
0.8734364463797848	0.4287443711105719	0.7254765776084066	T	T	T
0.8014712398194213	0.4718604038889766	0.5840721057466711	T	T	T
0.7020222777394534	0.4184670321013384	0.4799344215817502	T	T	T
0.6036559191367981	0.4364769434911071	0.6076176733145083	T	T	T
0.6006720536602533	0.4276117147245512	0.8041849532890616	T	T	T
0.7322586562735296	0.4226724236898978	0.7685233080261888	T	T	T
0.8644156667186852	0.6705991644567914	0.7334631939235351	T	T	T
0.7907336740783126	0.6305089355139510	0.5842872736377693	T	T	T
0.6905226387276353	0.6499845997994128	0.4585418736117099	T	T	T
0.5979567195748045	0.6566578312950481	0.6007670243315607	T	T	T
0.6038092808941256	0.6646009125132999	0.7980369970415560	T	T	T
0.7310516015888687	0.6760953157709895	0.7451322292425461	T	T	T
0.7949863917307454	0.5572811900298285	0.7498281161301980	T	T	T
0.5874313264152455	0.5464377183617961	0.7120168989986316	T	T	T
0.9285336066292009	0.3665424682507940	0.8896972984838039	T	T	T
0.8903533369557053	0.4941221901697718	0.8950839053881348	T	T	T
0.8873529555412430	0.6266535919195071	0.9182033607838522	T	T	T
0.6818147321675950	0.3774703595948405	0.9419699404282236	T	T	T
0.6821569806283290	0.5087301253483286	0.8972943973982087	T	T	T
0.7015644017451751	0.6376206904647913	0.9313183259738272	T	T	T

Structure files (CONTCAR) involved in this work:

0.4896721462291081	0.4555017536198973	0.7082116523812344	T	T	T
0.4886070321383220	0.6352028014399600	0.7100617757106629	T	T	T
0.6393216431124211	0.9392067010201380	0.2966951452256599	T	T	T
0.6907846314990889	0.9449978130541545	0.1164103271955831	T	T	T
0.7963057537909997	0.9471106487662008	0.9915974560581582	T	T	T
0.8995014441061100	0.9290229977334235	0.1132578394609300	T	T	T
0.8961676226759552	0.9428541139249852	0.3116677978827350	T	T	T
0.7697864250035171	0.9566782661225592	0.2697970482482874	T	T	T
0.6402153388632978	0.1779921471524672	0.2578919992842528	T	T	T
0.6980467878809927	0.1480241928979192	0.0900775589985893	T	T	T
0.8078438933667583	0.1477888387464587	0.9832005179168969	T	T	T
0.9059807118111576	0.1721611415337858	0.1130568442649236	T	T	T
0.8980333691793415	0.1552721349271998	0.3093747828545078	T	T	T
0.7717582607190144	0.1567087076137891	0.2549078877097269	T	T	T
0.6852321915693287	0.0554494320568545	0.2313810180885440	T	T	T
0.9153790026091079	0.0493391732742978	0.1908063880992660	T	T	T
0.5651482420715361	0.8757371090091997	0.4311374342600983	T	T	T
0.5787938637530765	0.0078900386729180	0.4439810413608777	T	T	T
0.6042194465938716	0.1385364426166565	0.4399148359591106	T	T	T
0.8078091017862057	0.8609763700796018	0.3982691787752758	T	T	T
0.8130566628261703	0.9881139552098751	0.4522396584798644	T	T	T
0.8053492555392517	0.1215582696402046	0.4408479799699266	T	T	T
0.0095428981669016	0.9555218088270178	0.2185463367773009	T	T	T
0.0137550051046889	0.1370313100251169	0.2178671189893322	T	T	T
0.8581798380970874	0.0692670653695795	0.7947697298413122	T	T	T
0.8065211002185323	0.0608664082731957	0.6139882550529409	T	T	T
0.6994760810899875	0.0503576096786351	0.4933724922113687	T	T	T
0.5963822860426725	0.0766768602872176	0.6123295113480024	T	T	T
0.6012262467138895	0.0572075540905979	0.8096548894211055	T	T	T
0.7280657126459200	0.0433997100210922	0.7673722637947183	T	T	T
0.8527656836514224	0.8259358713999702	0.7661977573243884	T	T	T
0.7987285471365007	0.8600660438724476	0.5947473785816475	T	T	T
0.6888812846396594	0.8497916355539281	0.4860696933066413	T	T	T
0.5888090897871855	0.8299574655408181	0.6145874051834148	T	T	T
0.5963421427830456	0.8528706672500942	0.8089319249243379	T	T	T
0.7238694695555191	0.8599082643273257	0.7584482615314768	T	T	T
0.8200582350270199	0.9514492008535240	0.7320509972030194	T	T	T
0.5804013469210701	0.9545808071877534	0.6829780282611549	T	T	T
0.9340917228438335	0.1226190536260474	0.9344264193196959	T	T	T
0.9150266920739829	0.9914834328283907	0.9378820805124891	T	T	T
0.8954511122666643	0.8605450887143794	0.9468156212837623	T	T	T
0.6892895182180344	0.1398858008191877	0.8932888440556364	T	T	T
0.6847985267282988	0.0134679520426626	0.9501784844344439	T	T	T
0.6863136333344639	0.8797698782366338	0.9484616161333205	T	T	T
0.4867307484836163	0.0465961610105468	0.7186824756415521	T	T	T
0.4808603761182657	0.8680663664498910	0.7167868807355630	T	T	T
0.3589902206476619	0.4428122559201681	0.7060454999008726	T	T	T
0.3049860972469139	0.4254842853450936	0.8827578248405287	T	T	T
0.2067836099602844	0.4445593385264844	0.0139001792178549	T	T	T
0.1069017162435732	0.4274024027461892	0.8831982626923626	T	T	T
0.1045562575603511	0.4526445774778838	0.6862951999277909	T	T	T
0.2309140014296140	0.4685705471958743	0.7310171670054828	T	T	T
0.3603947268176845	0.6638477754148080	0.7298362752124454	T	T	T

Structure files (CONTCAR) involved in this work:

0.3011396345967118	0.6670999289132628	0.9033353934945544	T	T	T
0.1926784736775028	0.6450853657416756	0.0124962994720649	T	T	T
0.0904667207095719	0.6733039064417755	0.8931473155497934	T	T	T
0.1030817703286861	0.6542402595744715	0.6970725527160903	T	T	T
0.2304196866895187	0.6365874095409330	0.7418660977872541	T	T	T
0.3194201675647045	0.5497914237563191	0.8125211534579337	T	T	T
0.0839445148552143	0.5506675486357295	0.8201804330377075	T	T	T
0.4328184012024897	0.3752876191898314	0.5757690831168047	T	T	T
0.4204599426872334	0.5067135853965257	0.5566802047471132	T	T	T
0.4085736029842726	0.6389865820204199	0.5492691931758917	T	T	T
0.1923025052066059	0.3724060290069670	0.6024982090189241	T	T	T
0.1846853749499502	0.5002602490914368	0.5481235559109559	T	T	T
0.1901365235538106	0.6343117836371859	0.5512409587793459	T	T	T
0.9943648237279789	0.4555807495990528	0.7812734474633164	T	T	T
0.9857226057782574	0.6362205991384032	0.7818122912470771	T	T	T
0.1424175690683613	0.5575169168454955	0.2118430219777251	T	T	T
0.2080742547728499	0.5685649830921433	0.3829670001327197	T	T	T
0.3005774173379790	0.5615615767287485	0.5305397291732789	T	T	T
0.3898680591339913	0.5669935763038960	0.3853615047481041	T	T	T
0.4000703297932841	0.5515149481038163	0.1901748754995784	T	T	T
0.2715605641474600	0.5294729164821337	0.2202696716585164	T	T	T
0.1443837447950533	0.3291725582461070	0.2343064277506109	T	T	T
0.1976239189358593	0.3366043533028885	0.4111914467951376	T	T	T
0.3093448956444410	0.3534540034571140	0.5142214279236758	T	T	T
0.4106788742170791	0.3253165227307974	0.3929271916979719	T	T	T
0.3965905105855953	0.3357936319222271	0.1955279738613870	T	T	T
0.2728196759629321	0.3572482644147489	0.2491112778830520	T	T	T
0.1834742684885800	0.4480079535731535	0.3058963264117593	T	T	T
0.4077010911163875	0.4449231619085813	0.3101862261789304	T	T	T
0.0701351508373054	0.6208241908346207	0.0747750426467960	T	T	T
0.0875650443302533	0.4902245158977623	0.0561180967666488	T	T	T
0.1075275279509105	0.3577522463862174	0.0484212619387737	T	T	T
0.3123253392003056	0.6236823983408507	0.0909782324530689	T	T	T
0.3270998859418220	0.4936000111724468	0.0488744317346860	T	T	T
0.3060510213734867	0.3604956638491976	0.0545446959258100	T	T	T
0.5064459725936745	0.5322108076749947	0.3040913103077573	T	T	T
0.5122159491157484	0.3628016482741324	0.2763023567290311	T	T	T
0.4410902004842885	0.7509194675267206	0.6414956774126283	T	T	T
0.1923028651704356	0.7489725078347352	0.6483309568120769	T	T	T
0.2734336722718139	0.7474514859530719	0.0553510194314480	T	T	T
0.1087322231214575	0.7466477842145016	0.0541307599547141	T	T	T
0.0620746141478434	0.2488506877124318	0.1360806392103904	T	T	T
0.3032561133053032	0.2453585547388145	0.1492840365965211	T	T	T
0.2271268404327216	0.2506113308098526	0.5561625216733194	T	T	T
0.3906213709717604	0.2506095527229922	0.5532874697269067	T	T	T
0.5595160594754151	0.2526677548101616	0.3639376474044324	T	T	T
0.8163900918410644	0.2473411596449641	0.3895382732680744	T	T	T
0.7246701569686824	0.2536342917832236	0.9728015206332359	T	T	T
0.8919114181431259	0.2473544341013639	0.9489934695203077	T	T	T
0.9323225337101788	0.7450956200270843	0.8660249738304340	T	T	T
0.6799285181121905	0.7600863652317588	0.8764752076786021	T	T	T
0.7764159385793614	0.7491010304418408	0.4953871042904052	T	T	T
0.6013290804822650	0.7497611739482914	0.4591664168400845	T	T	T

Structure files (CONTCAR) involved in this work:

0.8878490526900540	0.4277089600135552	0.5795778502074879	T	T	T
0.9551446832146236	0.6245810794638120	0.5298860060451245	T	T	T
0.8746958313972626	0.5773722765312421	0.5192679494879383	T	T	T
0.9340643400076415	0.5783913673399707	0.4097705036215736	T	T	T
0.9752886557423247	0.4665585831316066	0.4472985194959407	T	T	T
0.9520773410444490	0.5310607094225179	0.5428181003021250	T	T	T
0.0157002728828122	0.4719662996530701	0.5697638459167326	T	T	T
0.9243322553465398	0.5879812673070340	0.4892761132511534	T	T	T
0.9686610382145580	0.4748745312900833	0.5274977921766164	T	T	T

Figure 5(c) TS2

Si Al O Ga H C

1.0000000000000000

20.0219999999999985 0.0000000000000000 0.0000000000000000

0.0000000000000000 19.8990000000000009 0.0000000000000000

0.0000000000000000 0.0000000000000000 13.3829999999999991

93 3 192 1 6 2

Selective dynamics

Direct

0.4221048503143044	0.0568894069847847	0.6480589011657698	T	T	T
0.3008747925239770	0.0265906640044392	0.7888589464473542	T	T	T
0.2797914267509057	0.0602855202808203	0.0122704547533229	T	T	T
0.1201822904473666	0.0632255161053904	0.0127958271598750	T	T	T
0.0673098644207748	0.0294653821003215	0.8001575777140859	T	T	T
0.1758414061825570	0.0555347802862798	0.6508738780845710	T	T	T
0.4189513604418649	0.8270845319832221	0.6701136337780189	T	T	T
0.3012791167100349	0.8682682621867256	0.8091972518385480	T	T	T
0.2668798988383741	0.8280527188105032	0.0294618967424519	T	T	T
0.1119029074587596	0.8261698230636244	0.0173344115578426	T	T	T
0.0613760348559580	0.8705022182715276	0.8030242826676052	T	T	T
0.1785710203108682	0.8277905900783951	0.6734660212020678	T	T	T
0.0745947480182408	0.9426639839171436	0.1502527174210370	T	T	T
0.1957315851410470	0.9726549481835471	0.2929985312883977	T	T	T
0.2163456775867683	0.9367847728176317	0.5143607671450904	T	T	T
0.3756842588218620	0.9338928150777190	0.5157542530572405	T	T	T
0.4290971459064070	0.9697292328256087	0.3049435102419284	T	T	T
0.3203256299702470	0.9446151100698911	0.1546712098784531	T	T	T
0.0782533032821170	0.1725950094185754	0.1646884236841842	T	T	T
0.1956354528600245	0.1300366245506264	0.3073150474592632	T	T	T
0.2307380447408703	0.1727497254311160	0.5248048435555593	T	T	T
0.3853053027521907	0.1737253304134695	0.5131397966571501	T	T	T
0.4355334332220998	0.1278302660589628	0.3025813501047211	T	T	T
0.3184557782265689	0.1675424453892755	0.1708522873923329	T	T	T
0.5812252738449295	0.5554722500576676	0.3508282270894770	T	T	T
0.6925463028094642	0.5320469228750591	0.1895535898026987	T	T	T
0.7136864473218995	0.5654978233399026	0.9752358461544044	T	T	T
0.8719948037253026	0.5624788874577594	0.9786309770656051	T	T	T
0.9333212830769653	0.5310735965296235	0.1892602984000172	T	T	T
0.5753103771625803	0.3294611193918587	0.3373042595510184	T	T	T
0.7040545628938923	0.3758296002304813	0.2176736677215156	T	T	T
0.7330945320479418	0.3293368075575481	0.9992360022332746	T	T	T
0.8846427726251197	0.3267117607721496	0.9826717318840499	T	T	T
0.9385805847794234	0.3742795795253666	0.1925829413347424	T	T	T
0.9269390285057185	0.4393512397998640	0.8420956420392144	T	T	T

Structure files (CONTCAR) involved in this work:

0.7776735132432651	0.4445983200524805	0.4761376576196387	T	T	T
0.6218072456795080	0.4309358291554189	0.4923059251780078	T	T	T
0.5685002906035459	0.4679533848432492	0.7082820449932036	T	T	T
0.6721870326989081	0.4341728720534409	0.8583308025687943	T	T	T
0.9174602650331805	0.6731802998768113	0.8272370878975897	T	T	T
0.7985010953693329	0.6353174950013666	0.6964008876640053	T	T	T
0.7675025855891509	0.6687608790699213	0.4776694612461319	T	T	T
0.6116129544932261	0.6705064461686371	0.4879880884924176	T	T	T
0.5645036702701590	0.6267705365881719	0.7068680618993198	T	T	T
0.6814734765682160	0.6826487923622097	0.8268439860621349	T	T	T
0.5739438998550387	0.9434875213586222	0.3656889168762617	T	T	T
0.6946421601714431	0.9742606936725010	0.2243794430317420	T	T	T
0.7167001526567023	0.9433335976064009	0.0006882104395633	T	T	T
0.8768346292731994	0.9337914393056883	0.9957516425466912	T	T	T
0.9296570773262970	0.9703225258386121	0.2071424136264362	T	T	T
0.8202169670880947	0.9416162013250188	0.3578743814797035	T	T	T
0.5788361367593599	0.1747228992798689	0.3373525142348545	T	T	T
0.6975184271605818	0.1326508738337043	0.2039340698248639	T	T	T
0.7302226130215064	0.1727272389573143	0.9817539665088930	T	T	T
0.8845716029964167	0.1731710031207115	0.9941381394947018	T	T	T
0.9332061731468714	0.1289541139244035	0.2059039852327136	T	T	T
0.8199623301094258	0.1716863766568527	0.3430758245128387	T	T	T
0.9230647855151853	0.0576048510559504	0.8627599312089528	T	T	T
0.8034370900079160	0.0308031052798498	0.7237842752980091	T	T	T
0.7804537592157766	0.0596366301987714	0.4979493675802280	T	T	T
0.6205002710881123	0.0674789400171903	0.4952867163005303	T	T	T
0.5673846612230519	0.0321496604086458	0.7041568991443877	T	T	T
0.6764349983491451	0.0590757613353124	0.8564426305068016	T	T	T
0.9172407312900707	0.8259707334002080	0.8401781326065632	T	T	T
0.8009093610576765	0.8748778402800406	0.7072126634745330	T	T	T
0.7663102030565221	0.8301880803593531	0.4893297298074502	T	T	T
0.6112587069162949	0.8255468148193106	0.4971122254454417	T	T	T
0.5615562556701689	0.8752575207715242	0.7044119192041177	T	T	T
0.6760664025701262	0.8382721199102230	0.8406600947381184	T	T	T
0.4236873322036164	0.4452987182296417	0.6391556160092915	T	T	T
0.3041721875888239	0.4732309619911449	0.7869713324857591	T	T	T
0.2862998006555494	0.4331494966618601	0.0052836130229398	T	T	T
0.1281254006248224	0.4321383788821267	0.0027648188777077	T	T	T
0.0749322755273856	0.4724905388061189	0.7957435339873165	T	T	T
0.1818764380210376	0.4492802470029311	0.6441375267176637	T	T	T
0.4237810757318787	0.6722298030804599	0.6638229472752080	T	T	T
0.3012055654067342	0.6300649187085392	0.7988292130300546	T	T	T
0.2695570097997201	0.6720039826973991	0.0174879619159887	T	T	T
0.1151608143246114	0.6729660673472853	0.0083850699733042	T	T	T
0.0646687237120784	0.6298745190052861	0.7989083471014137	T	T	T
0.1788390422755840	0.6692518547855539	0.6629691083375628	T	T	T
0.0790873835899946	0.5530082872723269	0.1364492542003564	T	T	T
0.2011347839926069	0.5278828450579565	0.2801806634217601	T	T	T
0.2222194918318825	0.5678752404996531	0.5020567276557282	T	T	T
0.3825259480690991	0.5698316292310408	0.5049031570012897	T	T	T
0.4322678053079612	0.5270986980491682	0.2963304282919836	T	T	T
0.3278841360146872	0.5523481233546531	0.1415837143707789	T	T	T
0.0831030326109738	0.3275201302541418	0.1555914220532018	T	T	T

Structure files (CONTCAR) involved in this work:

0.1982658240463962	0.3698105346747855	0.3020587054861714	T	T	T
0.2317893768979684	0.3293405024749271	0.5220617966789938	T	T	T
0.3859599507738455	0.3270254795629311	0.5098164638904451	T	T	T
0.4329369088089829	0.3704188076799536	0.2957465865251194	T	T	T
0.3186699852036153	0.3258839644862873	0.1651260912191838	T	T	T
0.8153112473530308	0.5681431633726631	0.3206851920730353	T	T	T
0.8308446038345784	0.3315879049899838	0.3466139348978399	T	T	T
0.7891061607759552	0.4769969379243302	0.7270920610719763	T	T	T
0.3566919012652560	0.0620825107458622	0.7190447837159785	T	T	T
0.2991204397866690	0.0657018895293539	0.8950981025178482	T	T	T
0.1997339580397892	0.0510941688495852	0.0278943947147822	T	T	T
0.1013593124670971	0.0667796251237947	0.8953897302441649	T	T	T
0.1011394744920908	0.0571732992526943	0.6978877350279420	T	T	T
0.2277812650093165	0.0322297411184498	0.7373887752695101	T	T	T
0.3567983513988924	0.8259761622627064	0.7478127391338297	T	T	T
0.3037672700365510	0.8433253499614247	0.9241074752534089	T	T	T
0.1891681788679510	0.8519066644193648	0.0209276902231197	T	T	T
0.0837695013744288	0.8319634229962134	0.9043540884324027	T	T	T
0.1011956936103703	0.8376867696549558	0.7084889231295759	T	T	T
0.2272793779370569	0.8546489653268657	0.7626354501816489	T	T	T
0.3192970632958577	0.9477397703743462	0.8036158251794314	T	T	T
0.0804660553189739	0.9493794162691060	0.8117199966463566	T	T	T
0.4300645888486435	0.1265351163397011	0.5855385173362795	T	T	T
0.4162368043994042	0.9946631074336590	0.5695994705321183	T	T	T
0.3961805418922904	0.8626175286113374	0.5661092585879772	T	T	T
0.1930845255860674	0.1305746490446857	0.6114232183018731	T	T	T
0.1778962013462715	0.0023603580876140	0.5586803797587879	T	T	T
0.1922892125168320	0.8685951458693422	0.5704305328797773	T	T	T
0.9881841327912393	0.0461509405968893	0.7927136160263936	T	T	T
0.9812819524427486	0.8621818099103580	0.7870359554779295	T	T	T
0.1401622653034466	0.9390753280616586	0.2209323640757478	T	T	T
0.1978593230028790	0.9303476933427237	0.3967599747230580	T	T	T
0.2961872476764563	0.9473515244342301	0.5304042783341146	T	T	T
0.3947798706841023	0.9302060415265483	0.3982860298764578	T	T	T
0.3951432353428607	0.9451427181087549	0.2010308180604466	T	T	T
0.2686773180832578	0.9698412308089640	0.2405467939905225	T	T	T
0.1408292971937031	0.1698650119003118	0.2412856262886733	T	T	T
0.1937001572737197	0.1622960229529692	0.4183138833777234	T	T	T
0.3079912686902255	0.1478863502325820	0.5162170367219659	T	T	T
0.4126712950742605	0.1711173182722850	0.3994894535501417	T	T	T
0.3957064495060370	0.1557388503352194	0.2047524632337641	T	T	T
0.2697447005684727	0.1392000140106383	0.2590856000970418	T	T	T
0.1766421514370270	0.0508312518520225	0.3137681373055203	T	T	T
0.4167415224464601	0.0496652431052901	0.3215859861849932	T	T	T
0.0667015380626585	0.8711777070562934	0.0924639194174024	T	T	T
0.0805005774230678	0.0019443190042214	0.0667306490412437	T	T	T
0.0977420950118284	0.1342465406838480	0.0617147837995286	T	T	T
0.3029319074650010	0.8687047375196666	0.1193060294141264	T	T	T
0.3172535548891365	0.9949724769084100	0.0590238448988946	T	T	T
0.3042090074808296	0.1288893860785140	0.0663847321417178	T	T	T
0.5081871374270579	0.9536475551717974	0.2964840256161544	T	T	T
0.5154829217934218	0.1363298448971449	0.2857728717862468	T	T	T
0.6394727894290937	0.5636787333109902	0.2692532845844086	T	T	T

Structure files (CONTCAR) involved in this work:

0.6747388467691340	0.5654564221624345	0.0809923536573030	T	T	T
0.7929332445765995	0.5481695905535664	0.9895001421984436	T	T	T
0.9107764783927670	0.5663054725744516	0.0839158600313896	T	T	T
0.8990863057996715	0.5609581617039623	0.2870441865702044	T	T	T
0.7677043152763181	0.5501237436153649	0.2168445139556676	T	T	T
0.6413767618403424	0.3370514034150661	0.2698231286081086	T	T	T
0.7235188527683061	0.3313231395180851	0.1190845689077618	T	T	T
0.8087766322051624	0.3555810895470742	0.9713824846645632	T	T	T
0.9117829393404917	0.3320139390078051	0.0958288074669371	T	T	T
0.9093520347806789	0.3453759351260567	0.2960467618719748	T	T	T
0.7670032760724652	0.3778676913038699	0.2931190609156562	T	T	T
0.6800210285240191	0.4504587589794425	0.1838677319370764	T	T	T
0.9168802999987159	0.4514693861155553	0.1740524038893369	T	T	T
0.5682659877345567	0.6260700253770061	0.4089822379376605	T	T	T
0.6019238018443407	0.4991738503831314	0.4341872548645923	T	T	T
0.5841027269631353	0.3665624167522830	0.4451979871296046	T	T	T
0.8012453221981485	0.6451029068491607	0.3764142481356860	T	T	T
0.7964727237059743	0.5067464323630031	0.4113205842847724	T	T	T
0.8384655505037600	0.3828592331442544	0.4663101882049091	T	T	T
0.0140541350817071	0.5403911841512319	0.2046668309267047	T	T	T
0.0200197188461931	0.3700586115821968	0.1971994610924008	T	T	T
0.8728698750403898	0.4319442400308807	0.7437577884053717	T	T	T
0.8013185377257124	0.4622797385128196	0.5956794777971615	T	T	T
0.7026026520222008	0.4174413148208659	0.4839851714672989	T	T	T
0.6026447780346559	0.4359656339183113	0.6089974942501325	T	T	T
0.5987117814391828	0.4300613781656191	0.8059174680096222	T	T	T
0.7305420123835061	0.4251677431177545	0.7753109826399835	T	T	T
0.8635058137922569	0.6763003616266720	0.7373363788780862	T	T	T
0.8038101433423855	0.6340922466893282	0.5755131079874116	T	T	T
0.6887456362124506	0.6464495229937434	0.4851140396958671	T	T	T
0.5819965659314287	0.6595626136156217	0.5995413588674815	T	T	T
0.6046634317600638	0.6654124256812661	0.7954659469935765	T	T	T
0.7293315452386182	0.6729001998764672	0.7290343109989441	T	T	T
0.7992569799555169	0.5605892960549475	0.7451291522016159	T	T	T
0.5855133157080826	0.5478432492166195	0.7097440947289437	T	T	T
0.9306453188782731	0.3698743218871016	0.9034833137869871	T	T	T
0.9020903128664703	0.5005836558149315	0.9095486429263826	T	T	T
0.8869578117655269	0.6325018672764279	0.9215638256796377	T	T	T
0.6782941010802469	0.3760866471724869	0.9433001760407149	T	T	T
0.6792497274389059	0.5086666659725411	0.9057960130835773	T	T	T
0.7061680982002693	0.6376269207534957	0.9204739958766061	T	T	T
0.4883537016150443	0.4567813191273942	0.7092786444649068	T	T	T
0.4841666497236166	0.6352474299085914	0.7245626119939205	T	T	T
0.6391760128950889	0.9383418119677700	0.2944446438663637	T	T	T
0.6944077433146365	0.9375746969946012	0.1163984640754045	T	T	T
0.7973154746215655	0.9483915896808141	0.9881722696434614	T	T	T
0.8996377292454826	0.9297670084323668	0.1116836658778184	T	T	T
0.8947335641382275	0.9442606764093123	0.3096124254233351	T	T	T
0.7685145114103371	0.9659990649741537	0.2718282027572588	T	T	T
0.6406362944508043	0.1764670424019488	0.2597560862572039	T	T	T
0.6961041654581825	0.1540437974240344	0.0875040063866998	T	T	T
0.8077661734721897	0.1472116570613044	0.9838959627164888	T	T	T
0.9073149793141253	0.1726192570603533	0.1103873973386526	T	T	T

Structure files (CONTCAR) involved in this work:

0.8965735931569782	0.1558766434078996	0.3062471842121034	T	T	T
0.7704360954150204	0.1474673578507787	0.2521919039084390	T	T	T
0.6776891452027856	0.0537154157550034	0.2142348437724744	T	T	T
0.9161754819337296	0.0499828574208039	0.1882479096077725	T	T	T
0.5648747572778684	0.8740995357410235	0.4283581556328408	T	T	T
0.5795144463055448	0.0061015279441878	0.4435787784473446	T	T	T
0.6011165813761328	0.1376269344165337	0.4404267878400317	T	T	T
0.8034771036569991	0.8655203033469622	0.3944490779486590	T	T	T
0.8162269790044622	0.9930080701220941	0.4522908189907254	T	T	T
0.8050618536518878	0.1273817171746839	0.4427845283587788	T	T	T
0.0092337721950679	0.9558165052143848	0.2188404190704965	T	T	T
0.0136762314476423	0.1384431358483864	0.2180422292013504	T	T	T
0.8580054786858101	0.0695826037801433	0.7925053098486754	T	T	T
0.8021552590264047	0.0653651540317856	0.6144114666841639	T	T	T
0.6998642792866194	0.0519799570761972	0.4858856907167389	T	T	T
0.5991742740236696	0.0748873501657586	0.6119476029013377	T	T	T
0.6019791917438764	0.0538115161525869	0.8091024275411863	T	T	T
0.7291315908340056	0.0363337078456854	0.7708039657551228	T	T	T
0.8539658327714849	0.8271230531701164	0.7647264929019715	T	T	T
0.8020021153672933	0.8574994772645097	0.5899690627917463	T	T	T
0.6878811776041317	0.8523676696902455	0.4897479155346483	T	T	T
0.5862092585550880	0.8279668969627995	0.6126357977129779	T	T	T
0.5992977169621784	0.8521645627852733	0.8062083641796622	T	T	T
0.7261768361955609	0.8642976465125581	0.7525274624639458	T	T	T
0.8251328654037511	0.9522662842032575	0.7208604925984505	T	T	T
0.5797935872721124	0.9530299511483451	0.6798698793506298	T	T	T
0.9338620714040295	0.1251016243455646	0.9295435833585790	T	T	T
0.9157276444108515	0.9939361715888374	0.9378287241670012	T	T	T
0.8970404700734511	0.8626398759868853	0.9444232245832438	T	T	T
0.6905851157985451	0.1359619097409266	0.8911021537605047	T	T	T
0.6826864014906402	0.0103737824110943	0.9534343928063028	T	T	T
0.6902508604219669	0.8766011064579580	0.9448272546271990	T	T	T
0.4880405742460872	0.0471958655711161	0.7166843230870326	T	T	T
0.4813351398923172	0.8671769705159913	0.7205201408979865	T	T	T
0.3578659228830008	0.4428594589688338	0.7092770346520287	T	T	T
0.305462337754814	0.4277457437981135	0.8876376013932459	T	T	T
0.2067985742756963	0.4486380486011763	0.0175011161959664	T	T	T
0.1086751862253291	0.4287047778407087	0.8843809230425516	T	T	T
0.1053056958463310	0.4538943783726855	0.6863572984446304	T	T	T
0.2304403102132095	0.4697191640675056	0.7360105824698187	T	T	T
0.3557842878960523	0.6662753127200428	0.7286640184810553	T	T	T
0.3013775306107851	0.6677453993197676	0.9060219239157403	T	T	T
0.1921991824818431	0.6465965974730000	0.0131039480585157	T	T	T
0.0904033996314939	0.6744016509499098	0.8926212086497697	T	T	T
0.1017602892241482	0.6549372849787587	0.6971828056566923	T	T	T
0.2277621209953968	0.6359247115323270	0.7469423708167371	T	T	T
0.3201170648713094	0.5511646854032789	0.8142074643456582	T	T	T
0.0831393357288797	0.5514140963538701	0.8209076255580532	T	T	T
0.4319865051159448	0.3744447906068872	0.5803062471330706	T	T	T
0.4177527256628358	0.5050983646163443	0.5569942414355291	T	T	T
0.4119775350638342	0.6379145959049612	0.5547887737771943	T	T	T
0.1935786850193895	0.3727004912061799	0.6075661106749775	T	T	T
0.1892871894452822	0.5000821204628220	0.5500149710465092	T	T	T

Structure files (CONTCAR) involved in this work:

0.1909019721900926	0.6344357619269375	0.5544906957971992	T	T	T
0.9959167495293880	0.4529686239551777	0.7831186297038782	T	T	T
0.9845047402227469	0.6359726013626108	0.7844325165552836	T	T	T
0.1445781391190923	0.5594775840105238	0.2075753640126028	T	T	T
0.2033348842541067	0.5701083618166088	0.3843064201360450	T	T	T
0.3021404620757954	0.5655229037941211	0.5217021504357926	T	T	T
0.3996057139864305	0.5706718700720502	0.3869215985101976	T	T	T
0.4018287740427107	0.5553285977027369	0.1915520445449948	T	T	T
0.2737013543098175	0.5324937236248610	0.2273127943115801	T	T	T
0.1418606481175378	0.3304490046549670	0.2387211955882883	T	T	T
0.1952794035299055	0.3407695830687018	0.4151386466273319	T	T	T
0.3090132399513472	0.3542011850213886	0.5147406923686920	T	T	T
0.4111052626457706	0.3286186130560690	0.3949259539317646	T	T	T
0.3956467488395193	0.3388619587490912	0.1983299039113368	T	T	T
0.2712539613717797	0.3569200962446561	0.2529120766301006	T	T	T
0.1825963551907264	0.4499025471733962	0.3039140321144247	T	T	T
0.4112936917051244	0.4485261939904743	0.3108027836779003	T	T	T
0.0693932623233433	0.6224288288827465	0.0738960062242655	T	T	T
0.0858698559664535	0.4915096425707475	0.0562687316078178	T	T	T
0.1095180543631709	0.3594728632243828	0.0504355203444666	T	T	T
0.3112844347070448	0.6253975827685369	0.0943304073902630	T	T	T
0.3275852841533207	0.4949068041761910	0.0549801177588462	T	T	T
0.3041119929494510	0.3621315655482625	0.0584480071881631	T	T	T
0.5126209048076353	0.5336909213703472	0.2947893444178363	T	T	T
0.5127221782256559	0.3633747898905491	0.2777486567223759	T	T	T
0.4410356858336157	0.7506359003386274	0.6451023329566226	T	T	T
0.1930531246865187	0.7488822400015323	0.6519879713720820	T	T	T
0.2727590835171145	0.7488895062397205	0.0567319792549228	T	T	T
0.1083159822249286	0.7482937471192911	0.0532774994286067	T	T	T
0.0622088087438039	0.2501181553821981	0.1357820380918945	T	T	T
0.3040084599061649	0.2465657675195420	0.1515905249503576	T	T	T
0.2268363744934722	0.2514609965587655	0.5556455676651401	T	T	T
0.3900909048872497	0.2508048767370694	0.5522286984539193	T	T	T
0.5584563893719302	0.2515956862752067	0.3625128496056029	T	T	T
0.8114436819656411	0.2494926796846686	0.3708099353666418	T	T	T
0.7256162928044777	0.2526154648943064	0.9601034802886572	T	T	T
0.8899269540319950	0.2488226167392772	0.9485676410602824	T	T	T
0.9363269010772304	0.7483513553262153	0.8645684181483074	T	T	T
0.6868597177564334	0.7596006273652696	0.8635423449719331	T	T	T
0.7728511097717859	0.7500378001328812	0.4863561657419958	T	T	T
0.6042844705533242	0.7491005648122961	0.4569719203334677	T	T	T
0.8855077221369512	0.4213402036244497	0.6044016482681908	T	T	T
0.0143570838287473	0.5399736651774971	0.5177418802184132	T	T	T
0.9308250809122113	0.5477687981111493	0.5598053345826680	T	T	T
0.9464706575035935	0.5415384441291387	0.4302813942054321	T	T	T
0.9061542265301444	0.4159759255532579	0.4686524397232428	T	T	T
1.0000143754550754	0.4213279009947397	0.5513412868808031	T	T	T
0.9715355556860532	0.4222423365817654	0.4316110513964082	T	T	T
0.9629478423791824	0.5232257709843022	0.5038240795161386	T	T	T
0.9604035678967618	0.4458105492689368	0.5062816864834415	T	T	T

Figure 5(c) TS3

Si Al O Ga H C

1.00000000000000

Structure files (CONTCAR) involved in this work:

20.0219999999999985 0.0000000000000000 0.0000000000000000
0.0000000000000000 19.8990000000000009 0.0000000000000000
0.0000000000000000 0.0000000000000000 13.3829999999999991
93 3 192 1 6 2

Selective dynamics

Direct

0.4235412953019688	0.0554374313707159	0.6469928850560820	T	T	T
0.3024589422935418	0.0256768579179423	0.7881163702197397	T	T	T
0.2805462283809210	0.0602116234110479	0.0108245609093420	T	T	T
0.1210734891052040	0.0638624489021175	0.0118605684811139	T	T	T
0.0687684563132427	0.0293406385617833	0.8003318906911567	T	T	T
0.1774330515067217	0.0544001491829222	0.6501843894718699	T	T	T
0.4200417898156378	0.8264124783544883	0.6692657799721409	T	T	T
0.3034649609111290	0.8676307281704609	0.8100920975949732	T	T	T
0.2687080031951671	0.8282509954067240	0.0308924156341055	T	T	T
0.1137855508764259	0.8264913360672861	0.0183773165946223	T	T	T
0.0640171578288315	0.8708301269061358	0.8044114320328105	T	T	T
0.1806899763682384	0.8282758837775759	0.6733184067894044	T	T	T
0.0750458838480555	0.9434833908218337	0.1488969056029385	T	T	T
0.1962527416904113	0.9727250809311274	0.2925031867091702	T	T	T
0.2176726254460297	0.9366003220904368	0.5124965145155750	T	T	T
0.3769935661790691	0.9327288244987855	0.5143171202785317	T	T	T
0.4306716391619954	0.9704070202871578	0.3051028845140444	T	T	T
0.3214091519073095	0.9455478142210542	0.1544569471174823	T	T	T
0.0789453932112776	0.1723897744941649	0.1653840133392916	T	T	T
0.1960347433017164	0.1297676595681424	0.3084527211546674	T	T	T
0.2320145575326664	0.1724965335596220	0.5258017888910002	T	T	T
0.3867722801269246	0.1732904913248446	0.5135077358011471	T	T	T
0.4359869710589581	0.1278910202984506	0.3032004415709524	T	T	T
0.3186373188461228	0.1667011671041385	0.1705384486789013	T	T	T
0.5842803781654079	0.5525004002062823	0.3525546251376182	T	T	T
0.6935348090219358	0.5305100500350568	0.1885225393804068	T	T	T
0.7201930189116827	0.5664266861083407	0.9750349944398116	T	T	T
0.8774577858382162	0.5668145785561585	0.9924284716040128	T	T	T
0.9335755297858588	0.5301765649258242	0.1958646469428534	T	T	T
0.5763760015186158	0.3293637127541594	0.3343099176313914	T	T	T
0.6979329099437203	0.3763091185858778	0.2034392266377884	T	T	T
0.7327484974639571	0.3286708864738749	0.9896837149023503	T	T	T
0.8843805968394665	0.3270314127879130	0.9833731420283646	T	T	T
0.9361929318267030	0.3744031661040347	0.1913085860807920	T	T	T
0.9333454439428102	0.4463667500235277	0.8630349973792948	T	T	T
0.7847279620930203	0.4389837068006599	0.4957618925752063	T	T	T
0.6277183807704187	0.4283028657949266	0.4939368549478766	T	T	T
0.5697618566706381	0.4702111208579436	0.7049343647453181	T	T	T
0.6748637958886793	0.4373155471397702	0.8552617302116137	T	T	T
0.9214660053451160	0.6720899581785333	0.8331064032828903	T	T	T
0.8014131813126989	0.6373943444296378	0.6928658055164779	T	T	T
0.7717219825271756	0.6710348036377776	0.4724209291132712	T	T	T
0.6162420398654461	0.6708031627201163	0.4875507193849327	T	T	T
0.5694664919834385	0.6282961671922660	0.7047694247662124	T	T	T
0.6867075125829909	0.6832489420471703	0.8259943702854420	T	T	T
0.5755121078368074	0.9434947277930027	0.3628403053288345	T	T	T
0.6947270586946843	0.9747194411773302	0.2200591003851423	T	T	T

Structure files (CONTCAR) involved in this work:

0.7183531514269582	0.9431663627426611	0.9983127959914250	T	T	T
0.8780563711552858	0.9333541112510111	0.9936373661303868	T	T	T
0.9298990287185278	0.9711667756567153	0.2034130117934521	T	T	T
0.8202650033768637	0.9474859302740134	0.3558122212887746	T	T	T
0.5794283174040007	0.1743638211523011	0.3345258077596253	T	T	T
0.6959158783232327	0.1301893847195967	0.1969626829623583	T	T	T
0.7309359928185499	0.1728696937775495	0.9764878022800313	T	T	T
0.8853745991927441	0.1739098610098949	0.9904152362022045	T	T	T
0.9333980841691533	0.1288600961592853	0.2014379081190266	T	T	T
0.8173570788159678	0.1688042731048693	0.3336236846210576	T	T	T
0.9241959927475016	0.0567272854548769	0.8610013405662196	T	T	T
0.8040321634479564	0.0295995414217577	0.7198452398796912	T	T	T
0.7808292159028397	0.0636501748967838	0.4967923223473096	T	T	T
0.6210482375877199	0.0678749335986983	0.4934394808667566	T	T	T
0.5687465980713614	0.0309779140224842	0.7019488715521393	T	T	T
0.6778809690755796	0.0573508352306716	0.8547435803900519	T	T	T
0.9197419710951128	0.8261466479293980	0.8383164398510066	T	T	T
0.8029782335232831	0.8729073343193618	0.7017692526999563	T	T	T
0.7670671597280719	0.8312051495728084	0.4823249796075766	T	T	T
0.6124872660306450	0.8249683215038450	0.4925552048610052	T	T	T
0.5629170492996933	0.8743561236024268	0.6998255571580584	T	T	T
0.6778806191727798	0.8378015901027075	0.8374874140992193	T	T	T
0.4249702542761299	0.4450797754371261	0.6449964835139518	T	T	T
0.3047407223685447	0.4738413556130155	0.7912261345629434	T	T	T
0.2894333418899404	0.4335829029904646	0.0113570775582872	T	T	T
0.1329568110973445	0.4332855311471082	0.0126897832057977	T	T	T
0.0822029577142429	0.4741697158269910	0.8064780636625813	T	T	T
0.1824282986477088	0.4491070811940999	0.6464975087394812	T	T	T
0.4268073035808748	0.6715651843739652	0.6667851705804025	T	T	T
0.3028755506131812	0.6305916774535149	0.8015950047081555	T	T	T
0.2713916977779405	0.6723932885273635	0.0210104824517137	T	T	T
0.1177164246075040	0.6738174620535308	0.0137669471975797	T	T	T
0.0693366576021531	0.6304389321370160	0.8050197868620190	T	T	T
0.1801563266112493	0.6699461417364023	0.6639540646706884	T	T	T
0.0803393975062047	0.5546371170374499	0.1418363111962827	T	T	T
0.2033774146388047	0.5283907483517637	0.2825158318431670	T	T	T
0.2226706907969788	0.5671358629951915	0.5059667757143352	T	T	T
0.3819670164945069	0.5681093214069106	0.5100832940876785	T	T	T
0.4317622255044753	0.5266158189662504	0.3027150419070136	T	T	T
0.3312164889790271	0.5529506678529246	0.1433904080069421	T	T	T
0.0825926098526353	0.3273913137669121	0.1601548873848249	T	T	T
0.1986233773144937	0.3701396918800955	0.3045578153746903	T	T	T
0.2329717476804244	0.3292277097687047	0.5265821877490017	T	T	T
0.3870369986858441	0.3265781204668385	0.5185438426215573	T	T	T
0.4314388506479242	0.3709041840758975	0.3031622452584660	T	T	T
0.3200735141357577	0.3248162303588973	0.1672728456086500	T	T	T
0.8212084558148074	0.3303041863612715	0.3276947189773586	T	T	T
0.7984001113272501	0.4750396274248104	0.7278856326100365	T	T	T
0.8148145104345476	0.5583369654413217	0.3335540264139406	T	T	T
0.3580791593131684	0.0611321335461577	0.7178787957567008	T	T	T
0.3000606145066108	0.0656471376600443	0.8936819250049105	T	T	T
0.2005218327199481	0.0508010155584712	0.0260329197630741	T	T	T
0.1019221767153242	0.0686183156148972	0.8946189516162092	T	T	T

Structure files (CONTCAR) involved in this work:

0.1028279675331286	0.0555478979667603	0.6973842212229870	T	T	T
0.2294666818274420	0.0299121110507751	0.7359210848348069	T	T	T
0.3590502256880225	0.8252532868011657	0.7490710065940882	T	T	T
0.3052759758112809	0.8425230026702967	0.9249827106252237	T	T	T
0.1910072314224321	0.8522609710592401	0.0224447837350079	T	T	T
0.0864328972563023	0.8308610972426951	0.9047242084678701	T	T	T
0.1036049303559849	0.8389419654281084	0.7089571264770848	T	T	T
0.2296927691263007	0.8541254120729729	0.7626218224543353	T	T	T
0.3215617946491534	0.9471123152503698	0.8047026026514845	T	T	T
0.0830247782679414	0.9496147490520200	0.8156723528199398	T	T	T
0.4316846332212866	0.1245421701883022	0.5832829885158280	T	T	T
0.4177338093469339	0.9928048306614787	0.5693379271650618	T	T	T
0.3955830138094357	0.8612078606242262	0.5655513618656041	T	T	T
0.1948623727330722	0.1297193498183695	0.6122272566177756	T	T	T
0.1792631228304088	0.0022338843882919	0.5566693845154189	T	T	T
0.1944160244381549	0.8687718935824787	0.5701490404686878	T	T	T
0.9895864304932479	0.0451510796221455	0.7914379160674117	T	T	T
0.9840623278101174	0.8630518578386701	0.7872457907567858	T	T	T
0.1404456182993294	0.9401727612540418	0.2198739138720092	T	T	T
0.1983477919413269	0.9291978789962008	0.3952430644562908	T	T	T
0.2975776404701179	0.9475575362452195	0.5265473384969040	T	T	T
0.3976402424989863	0.9286865618927291	0.3974134002815620	T	T	T
0.3960995731705197	0.9474487289526069	0.2008613414653665	T	T	T
0.2691145421537101	0.9705594788932118	0.2396595571317995	T	T	T
0.1405806708488520	0.1694221249679163	0.2435340124789683	T	T	T
0.1950615184256178	0.1625132943551094	0.4191437621638420	T	T	T
0.3092988181816598	0.1479633779866332	0.5163761778823938	T	T	T
0.4135599295796991	0.1725454781376368	0.3992676426177296	T	T	T
0.3955974309288063	0.1541577923487558	0.2049263894949117	T	T	T
0.2695800307666959	0.1384674134810413	0.2583029162498699	T	T	T
0.1771764920040831	0.0505736794672940	0.3157316873421356	T	T	T
0.4175179750455992	0.0499070960833090	0.3255057676549024	T	T	T
0.0675904014523427	0.8718764626814821	0.0914071933966833	T	T	T
0.0810598256110593	0.0025402174534794	0.0651231470731010	T	T	T
0.0994919273618244	0.1345702907981926	0.0624978208268052	T	T	T
0.3050788989815676	0.8691763297554498	0.1201135473044779	T	T	T
0.3179513782688100	0.9949639459751868	0.0578132909551701	T	T	T
0.3046187333293873	0.1287768359517358	0.0654053780573057	T	T	T
0.5097439592664122	0.9550436984367547	0.2940664456970550	T	T	T
0.5156738525793387	0.1360771369109366	0.2838213336312343	T	T	T
0.6372414852545994	0.5624710665512233	0.2632360494425957	T	T	T
0.6862327967693976	0.5726536251167293	0.0841644672981228	T	T	T
0.7994429007282020	0.5462543911865922	0.9847429032303758	T	T	T
0.9031128914185540	0.5768448980372733	0.1068443139738333	T	T	T
0.9015093077688211	0.5471706947273889	0.3044861405467648	T	T	T
0.7678658747683593	0.5379295125796094	0.2304232304522300	T	T	T
0.6351538232895699	0.3367333704104167	0.2533391238090088	T	T	T
0.7202710879528246	0.3298795589445440	0.1087569804508898	T	T	T
0.8088893894093396	0.3555242196819756	0.9663668425661331	T	T	T
0.9061722783218822	0.3297852854484375	0.0996818172220165	T	T	T
0.9027632327337487	0.3504223239608910	0.2942046983691422	T	T	T
0.7592307150043580	0.3802990078361068	0.2806261208592456	T	T	T
0.6749033740137595	0.4511330365351042	0.1675909916423927	T	T	T

Structure files (CONTCAR) involved in this work:

0.9204090795004788	0.4526503970219518	0.1644266947373879	T	T	T
0.5732521926398431	0.6224351897149524	0.4134303027620932	T	T	T
0.6121199679561258	0.4952701510385042	0.4293839611227842	T	T	T
0.5959973997544759	0.3626668090553706	0.4412328161216705	T	T	T
0.8052559946925066	0.6395043413754324	0.3754369427990518	T	T	T
0.8008267549640290	0.5029257765108883	0.4319873170267527	T	T	T
0.8285466408857496	0.3695818937870524	0.4545380612081890	T	T	T
0.0140552363821070	0.5437567338246924	0.2102155026846280	T	T	T
0.0172361642897706	0.3674164941152332	0.1991599452379640	T	T	T
0.8803970981558256	0.4481712000996021	0.7688343218729905	T	T	T
0.8202611065971910	0.4453715749472700	0.6060874116797084	T	T	T
0.7082268633138253	0.4162600523275565	0.5047794573291033	T	T	T
0.5967808890853348	0.4336740294155837	0.6046939754236297	T	T	T
0.6013097588837548	0.4352563917510879	0.8032397958228171	T	T	T
0.7332554053589987	0.4300049384741181	0.7733796739492439	T	T	T
0.8677711415625413	0.6706511604701357	0.7437140114014663	T	T	T
0.8111871749164109	0.6465560811128754	0.5733958251496134	T	T	T
0.6936322086975742	0.6473446025825299	0.4856409134118250	T	T	T
0.5869480418988903	0.6650480239795713	0.6002092441264426	T	T	T
0.6104227131203975	0.6627193761927735	0.7961135963687744	T	T	T
0.7345446308904184	0.6785963878238527	0.7275478939178116	T	T	T
0.7947210522292307	0.5605009313379128	0.7279703691772575	T	T	T
0.5894729206051822	0.5493189062179086	0.6987007173782411	T	T	T
0.9344408106062241	0.3734657261584400	0.9162130020267243	T	T	T
0.9211120731186978	0.5060128894436928	0.9418010990955276	T	T	T
0.8929674665577065	0.6359544013397339	0.9331240558182649	T	T	T
0.6782003493738074	0.3751463583161502	0.9339508610054348	T	T	T
0.6814336011141593	0.5087550024526675	0.9131021726880212	T	T	T
0.7145288044993712	0.6375302342710258	0.9168905584057876	T	T	T
0.4893537485569183	0.4614817213772267	0.7130496836008157	T	T	T
0.4893873684981616	0.6368524291860642	0.7249733494067765	T	T	T
0.6406475312007018	0.9378725182297989	0.2914513915945633	T	T	T
0.6987055635718424	0.9346125463001331	0.1148391797920691	T	T	T
0.7987781867800926	0.9481051201927143	0.9828956372819697	T	T	T
0.8993856840739386	0.9285422254687498	0.1102469026064907	T	T	T
0.8946542175263462	0.9485909673808396	0.3071807326933529	T	T	T
0.7680423477528799	0.9735512608026369	0.2713867387393938	T	T	T
0.6417491847863329	0.1747978293543655	0.2576258017139900	T	T	T
0.6958631010615420	0.1566223975415449	0.0827029845624311	T	T	T
0.8085813886790136	0.1477127476815480	0.9812339219665580	T	T	T
0.9087026928737882	0.1735749499090893	0.1065175302496714	T	T	T
0.8950363055856742	0.1533470147459935	0.3017204492133258	T	T	T
0.7697758497654457	0.1364917375079783	0.2462382794192374	T	T	T
0.6720992029369963	0.0520413140224688	0.2011210685180205	T	T	T
0.9174063265862834	0.0502452737339464	0.1792928508382704	T	T	T
0.5660526070128189	0.8732980216579498	0.4234332648665181	T	T	T
0.5815016744956569	0.0054920038866557	0.4417781657916247	T	T	T
0.6006118305750227	0.1377402577847317	0.4385674496452681	T	T	T
0.8027674114982277	0.8716250674598636	0.3912379917975801	T	T	T
0.8184458810914170	0.9978902684499488	0.4514160937090615	T	T	T
0.8037589759374911	0.1318388408407600	0.4405764448394314	T	T	T
0.0092895717396866	0.9561198892758250	0.2167184242573687	T	T	T
0.0135976939730993	0.1386570772420561	0.2169970588511635	T	T	T

Structure files (CONTCAR) involved in this work:

0.8590956270636840	0.0660607903902263	0.7903097240259379	T	T	T
0.8013295020948384	0.0691279843062933	0.6139275433857273	T	T	T
0.7005790748743672	0.0537650089982515	0.4837624199784192	T	T	T
0.5997870825719243	0.0747525294303141	0.6102339668072936	T	T	T
0.6035107123860759	0.0513589967977926	0.8073047630208970	T	T	T
0.7305229682552791	0.0322580352313493	0.7703844157216145	T	T	T
0.8574174494191840	0.8277823921543099	0.7613273752131233	T	T	T
0.8037886945740224	0.8502288807251899	0.5863642928258164	T	T	T
0.6887427218204212	0.8532649927291225	0.4887141759660429	T	T	T
0.5857340027540303	0.8269538565889477	0.6071901703633232	T	T	T
0.6014954706396011	0.8505046870638764	0.8003805907886186	T	T	T
0.7290028123744653	0.8624336030287224	0.7498007720716238	T	T	T
0.8254338221854194	0.9513247651729974	0.7078508450794653	T	T	T
0.5813369163583313	0.9521559878508048	0.6755756240635024	T	T	T
0.9340623786682055	0.1254064735545973	0.9254094406077725	T	T	T
0.9179598766002722	0.9937313443146524	0.9377255902273367	T	T	T
0.8985316823473869	0.8622250321384243	0.9425319921220043	T	T	T
0.6922052432160433	0.1346833301445928	0.8862967411293087	T	T	T
0.6840462225023655	0.0112411741887231	0.9547111095939937	T	T	T
0.6901911333111187	0.8782368969346092	0.9402627555246224	T	T	T
0.4894337829094516	0.0459008277070179	0.7156921897203219	T	T	T
0.4827675045902517	0.8669701959718688	0.7176463514486113	T	T	T
0.3604981480570365	0.4429517815389275	0.7177388950196663	T	T	T
0.3016580582305090	0.4285592839016170	0.8918316222866639	T	T	T
0.2109375893566446	0.4490237034571978	0.0357130443663342	T	T	T
0.1204422813404191	0.4316178647709588	0.8924136635060202	T	T	T
0.1073704812605524	0.4545144443699745	0.6941939314447239	T	T	T
0.2332016393323861	0.4710250105109816	0.7342458279614382	T	T	T
0.3605313177678763	0.6650873860350353	0.7353817267127167	T	T	T
0.3001635503859497	0.6692334776841717	0.9078411776970324	T	T	T
0.1941451661721958	0.6460449201861630	0.0220069293811751	T	T	T
0.0950183204163233	0.6763528695848257	0.8972573738638416	T	T	T
0.1035692786661758	0.6565262904671075	0.7015018186196340	T	T	T
0.2309238553305387	0.6370686152291239	0.7454801479924982	T	T	T
0.3197192942239528	0.5516050309373772	0.8201378735363200	T	T	T
0.0927455550179964	0.5534940889343700	0.8275130443178964	T	T	T
0.4337700527058399	0.3726794368883715	0.5901189157237628	T	T	T
0.4164692582047865	0.5018320191070725	0.5584344038794887	T	T	T
0.4131429912073463	0.6353483659583170	0.5596807734370708	T	T	T
0.1924195220823162	0.3723134949665484	0.6101094924811495	T	T	T
0.1870027298203756	0.4995341577820802	0.5509127218456067	T	T	T
0.1895462100090587	0.6337326401798652	0.5557499593392796	T	T	T
0.0034651336633206	0.4555096358024123	0.8035833175965378	T	T	T
0.9887955168162889	0.6333379830735589	0.7935792334956007	T	T	T
0.1439740292879188	0.5617594798343151	0.2163109632425396	T	T	T
0.2079580843119611	0.5697748538449291	0.3870458097938028	T	T	T
0.3018212278987287	0.5645972379563227	0.5310997958797087	T	T	T
0.3967466712735586	0.5702271557943528	0.3914365149147845	T	T	T
0.4039247547697645	0.5564156287346995	0.1971074981593358	T	T	T
0.2742176281071885	0.5333664962669803	0.2253828316975570	T	T	T
0.1389410570325067	0.3314685653105295	0.2470616331322552	T	T	T
0.1994110510532207	0.3418943675010847	0.4179327385177881	T	T	T
0.3102750316865541	0.3541476410386977	0.5260966099727439	T	T	T

Structure files (CONTCAR) involved in this work:

0.4101099552878337	0.3300247718850527	0.4030143939139840	T	T	T
0.3959099265318197	0.3362753734428435	0.2066271946342249	T	T	T
0.2697295507835840	0.3565013740118667	0.2506158816979847	T	T	T
0.1838240869910662	0.4505982529065339	0.3059205164764838	T	T	T
0.4075722457759202	0.4486930515882394	0.3139921996029981	T	T	T
0.0704738114349148	0.6233004966880125	0.0777440126454623	T	T	T
0.0883071793788412	0.4920586141595631	0.0643516575622883	T	T	T
0.1112518743439947	0.3607740489082855	0.0573147870534264	T	T	T
0.3155759329276724	0.6258002487515101	0.0946941607068735	T	T	T
0.3331667369714511	0.4950409072257069	0.0573244321407115	T	T	T
0.3101579281668731	0.3619798736079582	0.0601304461746725	T	T	T
0.5121948012315347	0.5305760699671463	0.3068746562706186	T	T	T
0.5112908089983588	0.3670711479180370	0.2878260998279555	T	T	T
0.4418616434322936	0.7499316338221999	0.6443099697765068	T	T	T
0.1942786790040654	0.7493230913310081	0.6505484931811417	T	T	T
0.2743888855688546	0.7493074618333808	0.0599400628662762	T	T	T
0.1104080952447346	0.7492285657000468	0.0578566157621462	T	T	T
0.0638233570867448	0.2500778762597631	0.1367489565948587	T	T	T
0.3045588865388014	0.2458766742395674	0.1518217748359607	T	T	T
0.2274115016043040	0.2509989105321430	0.5577363363863372	T	T	T
0.3916249883493531	0.2494197710884383	0.5566471680270925	T	T	T
0.5588517199072189	0.2514110024445193	0.3578622877591031	T	T	T
0.8039192493295541	0.2474340940156070	0.3450299192646312	T	T	T
0.7266429024075897	0.2520049358065046	0.9500853086553906	T	T	T
0.8912797446280312	0.2498301201461135	0.9458764369159363	T	T	T
0.9398884800072977	0.7488609309953834	0.8626178573666785	T	T	T
0.6883117789779062	0.7598142568683875	0.8656754428066062	T	T	T
0.7740845168360861	0.7522326998780097	0.4626577051226312	T	T	T
0.6079433593217147	0.7484720541049474	0.4512240382003196	T	T	T
0.9216119251531019	0.4338543337927124	0.6285984116230330	T	T	T
0.0388549112728947	0.4838842683585016	0.5626726823917191	T	T	T
0.8769474863984470	0.3759617582868739	0.4611810766865139	T	T	T
0.0274006873269737	0.4494516226976473	0.4351098511766169	T	T	T
0.0253539800200423	0.5655768248254397	0.3799395463188571	T	T	T
0.9940918293041507	0.5953151798121185	0.5030905424091671	T	T	T
0.9503232668373126	0.5489867765292463	0.3940082502530746	T	T	T
0.0203272925150053	0.4916048199286949	0.4868707457270718	T	T	T
0.9980867413730142	0.5534447735916834	0.4505334256481044	T	T	T

Figure 7(a) ①

Si O Al Zn C H

1.0000000000000000

20.0219999999999985 0.0000000000000000 0.0000000000000000

0.0000000000000000 19.8990000000000009 0.0000000000000000

0.0000000000000000 0.0000000000000000 13.3829999999999991

93 194 3 2 2 8

Selective dynamics

Direct

0.4229895333669044 0.0598578222190368 0.6483589071279581 T T T

0.3056756877159781 0.0317690970281843 0.7922157090329456 T T T

0.2829479608427121 0.0556946078383812 0.0170793941906004 T T T

0.1239937795494480 0.0621469703191157 0.0122483486412374 T T T

0.0682021600700912 0.0310237266111110 0.8013696391344726 T T T

Structure files (CONTCAR) involved in this work:

0.1809222379907953	0.0644684492929312	0.6653309872984089	T	T	T
0.4192469781254792	0.8269962591559318	0.6689599523969082	T	T	T
0.3012841805033724	0.8728090008765468	0.8004194503923154	T	T	T
0.2675994114471266	0.8307676660538830	0.0198154063107731	T	T	T
0.1118547692193055	0.8270548190932728	0.0129539449824069	T	T	T
0.0661047031998504	0.8740642527025868	0.7989467806950713	T	T	T
0.1792813473565433	0.8283727389018769	0.6649058883218573	T	T	T
0.0761450614834507	0.9409531905025673	0.1495163088624790	T	T	T
0.1953217851728209	0.9695369701603623	0.2907334253733050	T	T	T
0.2171603810610050	0.9431458216157010	0.5165491345052583	T	T	T
0.3775368937626946	0.9349828754432772	0.5140450132560146	T	T	T
0.4338625886279458	0.9684244694575619	0.3018553861649701	T	T	T
0.3209208323607295	0.9352172302178474	0.1648448006721812	T	T	T
0.0830019634144595	0.1715806264668985	0.1662187607472573	T	T	T
0.1984408369071068	0.1281888358925229	0.3018811254339415	T	T	T
0.2320249948103819	0.1690259371952706	0.5191041659174480	T	T	T
0.3875802665825491	0.1734150141269470	0.5083657115246480	T	T	T
0.4352106137494769	0.1266179246918322	0.2948697926591325	T	T	T
0.3186995562222226	0.1720160299713188	0.1660875573107772	T	T	T
0.5772320115587474	0.5547122332697637	0.3604934013046815	T	T	T
0.6905472011944492	0.5260230740651460	0.2056587760547406	T	T	T
0.7135248595880412	0.5679264831028734	0.9917841754624607	T	T	T
0.8728865891470005	0.5732149262996226	0.9870478336116633	T	T	T
0.8102580601649825	0.5504430212020224	0.3448103980606872	T	T	T
0.5731059789847162	0.3282815700135230	0.3320657980800034	T	T	T
0.6931797564199091	0.3722122276590810	0.1926689908387656	T	T	T
0.7302362411959519	0.3280321104338044	0.9797104506898795	T	T	T
0.8852140384798134	0.3263880161677911	0.9950121632093081	T	T	T
0.9420115141549946	0.3742357102635310	0.1928596027098866	T	T	T
0.9188770027867932	0.4457586292198374	0.8604579098905958	T	T	T
0.8006129810136563	0.4736984312919748	0.7186895992872337	T	T	T
0.7749146268950073	0.4370274135829125	0.4957687596098119	T	T	T
0.6176987322933701	0.4276900704615111	0.4917712654616653	T	T	T
0.5695585766745654	0.4684028264811039	0.7027737590031424	T	T	T
0.6771898941553564	0.4495114337302780	0.8578710812184155	T	T	T
0.9204712793369326	0.6779589347972118	0.8279663975392726	T	T	T
0.7679233409873865	0.6684823913458919	0.4632121236954432	T	T	T
0.6130422522377671	0.6735208838047261	0.4885110965943720	T	T	T
0.5620802024914113	0.6266093595781426	0.6987457939798617	T	T	T
0.6756761181592980	0.6732293926604046	0.8286113168502997	T	T	T
0.5784178487314120	0.9454771252742717	0.3585829291745204	T	T	T
0.6985228427257744	0.9736972026188176	0.2144521845553417	T	T	T
0.7197181225616140	0.9377975021564370	0.9931873660501586	T	T	T
0.8796720194513373	0.9345938581996793	0.9950116446892429	T	T	T
0.9313994077695206	0.9704032364165917	0.2048726746841065	T	T	T
0.8221593057704446	0.9464459247872706	0.3546047890177491	T	T	T
0.5778855435296834	0.1732894312116914	0.3293241665322043	T	T	T
0.6983446555762736	0.1315736386565251	0.1936238942148979	T	T	T
0.7322974532561992	0.1720598064207174	0.9723003765124684	T	T	T
0.8871522637881869	0.1740806752238045	0.9828316315541507	T	T	T
0.9361677801825522	0.1282486258026627	0.1962718443935083	T	T	T
0.8210921406095084	0.1730453006366237	0.3302815770709610	T	T	T
0.9232583488437517	0.0545066340190171	0.8560288450295894	T	T	T

Structure files (CONTCAR) involved in this work:

0.8019732616306238	0.0257657038854117	0.7096293902273790	T	T	T
0.7814749251755722	0.0662544146829339	0.4916151219369715	T	T	T
0.6211157774656193	0.0702436774895322	0.4902735990855237	T	T	T
0.5684592889189702	0.0323423934648345	0.6992370527693311	T	T	T
0.6787084060748380	0.0537295973343503	0.8499462552763505	T	T	T
0.9230226548426559	0.8305535056593389	0.8369034019744747	T	T	T
0.8026804170480584	0.8682867760253176	0.6944250466460015	T	T	T
0.7695334177273190	0.8260307125329301	0.4770625649325468	T	T	T
0.6146420605478187	0.8268738991038614	0.4901710991462593	T	T	T
0.5639789632342165	0.8751451306414400	0.6982093816635562	T	T	T
0.6787309059934808	0.8325271663367306	0.8327768686180960	T	T	T
0.4232628349115982	0.4409839262879968	0.6482850138450630	T	T	T
0.3046623235696873	0.4686295404472010	0.7906248739686720	T	T	T
0.2792161673899784	0.4457733986830846	0.0175348527865488	T	T	T
0.1213887210104753	0.4377366000133109	0.0182000873833635	T	T	T
0.0644566531519634	0.4680362221134450	0.8046414445520454	T	T	T
0.1774137710494139	0.4353252996931579	0.6644623957915525	T	T	T
0.4169267823177950	0.6729517437676322	0.6685295503564492	T	T	T
0.3008152252125669	0.6272682191800307	0.8010618464392716	T	T	T
0.2683986108183547	0.6693126203478155	0.0212535246270612	T	T	T
0.1137814437935347	0.6733375258640554	0.0126451233851896	T	T	T
0.0659414802859687	0.6268108923540886	0.8001137419378337	T	T	T
0.1790327314370695	0.6707660262120645	0.6642774447755061	T	T	T
0.0780925585564259	0.5599557582561052	0.1505505573690809	T	T	T
0.1969927083641790	0.5283179137453137	0.2901393601474708	T	T	T
0.2148213541692296	0.5552249302835833	0.5168282672645459	T	T	T
0.3745112083621240	0.5648018706357711	0.5160285432999757	T	T	T
0.4312815341095956	0.5307370492770253	0.3051261193293852	T	T	T
0.3223439180873646	0.5639527012856360	0.1636992959413478	T	T	T
0.0860747232060938	0.3238276682333810	0.1644770073495837	T	T	T
0.1987597894947753	0.3702246486285050	0.3019137413803402	T	T	T
0.2306096881976337	0.3304451618259749	0.5198924432914429	T	T	T
0.3858007633877648	0.3275357677082590	0.5073795373119960	T	T	T
0.4314784040306674	0.3736343630112312	0.2934628701207281	T	T	T
0.3169496909673892	0.3291663859641624	0.1643565927995745	T	T	T
0.0115271974397981	0.5582939984834047	0.2299884146922594	T	T	T
0.3593272235865643	0.0704534505361719	0.7220504764537609	T	T	T
0.3176050317310756	0.0536104072774043	0.9074776865759078	T	T	T
0.2029974813936762	0.0450829125344854	0.0064758614506398	T	T	T
0.0930589583540772	0.0697708166481095	0.9012833951182453	T	T	T
0.1041748258460412	0.0638887497304314	0.7041706821050895	T	T	T
0.2300159375124115	0.0522700484253555	0.7606321493663701	T	T	T
0.3602001811370835	0.8277634591266713	0.7521222103595521	T	T	T
0.3013139516576119	0.8614649379944679	0.9199077320509944	T	T	T
0.1890669216333045	0.8516749093679465	0.0224401400812290	T	T	T
0.0881379019340701	0.8318069454595058	0.8975824858085607	T	T	T
0.1027054077719031	0.8409796825631326	0.7017891626685776	T	T	T
0.2291789411570635	0.8499025924186960	0.7555983460979895	T	T	T
0.3156493715238662	0.9513072539518800	0.7756310499563049	T	T	T
0.0889873048919051	0.9519597532794198	0.8108738628659016	T	T	T
0.4331750378976637	0.1270034912580599	0.5808418162355157	T	T	T
0.4124780334360296	0.9957838447131577	0.5751018283855072	T	T	T
0.3935158264205216	0.8636636096879757	0.5676336938963631	T	T	T

Structure files (CONTCAR) involved in this work:

0.1965103399323012	0.1376832531350940	0.6172973526759244	T	T	T
0.1904963822000766	0.0052318999590442	0.5835321656707115	T	T	T
0.1947020118141140	0.8716058060035349	0.5648430672965226	T	T	T
0.9882995718626033	0.0394830849120853	0.7869284419530199	T	T	T
0.9856627283626701	0.8698025048132459	0.7846604669232345	T	T	T
0.1405171605226615	0.9312413589814611	0.2219834774420633	T	T	T
0.1838170106260091	0.9487607264324486	0.4064175441615717	T	T	T
0.2976646384853671	0.9474692034571056	0.5091048091318552	T	T	T
0.4080103655032456	0.9313712056757277	0.4025164112962519	T	T	T
0.3970736223129401	0.9349688250869801	0.2057667438751878	T	T	T
0.2703794030437653	0.9475539016124026	0.2584572820895613	T	T	T
0.1393777171799479	0.1728712069295747	0.2532798207087525	T	T	T
0.1954108071362969	0.1376403678467611	0.4216944540695449	T	T	T
0.3103835196899921	0.1479754906417331	0.5160487599149172	T	T	T
0.4131227982628682	0.1682182117249773	0.3939250490204362	T	T	T
0.3958200156397455	0.1579353192076288	0.1987815474927172	T	T	T
0.2709636811747914	0.1528017372775445	0.2608489736746392	T	T	T
0.1860651735837045	0.0498735055169259	0.2730462924876049	T	T	T
0.4152378364361016	0.0479706074872893	0.3085278672120086	T	T	T
0.0651656287184748	0.8724030522157751	0.0851673548234033	T	T	T
0.0859355525201979	0.0023097334406959	0.0712516906989193	T	T	T
0.1119620003304306	0.1327740055240721	0.0690689441545291	T	T	T
0.3055579438757610	0.8621878884098400	0.1157694497123085	T	T	T
0.3130198138056026	0.9946078075003403	0.0829269863049157	T	T	T
0.2991374463163007	0.1277005859859964	0.0686101143963388	T	T	T
0.5134744535668009	0.9569772069326931	0.2878885365445859	T	T	T
0.5153175505368958	0.1333695509258441	0.2779010033203826	T	T	T
0.6404266974740448	0.5598586983805881	0.2861182382796452	T	T	T
0.6936543113949526	0.5751886979498865	0.1091080329788294	T	T	T
0.7933729125285222	0.5571328991280305	0.9774894566922474	T	T	T
0.8960669371698434	0.5817179933999099	0.1014175325237190	T	T	T
0.8873252948461094	0.5371781108369375	0.3148852952216175	T	T	T
0.7646314933310510	0.5217622773276387	0.2552584587376266	T	T	T
0.6393127428730192	0.3345803292935671	0.2646852373124834	T	T	T
0.6893520143015736	0.3358179200135508	0.0835030842041041	T	T	T
0.8077573559454749	0.3508881298992408	0.9955054785750928	T	T	T
0.9127791883181482	0.3221438322096037	0.1095416818886956	T	T	T
0.9052697689598537	0.3604966901308864	0.3009197789851261	T	T	T
0.7666256725662091	0.3680371555510489	0.2394033256372579	T	T	T
0.6679999675627439	0.4501426803306221	0.1777247550838995	T	T	T
0.9321800658687196	0.4498559759225065	0.1558012247753423	T	T	T
0.5674166625028207	0.6263534941904748	0.4167236331347690	T	T	T
0.5874068479474034	0.4963695915447600	0.4440449305333341	T	T	T
0.5825363353669729	0.3624730203647358	0.4418269082717970	T	T	T
0.7960426680179928	0.6301515274626450	0.3639388889245367	T	T	T
0.7933744110769583	0.5134308675279983	0.4531345250917339	T	T	T
0.8221676328135598	0.3825623413256276	0.4405566147266355	T	T	T
0.0213500747300630	0.3603028122913754	0.2111785967669441	T	T	T
0.8548647757214896	0.4342876264305011	0.7873359076729289	T	T	T
0.7863438201272397	0.4335400254840752	0.6152332056230853	T	T	T
0.6972208096517458	0.4232757515067409	0.4688371691305817	T	T	T
0.6031989457001834	0.4268822340805594	0.6107980809978067	T	T	T
0.6037828053214945	0.4453227775125203	0.8068290451833575	T	T	T

Structure files (CONTCAR) involved in this work:

0.7300936663526688	0.4797827567592233	0.7771423334655354	T	T	T
0.8689781857332824	0.6807176015220312	0.7360104744608489	T	T	T
0.8129569447395063	0.6438921918668806	0.5580974909787941	T	T	T
0.6903609798925346	0.6480716580498878	0.4845653461345573	T	T	T
0.5855568661135238	0.6695766203889602	0.6019061950883491	T	T	T
0.5980077339893146	0.6571676980602330	0.7974266714138737	T	T	T
0.7250257087552255	0.6500352957469887	0.7401381853456385	T	T	T
0.8283484475884814	0.5490575906092058	0.6919975433485328	T	T	T
0.5813061294219424	0.5480685976769142	0.6825712311601990	T	T	T
0.9290752089843131	0.3789088739673599	0.9289723113396503	T	T	T
0.9119275012711747	0.5116856797439253	0.9308130468763942	T	T	T
0.8901728640910075	0.6423738087219926	0.9268427054032597	T	T	T
0.6977259938933763	0.3744435170025482	0.8927885739788654	T	T	T
0.6745465658969175	0.5012858843703445	0.9513570058622441	T	T	T
0.6902683380841161	0.6352687005799268	0.9341342121758610	T	T	T
0.4904821349788300	0.4512758858697387	0.7133917854265055	T	T	T
0.4813394087463225	0.6328003282935533	0.7115253023577591	T	T	T
0.6440266242948915	0.9400023840476067	0.2885211850612986	T	T	T
0.6987789882736820	0.9323744691853475	0.1099276716731295	T	T	T
0.8001228797138503	0.9463481853052956	0.9809055926084701	T	T	T
0.8993348373604352	0.9283345749408514	0.1122308169380593	T	T	T
0.8975571830599719	0.9481219674993647	0.3098477280816995	T	T	T
0.7719117145764277	0.9681474544176955	0.2649908256331979	T	T	T
0.6410575283677494	0.1723498987961258	0.2540686509193599	T	T	T
0.6971581663908019	0.1583090532390606	0.0794177859735637	T	T	T
0.8100934727895793	0.1481333852126229	0.9781627446440102	T	T	T
0.9141423421851345	0.1686821032637544	0.0965223714213798	T	T	T
0.8978157194889265	0.1573300985493176	0.2936020951346398	T	T	T
0.7712678982553869	0.1433306019416914	0.2433188162353972	T	T	T
0.6798760565685930	0.0519395287858528	0.1954154344994266	T	T	T
0.9187287615088205	0.0492787494708657	0.1816115163806281	T	T	T
0.5695455061834259	0.8756205457478786	0.4202194959548574	T	T	T
0.5832424866340469	0.0069777286077532	0.4382248691021146	T	T	T
0.5979437521873370	0.1392782823653567	0.4357280343656435	T	T	T
0.8076317086027754	0.8706266699649465	0.3934967868347549	T	T	T
0.8159478106019591	0.9983438207471107	0.4475222119046882	T	T	T
0.8081127598467147	0.1325243446107847	0.4346602649482940	T	T	T
0.0106014259614790	0.9543890399291789	0.2171546674954057	T	T	T
0.0164779462922216	0.1365481229360596	0.2116615329640657	T	T	T
0.8577598695627531	0.0549887628002119	0.7854982916844350	T	T	T
0.8013798557555655	0.0715405265232444	0.6092063517118156	T	T	T
0.7009443208210246	0.0594179551503476	0.4785253527749122	T	T	T
0.5999895692784906	0.0755570245342214	0.6072261067973095	T	T	T
0.6036554782721105	0.0521159635007945	0.8042877798205693	T	T	T
0.7291870097977217	0.0287384427827189	0.7624571102037787	T	T	T
0.8598267755630203	0.8334634048164921	0.7620856789395469	T	T	T
0.8053977820206367	0.8325938532762787	0.5854997152059942	T	T	T
0.6923244900061756	0.8512830356732012	0.4856851239423737	T	T	T
0.5886419174817850	0.8292692280487252	0.6048829429236290	T	T	T
0.6030460774157297	0.8527267184065275	0.7991616273434947	T	T	T
0.7296884577995362	0.8570007387769961	0.7446851358638930	T	T	T
0.8182717108436062	0.9479378097971743	0.6820305531602859	T	T	T
0.5793820878101783	0.9533309157366241	0.6727957886919894	T	T	T

Structure files (CONTCAR) involved in this work:

0.9320293363685115	0.1276946375443691	0.9086347608460194	T	T	T
0.9185611355339223	0.9974543733126282	0.9432241736179074	T	T	T
0.9031794849021163	0.8648426107766263	0.9428329839716012	T	T	T
0.6950982785503369	0.1298531329345040	0.8849079484300280	T	T	T
0.6833860619790104	0.0035020089059171	0.9455016620923644	T	T	T
0.6962287493942877	0.8695231172211876	0.9376091798171978	T	T	T
0.4895808394636000	0.0484125553224927	0.7146278920707612	T	T	T
0.4842447610330884	0.8644782509414523	0.7154977775244992	T	T	T
0.3601463692710285	0.4300249806568548	0.7234897120990693	T	T	T
0.3111247450714424	0.4454272334489523	0.9062411512804391	T	T	T
0.1991154084402910	0.4614392478644506	0.0148336756755305	T	T	T
0.0908896409210819	0.4335230509840833	0.9070887683158623	T	T	T
0.1020602733272643	0.4344955729542702	0.7091314581102987	T	T	T
0.2294566897075708	0.4500024226772618	0.7548044002175073	T	T	T
0.3590048723766567	0.6736389411796855	0.7537733549842940	T	T	T
0.3004401792902318	0.6379483306010713	0.9206577135453118	T	T	T
0.1900439382149772	0.6474650225441900	0.0267062524946391	T	T	T
0.0926380634653218	0.6679015658882510	0.8965160915183994	T	T	T
0.1018646558574569	0.6565793334332064	0.6994517010086411	T	T	T
0.2282062616253426	0.6482451837425187	0.7553121439445986	T	T	T
0.3165151479587219	0.5489952564881018	0.7763658760507715	T	T	T
0.0834962491250458	0.5476685859697675	0.8104904451013185	T	T	T
0.4320070915339351	0.3752301259549169	0.5772904630401358	T	T	T
0.4128803320743187	0.5062593306456015	0.5771705229998718	T	T	T
0.3870907360353355	0.6371751088212849	0.5685348522418036	T	T	T
0.1929622056370172	0.3621368571004794	0.6163080625338569	T	T	T
0.1822314505489497	0.4943385616529938	0.5806394683853832	T	T	T
0.1938566943429282	0.6276077104682459	0.5635843648137387	T	T	T
0.9852316302441946	0.4558334289267641	0.7912383868131411	T	T	T
0.9862641552325165	0.6363782918341229	0.7868172884953470	T	T	T
0.1432534492708805	0.5685972954189139	0.2204321411924695	T	T	T
0.1838597682163314	0.5514632811946781	0.4044369616333258	T	T	T
0.2951579690604799	0.5471622812299315	0.5138740760630377	T	T	T
0.4032753041540644	0.5692968709420921	0.4034109762361181	T	T	T
0.3979234197419415	0.5644701818784722	0.2062737380973120	T	T	T
0.2718562149668252	0.5487390118091773	0.2570189169583101	T	T	T
0.1432411004645685	0.3226755824350793	0.2505232439224809	T	T	T
0.1945112995945255	0.3614895353372496	0.4215840314922944	T	T	T
0.3086400908246915	0.3528323859727551	0.5189291467950300	T	T	T
0.4083301702964874	0.3308405249113152	0.3911081249951119	T	T	T
0.3940796434510152	0.3454369294934393	0.1936357611865550	T	T	T
0.2723625919206314	0.3488908532652035	0.2624215132352702	T	T	T
0.1834331774559327	0.4486126068095498	0.2736687086177119	T	T	T
0.4108328864611808	0.4517418353775430	0.3119661893447667	T	T	T
0.0662872608718795	0.6256132007442292	0.0818932846378669	T	T	T
0.0785322402315926	0.4922563436974872	0.0850512615523612	T	T	T
0.1145910180130675	0.3640021966435124	0.0675981919063282	T	T	T
0.3065884555115455	0.6375562440665908	0.1169835405681708	T	T	T
0.3148381959711291	0.5055332062180482	0.0801395566000290	T	T	T
0.2929481378867886	0.3729879856675755	0.0683664524258405	T	T	T
0.5111725864061191	0.5390046938941198	0.2945937366932300	T	T	T
0.5110981423296276	0.3655873457542773	0.2753488849125263	T	T	T
0.4368960143479211	0.7496607655999616	0.6411410634370891	T	T	T

Structure files (CONTCAR) involved in this work:

0.1891889687542297	0.7494116271368082	0.6372637034214722	T	T	T
0.2757858181547516	0.7499137995179175	0.0223930178218928	T	T	T
0.1050518407040765	0.7497247414961661	0.0507215933494769	T	T	T
0.0678304856405495	0.2480492994347053	0.1309489160814244	T	T	T
0.3082576059196603	0.2504532729911669	0.1362379861647599	T	T	T
0.2232896395374306	0.2497884445106343	0.5218942950642503	T	T	T
0.3930273039208497	0.2506930047487337	0.5459013458579599	T	T	T
0.5550367051216185	0.2499522504516867	0.3508122233899492	T	T	T
0.8106954217700592	0.2513604397066245	0.3481535904566821	T	T	T
0.7266726188823383	0.2506315606451243	0.9420507851410351	T	T	T
0.8923029021703616	0.2517771369581166	0.9462007009591071	T	T	T
0.9448542789259403	0.7533733257638158	0.8584843092159866	T	T	T
0.6841754055769151	0.7529003634205207	0.8511794484739162	T	T	T
0.7740774320404771	0.7483139180529773	0.4418720882526584	T	T	T
0.6077566304829496	0.7504649402610426	0.4491140390545580	T	T	T
0.9249355374875950	0.4743603419223367	0.5394215030999614	T	T	T
0.9530670906357721	0.6352379213500312	0.5687884656825821	T	T	T
0.9228697297298790	0.5304222374119694	0.1962473366601957	T	T	T
0.8204502829254385	0.3355789223414272	0.3273870650066336	T	T	T
0.8018585305629032	0.6349903719109454	0.6897190734114602	T	T	T
0.9264639743731783	0.4170713128776619	0.4303865793971628	T	T	T
0.8838871605523152	0.5565270910924490	0.5585267167820825	T	T	T
0.0296349217734152	0.4075671606550700	0.4358901990725396	T	T	T
0.0155341059930573	0.6006003567339573	0.3214725731317777	T	T	T
0.0438902355636646	0.4262561056136862	0.5094773704596373	T	T	T
0.0485847544150841	0.4369846249648092	0.3729357555917028	T	T	T
0.0351806513540696	0.3532218225737465	0.4252597087841696	T	T	T
0.0058872231898917	0.5677497931830326	0.3855256122306612	T	T	T
0.9773165074339293	0.6398202940348922	0.3164733434699690	T	T	T
0.0654626125692582	0.6226945727468602	0.3263369324878910	T	T	T
-0.0071390228549286	0.6226365655556664	0.6068791321655317	T	T	T
0.9302828219363530	0.6687082932988552	0.6115045691770247	T	T	T

Figure 7(a) ②

Si O Al Zn C H

1.0000000000000000

20.0219999999999985 0.0000000000000000 0.0000000000000000

0.0000000000000000 19.8990000000000009 0.0000000000000000

0.0000000000000000 0.0000000000000000 13.3829999999999991

93 194 3 2 2 8

Selective dynamics

Direct

0.4225145910203926	0.0595462020279037	0.6485790971729672	T	T	T
0.3046527330769712	0.0318463983893104	0.7919043640066751	T	T	T
0.2818899259769772	0.0552575296050650	0.0173199165380797	T	T	T
0.1225919070944530	0.0633013615570602	0.0125182209039261	T	T	T
0.0676461373429475	0.0311613610307614	0.8014393905950192	T	T	T
0.1803106424296463	0.0658254370393375	0.6658202060950762	T	T	T
0.4188690453185726	0.8275709831554494	0.6697123491556956	T	T	T
0.2996188299079197	0.8730636108760490	0.7987406948722796	T	T	T
0.2675371073269232	0.8310181912398678	0.0186560237244745	T	T	T
0.1114524012208293	0.8273177061370803	0.0148853352520468	T	T	T
0.0659690091405128	0.8745516316693552	0.8003938313738951	T	T	T

Structure files (CONTCAR) involved in this work:

0.1775004814913359	0.8281947968087702	0.6637394184448145	T	T	T
0.0750879838158960	0.9419974909358284	0.1505225682951956	T	T	T
0.1954957824146162	0.9696686431034366	0.2909158229845983	T	T	T
0.2163734241615811	0.9438216965367501	0.5173266638188068	T	T	T
0.3768563353435632	0.9346684952158603	0.5140671134908527	T	T	T
0.4327939452427373	0.9691126229954596	0.3020591936796849	T	T	T
0.3200707593997223	0.9341038671897350	0.1655308051932691	T	T	T
0.0814135831191259	0.1723801066486233	0.1673265695480100	T	T	T
0.1993442043147791	0.1283700395527703	0.2994747886882900	T	T	T
0.2311378082623752	0.1693642370200545	0.5176669321674392	T	T	T
0.3873743240106788	0.1737949974664249	0.5095335089772388	T	T	T
0.4340829010045409	0.1269678634599176	0.2955596353645836	T	T	T
0.3194458774840515	0.1729231388601215	0.1631845463214354	T	T	T
0.5762254684470663	0.5561967669727842	0.3587004314194410	T	T	T
0.6892145014505769	0.5269899442584213	0.2081244012539540	T	T	T
0.7140889038730488	0.5659421028108993	0.9912944918083224	T	T	T
0.8726871860019290	0.5727621040633052	0.9841058946021972	T	T	T
0.8112523032824268	0.5532442073164759	0.3444511695242868	T	T	T
0.5730503941455515	0.3286875442647796	0.3315271961378707	T	T	T
0.6918077789123380	0.3735441223855412	0.1934058376426763	T	T	T
0.7327469730810638	0.3300199658369773	0.9783456244091818	T	T	T
0.8878339143968322	0.3263538315981843	0.9886022652062167	T	T	T
0.9418734735978145	0.3739661128171693	0.1886212241862313	T	T	T
0.9202296177386901	0.4471350660967705	0.8568728492474786	T	T	T
0.8005068937148294	0.4770461200614841	0.7181969724941075	T	T	T
0.7801074081280237	0.4396971402939370	0.4946494614271119	T	T	T
0.6227020106157567	0.4295058847046270	0.4884633821978686	T	T	T
0.5716294397602319	0.4690795150599087	0.6993918351134321	T	T	T
0.6774712508361648	0.4492331182159207	0.8558441313649812	T	T	T
0.9196754287540166	0.6791745798324608	0.8270303106104885	T	T	T
0.7639296447847854	0.6706129653776188	0.4622002896615345	T	T	T
0.6095006863463263	0.6745126710619087	0.4881002237626965	T	T	T
0.5612419693483882	0.6273047151331043	0.6995096116651536	T	T	T
0.6736025752969880	0.6742264978006299	0.8328046639131765	T	T	T
0.5774132611650911	0.9471785476771991	0.3593109035835302	T	T	T
0.6978823152267047	0.9753506120366046	0.2160575108798184	T	T	T
0.7189005305383669	0.9397628775895174	0.9945181648895631	T	T	T
0.8786084710299499	0.9354913543067658	0.9960369212017353	T	T	T
0.9297055372118715	0.9721927533946116	0.2063805265472781	T	T	T
0.8213420196820720	0.9475424606791965	0.3564461032597717	T	T	T
0.5766176086714191	0.1742236525022295	0.3316235100697348	T	T	T
0.6974385254877227	0.1334024910934448	0.1957066572418414	T	T	T
0.7318001095412107	0.1733853688577835	0.9738208401017657	T	T	T
0.8865077932307541	0.1741258550780655	0.9806794966428488	T	T	T
0.9342123131523314	0.1305828901340935	0.1967184222026102	T	T	T
0.8198400394989040	0.1760157787644429	0.3329368113423026	T	T	T
0.9228957033906058	0.0536148252929104	0.8557640195388614	T	T	T
0.8000633372044272	0.0258300156656320	0.7105565961656976	T	T	T
0.7816061521470823	0.0675510106210622	0.4928575447888789	T	T	T
0.6211294990723116	0.0715469833770051	0.4916043570730387	T	T	T
0.5683950264727412	0.0326769079831831	0.7004350184364025	T	T	T
0.6772599503178905	0.0556575494557217	0.8519990106945103	T	T	T
0.9221764969912237	0.8316488813269628	0.8382502055351967	T	T	T

Structure files (CONTCAR) involved in this work:

0.8006496490435060	0.8675575312862540	0.6954881435740958	T	T	T
0.7666722422019481	0.8273333039993364	0.4777974389670526	T	T	T
0.6118646167326723	0.8279962995553666	0.4905326235319719	T	T	T
0.5629995570812544	0.8756787426653292	0.6996359804682074	T	T	T
0.6769590128961338	0.8323555388947457	0.8365252632996319	T	T	T
0.4245431326525159	0.4420458595039942	0.6436919940968739	T	T	T
0.3056586642024521	0.4689786708345285	0.7867008403037957	T	T	T
0.2796317962619853	0.4460712908713183	0.0132810665150286	T	T	T
0.1216531054687710	0.4365066127883552	0.0152667054003297	T	T	T
0.0649903305696005	0.4693293678707556	0.8031725495008682	T	T	T
0.1777669058285070	0.4353755477202273	0.6615838321055951	T	T	T
0.4167493791829522	0.6734831444679725	0.6677072224206095	T	T	T
0.2993425878703321	0.6274515690153601	0.7973183552904187	T	T	T
0.2683179790176683	0.6696932947415222	0.0180533991029612	T	T	T
0.1134738665310865	0.6738331740322149	0.0109117223699035	T	T	T
0.0653981220299066	0.6278649351145219	0.7992458572971713	T	T	T
0.1771700901195886	0.6707600593303805	0.6608849031397231	T	T	T
0.0783761900705689	0.5591667799252381	0.1472115205788861	T	T	T
0.1975666560574821	0.5286999523872088	0.2865206227027667	T	T	T
0.2145684638395325	0.5555817806422297	0.5139676757118395	T	T	T
0.3745351880656724	0.5664356738628457	0.5135022915649322	T	T	T
0.4298380790699161	0.5307239031677784	0.3033627682192070	T	T	T
0.3224768248106831	0.5645934550522835	0.1602776213256508	T	T	T
0.0858813797948039	0.3252775963271245	0.1641861184358077	T	T	T
0.1997548598957511	0.3708265361654586	0.2986580502941029	T	T	T
0.2299114760298229	0.3304316088088942	0.5179094271728476	T	T	T
0.3853704671342000	0.3272561510155288	0.5067066819531694	T	T	T
0.4297732894450557	0.3741586746909886	0.2935895815273328	T	T	T
0.3181467012839354	0.3294478999387149	0.1600278728113342	T	T	T
0.0117488101066908	0.5574803908492393	0.2261243631184005	T	T	T
0.3594579226770653	0.0702531389312663	0.7233184146618660	T	T	T
0.3171747962483373	0.0503320196616003	0.9082787787068257	T	T	T
0.2017633487454119	0.0474131298289725	0.0055681125621662	T	T	T
0.0911660258511856	0.0702363098156339	0.9017021542102335	T	T	T
0.1035922128270753	0.0645370744434608	0.7046734172771851	T	T	T
0.2297618632602699	0.0557656001762172	0.7613904818888640	T	T	T
0.3593682125991771	0.8282655345357972	0.7521317463048164	T	T	T
0.2993661550199210	0.8635670516284408	0.9185862414285981	T	T	T
0.1888793491643451	0.8511828526146047	0.0254073610430457	T	T	T
0.0884636644363800	0.8328215834606678	0.8992101335586302	T	T	T
0.1013301491456904	0.8405896469129470	0.7028209995006789	T	T	T
0.2281206671584385	0.8482166759079289	0.7542126938038760	T	T	T
0.3122739302237019	0.9514730438452219	0.7712841987458581	T	T	T
0.0895169561670081	0.9523355718683896	0.8107831207227451	T	T	T
0.4328870078516881	0.1266232723518969	0.5809871584285755	T	T	T
0.4113911877801665	0.9956949160107953	0.5751383683004959	T	T	T
0.3935541730506637	0.8634520585183237	0.5675422622091203	T	T	T
0.1943567984958101	0.1385622432328321	0.6152133597653008	T	T	T
0.1912184028323463	0.0054313419704168	0.5863698316525721	T	T	T
0.1924070251028027	0.8723212357382680	0.5643162144850555	T	T	T
0.9876359295859709	0.0382878540947325	0.7862059829965891	T	T	T
0.9853603081489091	0.8708289163086783	0.7877468063793135	T	T	T
0.1387320303633902	0.9325881509823810	0.2243496831267742	T	T	T

Structure files (CONTCAR) involved in this work:

0.1830411044172982	0.9520044102379080	0.4075542114993509	T	T	T
0.2969054357160284	0.9462005446887886	0.5092460999948523	T	T	T
0.4072310290641209	0.9314887754727207	0.4024324623322789	T	T	T
0.3964286543749770	0.9355274924587574	0.2056907088093440	T	T	T
0.2693572498520178	0.9430536973488859	0.2598622793047786	T	T	T
0.1380236975770374	0.1714209164792396	0.2541277837438081	T	T	T
0.1975316560208675	0.1355940643768372	0.4196756698124023	T	T	T
0.3099185995201876	0.1498113789241927	0.5196280287849676	T	T	T
0.4111403326890822	0.1683015143689392	0.3943040730679888	T	T	T
0.3959901713102618	0.1582784679201091	0.1984481099713327	T	T	T
0.2702419457047465	0.1566959141824515	0.2574135587404235	T	T	T
0.1904234401549177	0.0498972536658795	0.2686018853705662	T	T	T
0.4133774511605649	0.0484609309668045	0.3088097190190935	T	T	T
0.0648319646036462	0.8727904950825210	0.0871385919621269	T	T	T
0.0856430184039950	0.0027260126657785	0.0714983852170711	T	T	T
0.1095123702566347	0.1337310265402096	0.0692507508981859	T	T	T
0.3069721461493157	0.8613341108623355	0.1140644402228683	T	T	T
0.3095028089349557	0.9943524689789294	0.0858151737419598	T	T	T
0.3003573462688286	0.1273129959948326	0.0668862890932457	T	T	T
0.5126348816032129	0.9591308170321412	0.2884930828892335	T	T	T
0.5143545368623825	0.1336131482694247	0.2807034027818142	T	T	T
0.6375978607594976	0.5657207393821346	0.2815758796988459	T	T	T
0.6973149650318446	0.5733092494828613	0.1093565869900426	T	T	T
0.7935959831681338	0.5545617232606228	0.9733269401110540	T	T	T
0.8959540618687050	0.5824010530425527	0.0979032060419667	T	T	T
0.8870128606666486	0.5426909399644914	0.3095261344559372	T	T	T
0.7611708257155627	0.5208554699517828	0.2639007795042151	T	T	T
0.6361225684983114	0.3321011162043290	0.2572700627966023	T	T	T
0.6922564566274237	0.3412148280549243	0.0814849958077968	T	T	T
0.8106164298722563	0.3521526084079726	0.9920461622370497	T	T	T
0.9185830510405668	0.3222017925351647	0.1002441330722285	T	T	T
0.9040769368543244	0.3548804294122637	0.2915619299145594	T	T	T
0.7634832388760497	0.3698987755863433	0.2454475281961039	T	T	T
0.6645659589915575	0.4513091774444020	0.1834660874911869	T	T	T
0.9284450273709471	0.4496952354357753	0.1529094881820035	T	T	T
0.5635526034088633	0.6265670883077297	0.4177066006825426	T	T	T
0.5919500342801458	0.4975276081139636	0.4398104805060397	T	T	T
0.5887414793083848	0.3634713568452818	0.4394078873601125	T	T	T
0.7945654096772556	0.6322591576186611	0.3648245727600972	T	T	T
0.8010746635768876	0.5167947167622960	0.4564050761252614	T	T	T
0.8296190454014568	0.3863949866836478	0.4402595002804934	T	T	T
0.0220962609358456	0.3647042365835393	0.2075618277263933	T	T	T
0.8553475941830794	0.4377091406345914	0.7851887059960379	T	T	T
0.7910834207410457	0.4361040706216401	0.6140734058490156	T	T	T
0.7027804414865740	0.4263093303086863	0.4660271557334926	T	T	T
0.6080764448711851	0.4296284301086042	0.6075704790570829	T	T	T
0.6043290039861718	0.4446783517313606	0.8040798819444457	T	T	T
0.7293225510557937	0.4812086920348845	0.7745145021034012	T	T	T
0.8692440774983828	0.6835720969047536	0.7331610594033325	T	T	T
0.8077368905583785	0.6474558265956645	0.5593749277091422	T	T	T
0.6867037152114064	0.6486672384609581	0.4814713887943572	T	T	T
0.5840272289297427	0.6707297801472042	0.6026045037184290	T	T	T
0.5965730855403242	0.6579111772860207	0.7987315666963698	T	T	T

Structure files (CONTCAR) involved in this work:

0.7238124793452678	0.6546378443595930	0.7435077933985816	T	T	T
0.8266981540914763	0.5530655470520909	0.6926021042815810	T	T	T
0.5822554758625770	0.5492813477615857	0.6827099423889796	T	T	T
0.9309625321583577	0.3782586823793010	0.9198559419062636	T	T	T
0.9141295372289736	0.5121272601021477	0.9292033757053073	T	T	T
0.8868049629111436	0.6422258329929178	0.9226501428030738	T	T	T
0.7001963585218177	0.3745342439078115	0.8889351527650740	T	T	T
0.6742936389671554	0.4997371193618460	0.9509454652559087	T	T	T
0.6890633791374295	0.6333411301688794	0.9354470511093148	T	T	T
0.4927027899142176	0.4512232456341550	0.7068407329062888	T	T	T
0.4803585334339078	0.6324352451078880	0.7120870801935784	T	T	T
0.6429579286601752	0.9413086269526595	0.2891734013765245	T	T	T
0.6988834818244014	0.9339975784514110	0.1115115777200411	T	T	T
0.7992461093181717	0.9480131621463355	0.9803882379153724	T	T	T
0.8973515056561536	0.9303468059883346	0.1135828999556528	T	T	T
0.8965621814968013	0.9480495086377919	0.3110920149284082	T	T	T
0.7709659734831651	0.9698866786138691	0.2674225022810893	T	T	T
0.6393410325579019	0.1733161726742510	0.2556314417988882	T	T	T
0.6972187115633675	0.1604661950604331	0.0815952304059060	T	T	T
0.8092852127905552	0.1482147964210252	0.9772016752466254	T	T	T
0.9133708876985147	0.1689342027593486	0.0944540360086220	T	T	T
0.8961215116702188	0.1628090805437427	0.2921388845015487	T	T	T
0.7697565570018563	0.1458188562724982	0.2465991607130600	T	T	T
0.6794389631833411	0.0535951968120236	0.1967076001546045	T	T	T
0.9159255125174102	0.0513061169167081	0.1863656345039547	T	T	T
0.5673339855120049	0.8773099212100768	0.4207444460813269	T	T	T
0.5831787141258121	0.0083828312656065	0.4392898252926091	T	T	T
0.5970986580046050	0.1407033994294250	0.4382508328395435	T	T	T
0.8056961633677101	0.8720117160419908	0.3955608588203229	T	T	T
0.8159105561296204	0.9993537348682651	0.4494955840568959	T	T	T
0.8096430531863390	0.1332899155072464	0.4362271482671754	T	T	T
0.0090383753736653	0.9563319640499818	0.2166231886757581	T	T	T
0.0145826356926501	0.1377401793712930	0.2123649767648930	T	T	T
0.8570880697249891	0.0525026982554688	0.7861364393279399	T	T	T
0.8005883256155597	0.0722815648375977	0.6108649354526071	T	T	T
0.7010055059092217	0.0615617691531061	0.4784816985909079	T	T	T
0.6006473099190056	0.0758286876581517	0.6089407180222890	T	T	T
0.6022439325842112	0.0531068432791698	0.8062578948881453	T	T	T
0.7278046795913922	0.0310968012234590	0.7644401680629495	T	T	T
0.8600082657290088	0.8350958178781162	0.7615289795642919	T	T	T
0.8025545831523184	0.8316446677819287	0.5865632854037538	T	T	T
0.6895314840161935	0.8526098232329257	0.4865407181210183	T	T	T
0.5863750895989640	0.8298642182182068	0.6055160487240674	T	T	T
0.6017762378249167	0.8522434217676412	0.8002900732582829	T	T	T
0.7289152076437475	0.8532218484076523	0.7478955489546733	T	T	T
0.8130408923460943	0.9475805269941829	0.6817682871240863	T	T	T
0.5801395756149256	0.9536000533154373	0.6749476246563690	T	T	T
0.9311694768379399	0.1271834404388211	0.9069556499734318	T	T	T
0.9189632923376133	0.9973564497785735	0.9442149535499864	T	T	T
0.9013507658322493	0.8651677927615135	0.9443850237477696	T	T	T
0.6927674568689312	0.1319307040354690	0.8872676695989922	T	T	T
0.6824181884538241	0.0056223897935359	0.9477418816432176	T	T	T
0.6944675504850012	0.8717953584650395	0.9391477224455705	T	T	T

Structure files (CONTCAR) involved in this work:

0.4892895717106039	0.0478509585815076	0.7141879910974193	T	T	T
0.4831264402009756	0.8660999295502895	0.7169629750797905	T	T	T
0.3622163673740463	0.4313530050485495	0.7203523396791784	T	T	T
0.3125801550981895	0.4466521572753087	0.9026102028548941	T	T	T
0.1993030236131044	0.4601355968885076	0.0082139053148981	T	T	T
0.0889794820842109	0.4325568176004940	0.9050186127452767	T	T	T
0.1026450632248399	0.4368816429717370	0.7072237513525247	T	T	T
0.2308508797333839	0.4485573608849620	0.7510295312489355	T	T	T
0.3573494903712869	0.6743071915324016	0.7505565348037851	T	T	T
0.2988236231240646	0.6374978671290797	0.9169521605912788	T	T	T
0.1898772212069550	0.6485463466398405	0.0255882306851235	T	T	T
0.0931700859781850	0.6700656666121606	0.8940096463072120	T	T	T
0.1000245023541465	0.6564214967742636	0.6967415605501415	T	T	T
0.2266721619139792	0.6481536502479066	0.7514975830444257	T	T	T
0.3156885429771634	0.5495036464927351	0.7714818732786440	T	T	T
0.0836561680630604	0.5489158749747163	0.8121872615198802	T	T	T
0.4327681641186228	0.3765102496373359	0.5722400816212665	T	T	T
0.4135310691371819	0.5075769116078932	0.5732439970552200	T	T	T
0.3885031994310638	0.6385402140536490	0.5660575232435561	T	T	T
0.1908337759714022	0.3618159318953311	0.6133500846815876	T	T	T
0.1829819136759087	0.4942299963108832	0.5777631363917235	T	T	T
0.1913656001095772	0.6275818050546721	0.5600055108380309	T	T	T
0.9854493090737246	0.4587436331751853	0.7846454450953799	T	T	T
0.9855113464428424	0.6372980302575992	0.7874131580147197	T	T	T
0.1435553954514324	0.5687149987945140	0.2168745898543407	T	T	T
0.1844590781752585	0.5509574363150199	0.4012417753351535	T	T	T
0.2950727612631022	0.5494526160635061	0.5134269272641618	T	T	T
0.4016298244711048	0.5710255430621854	0.3999717322185435	T	T	T
0.3981843622689578	0.5637931257158173	0.2027391572827214	T	T	T
0.272155551873975	0.5507600328524038	0.2541469896579658	T	T	T
0.1429600986821896	0.3234562213685072	0.2504596868184720	T	T	T
0.1979298039925634	0.3641285730609164	0.4186341546588756	T	T	T
0.3083301016769414	0.3510567399361810	0.5234330921369196	T	T	T
0.4043960788803144	0.3303164441538473	0.3889548026227888	T	T	T
0.3948771647373796	0.3463902662845555	0.1914819310703904	T	T	T
0.2723767884122906	0.3476980038907519	0.2572502428106400	T	T	T
0.1855501562656424	0.4490381706124679	0.2682437218154415	T	T	T
0.4081695178808178	0.4521113086367227	0.3120760816457875	T	T	T
0.0661100435827648	0.6243702453499080	0.0774929347909868	T	T	T
0.0794416744748275	0.4913735495277371	0.0820999723498257	T	T	T
0.1161295510054000	0.3630440502059174	0.0657030372185967	T	T	T
0.3076409203422937	0.6382507105603504	0.1130032806668256	T	T	T
0.3135001152368018	0.5063226207887151	0.0769005094165840	T	T	T
0.2946927845123992	0.3736077689203618	0.0640707528296076	T	T	T
0.5100258025596554	0.5372821178569780	0.2953079104656971	T	T	T
0.5098862946689221	0.3674635102259400	0.2803275496358839	T	T	T
0.4376503555288340	0.7503243520983151	0.6427908870659977	T	T	T
0.1868498990620228	0.7494707412277936	0.6339591427919167	T	T	T
0.2764039828120984	0.7502472630759989	0.0176419816879498	T	T	T
0.1036285928840937	0.7496908463856612	0.0511486351921624	T	T	T
0.0669638948416316	0.2491085543178077	0.1332287009625164	T	T	T
0.3109866162881198	0.2509389678724116	0.1298775850641234	T	T	T
0.2205675633534363	0.2499315207858686	0.5165671616897312	T	T	T

Structure files (CONTCAR) involved in this work:

0.3954239239392836	0.2509907036519893	0.5463306759114875	T	T	T
0.5535446746489975	0.2509475751970519	0.3531367974979703	T	T	T
0.8068279045058043	0.2536348993932090	0.3544246654554495	T	T	T
0.7275865757758849	0.2520709281656898	0.9440988105353308	T	T	T
0.8920191857868366	0.2511484204790323	0.9409422188287117	T	T	T
0.9435509171507848	0.7542089940776214	0.8597585462366979	T	T	T
0.6806862180393151	0.7532251703212226	0.8609756161881619	T	T	T
0.7694400759873374	0.7501111612448489	0.4400063191371150	T	T	T
0.6040319680091158	0.7516035811420778	0.4491599978849176	T	T	T
0.9335753894106854	0.4902831350697888	0.5287945236887172	T	T	T
0.9460865649606907	0.6472360818194992	0.5680220561753960	T	T	T
0.9228147142886108	0.5306238019827529	0.1927053694416401	T	T	T
0.8214737166791375	0.3367282956265946	0.3268684207265897	T	T	T
0.7996341479745730	0.6389627582261562	0.6915909560983643	T	T	T
0.9336340644332771	0.4011660086238127	0.4453860571714899	T	T	T
0.8787127344031220	0.5661051536158493	0.5568800445902616	T	T	T
0.0235844952140080	0.3707631595276496	0.4597547910915407	T	T	T
0.0162974622402650	0.5987651618262441	0.3186473434215709	T	T	T
0.9627541296941691	0.4787692690615368	0.5847051926163518	T	T	T
0.0616240637618981	0.3994327194410152	0.5003705076297766	T	T	T
0.0432432731295126	0.3251584697350350	0.4248539620591344	T	T	T
0.0053941812952037	0.5654221672266406	0.3817196803970244	T	T	T
0.9792137451577227	0.6390850442171933	0.3137795045061612	T	T	T
0.0667641976744068	0.6194403323599008	0.3244303837798602	T	T	T
0.9237166543585489	0.6752286785842543	0.6199957330437209	T	T	T
0.9902718343575949	0.6374054030191386	0.5955524963661005	T	T	T

Figure 7(a) ©

Si O Al Zn C H

1.0000000000000000

20.0219999999999985 0.0000000000000000 0.0000000000000000

0.0000000000000000 19.8990000000000009 0.0000000000000000

0.0000000000000000 0.0000000000000000 13.3829999999999991

93 194 3 2 2 8

Selective dynamics

Direct

0.4228869238444793 0.0613842205181538 0.6471076801860874 T T T

0.3054628920944850 0.0326637652947171 0.7906628493827049 T T T

0.2825300332243488 0.0557807897522120 0.0159565817747204 T T T

0.1233859272450944 0.0628899185230625 0.0118577803846818 T T T

0.0680244992506592 0.0319815011050474 0.8006547992380278 T T T

0.1804119467237610 0.0662273269851466 0.6644436623334122 T T T

0.4190793160890897 0.8290725342311656 0.6686128761259225 T T T

0.3013113935870256 0.8740721205615974 0.7997893678013562 T T T

0.2674285016735278 0.8319507691397386 0.0185995395168189 T T T

0.1122756339138637 0.8271836089696547 0.0118859665144261 T T T

0.0663999364944759 0.8751638818667893 0.7981276538764053 T T T

0.1795016232796128 0.8299382168702013 0.6640902019416208 T T T

0.0761308291477647 0.9410701021519187 0.1484461450278509 T T T

0.1951802499239234 0.9707211942358580 0.2897587238677564 T T T

0.2166191889126295 0.9450687033331850 0.5155945817074816 T T T

0.3767991550416533 0.9370087624711996 0.5128756611645214 T T T

0.4334840578013421 0.9689522379703719 0.3011890655242336 T T T

Structure files (CONTCAR) involved in this work:

0.3205074269826709	0.9354893361974520	0.1643105654145970	T	T	T
0.0829886686592220	0.1733416316373299	0.1654346954936597	T	T	T
0.1986959464345416	0.1294067171536163	0.3001963986989714	T	T	T
0.2314019574169744	0.1709833781275470	0.5180753107923033	T	T	T
0.3877467640262479	0.1755651967556749	0.5083094626036075	T	T	T
0.4347290974214814	0.1272338511545836	0.2947601142789048	T	T	T
0.3191471429104895	0.1724540072895951	0.1639482382867387	T	T	T
0.5765920049161979	0.5555627880738732	0.3563335232646699	T	T	T
0.6930588850726803	0.5264713288530137	0.2073298890386950	T	T	T
0.7157729802731487	0.5690669290380731	0.9904241923699384	T	T	T
0.8743155977500553	0.5735072875224636	0.9903765963728578	T	T	T
0.8140554463910994	0.5489981736214975	0.3505958425517758	T	T	T
0.5729328074612888	0.3293194819532767	0.3329942969580985	T	T	T
0.6932053398633879	0.3722444502207662	0.1924693528976635	T	T	T
0.7295089757535113	0.3281265539752661	0.9787912531620496	T	T	T
0.8842003694558762	0.3256297805551130	0.9922293022639671	T	T	T
0.9399389910367036	0.3745989386438109	0.1872895328565203	T	T	T
0.9189163357681689	0.4457278275009617	0.8619665593951541	T	T	T
0.7992392389891578	0.4733364958938792	0.7209377285985598	T	T	T
0.7751601156008380	0.4378891642771760	0.4988945098310583	T	T	T
0.6179144262462465	0.4296902116551805	0.4913724886496658	T	T	T
0.5693364612706979	0.4703833600606804	0.7035228878804956	T	T	T
0.6761096032263409	0.4493855121652702	0.8593645755182094	T	T	T
0.9203536876525125	0.6790854399483957	0.8322672269745280	T	T	T
0.7689672825414156	0.6691388183178801	0.4647881075075628	T	T	T
0.6134934363543909	0.6734499108652010	0.4857268461903204	T	T	T
0.5611561403964461	0.6286480790159228	0.6975512647270407	T	T	T
0.6709430983163991	0.6734505543757702	0.8319769063356683	T	T	T
0.5781247835624749	0.9463102140277350	0.3583187435951223	T	T	T
0.6986259032293377	0.9746174053016079	0.2147355993377573	T	T	T
0.7193417638397113	0.9386822098439269	0.9931483075801604	T	T	T
0.8791717898097631	0.9355978137803949	0.9948084227197029	T	T	T
0.9314364421717772	0.9709838773002379	0.2047314732320573	T	T	T
0.8223144786026186	0.9464977033569020	0.3543937333392795	T	T	T
0.5773133634854800	0.1743343346266658	0.3301443126629828	T	T	T
0.6979773515196183	0.1330130600917626	0.1946201744248956	T	T	T
0.7314615589228283	0.1720728467298855	0.9727744952410147	T	T	T
0.8860565773152397	0.1735846380643680	0.9816069341591626	T	T	T
0.9361974706353355	0.1292817699819870	0.1955532279635332	T	T	T
0.8213885248537792	0.1738483339733869	0.3314463050929802	T	T	T
0.9229809354395446	0.0544525363141585	0.8549581892851957	T	T	T
0.8008923354384250	0.0255951441759743	0.7094927724814899	T	T	T
0.7813998816255311	0.0659235484182406	0.4913995534131842	T	T	T
0.6210928711646554	0.0709533384408482	0.4899062946962580	T	T	T
0.5684866342322588	0.0326653249704840	0.6985930734758143	T	T	T
0.6776316053184643	0.0542709603975123	0.8501704536957683	T	T	T
0.9232726451010803	0.8317280161859595	0.8365927849080473	T	T	T
0.8022755803505028	0.8676295569071723	0.6941621102118501	T	T	T
0.7695170947988175	0.8262803757721496	0.4763804804432588	T	T	T
0.6144875250352446	0.8272107962674218	0.4896111573936472	T	T	T
0.5641962129914594	0.8755900782329539	0.6978852736729165	T	T	T
0.6784234481142136	0.8320297418031478	0.8337967151000503	T	T	T
0.4245205628955604	0.4442360167104871	0.6418766405617863	T	T	T

Structure files (CONTCAR) involved in this work:

0.3050975195647415	0.4700309027501945	0.7843200540591836	T	T	T
0.2823156617652523	0.4448763108733426	0.0092340272552848	T	T	T
0.1235811920282465	0.4387513004743827	0.0123900025838366	T	T	T
0.0634739947471440	0.4706034703076795	0.8013382459391251	T	T	T
0.1770268545398760	0.4383930087328246	0.6603786661432055	T	T	T
0.4169380089342543	0.6754028167300345	0.6613741113192021	T	T	T
0.3008770727157746	0.6290430439493758	0.7960701004551687	T	T	T
0.2680232828340654	0.6705642090924965	0.0140114796520042	T	T	T
0.1125305110428308	0.6729918368692699	0.0069265821431010	T	T	T
0.0636918714073117	0.6303209483486411	0.7931570339181128	T	T	T
0.1798827614651611	0.6726584245967958	0.6616936626241774	T	T	T
0.0749585167997209	0.5603538564998205	0.1504802999077844	T	T	T
0.1970399137608429	0.5321398505341509	0.2847089406957240	T	T	T
0.2180151358913026	0.5581463608104668	0.5139179369898181	T	T	T
0.3769376717367241	0.5673585179472465	0.5103929471473828	T	T	T
0.4301653350310670	0.5315884024610118	0.2984096298696531	T	T	T
0.3222216291901105	0.5643985209856296	0.1558315762286612	T	T	T
0.0857954685775683	0.3264728901959429	0.1591205492910484	T	T	T
0.1994615327644434	0.3731406797915868	0.2962430363669211	T	T	T
0.2299156870287151	0.3321048773003494	0.5167773662070237	T	T	T
0.3855947572090648	0.3292667339718722	0.5051273637878472	T	T	T
0.4305645351238453	0.3743948013592894	0.2910405421704338	T	T	T
0.3184488268731565	0.3294938902863699	0.1586017128125154	T	T	T
0.0103308496117254	0.5534076530404850	0.2197802101087283	T	T	T
0.3595609243039617	0.0716003459208587	0.7214879632081438	T	T	T
0.3171957934095110	0.0531496190419345	0.9064110410023497	T	T	T
0.2024346077437061	0.0462658335952158	0.0054684270217919	T	T	T
0.0921424746488654	0.0706131117020075	0.9010059576537508	T	T	T
0.1038332347416328	0.0657645052215236	0.7040088345548342	T	T	T
0.2300257604698079	0.0541399198272878	0.7591759512503448	T	T	T
0.3605160918012610	0.8286688461453868	0.7525703434933858	T	T	T
0.3014039856655079	0.8639538670029864	0.9194922296165249	T	T	T
0.1890553125412270	0.8533072494675263	0.0215281537977634	T	T	T
0.0883742373989209	0.8331868282064452	0.8966407205235655	T	T	T
0.1027270012336716	0.8419456801713984	0.7007579143614325	T	T	T
0.2291528299308286	0.8510453264774785	0.7553018627614846	T	T	T
0.3153901669135859	0.9523300186655607	0.7725720826889555	T	T	T
0.0894274321702552	0.9530974358171375	0.8091264030237991	T	T	T
0.4331808020183417	0.1290981505117281	0.5809675284518981	T	T	T
0.4121031359818204	0.9984231835226578	0.5719850794885635	T	T	T
0.3924266293780409	0.8664711958180400	0.5685714489220611	T	T	T
0.1955684418489276	0.1393962031125808	0.6158705186160692	T	T	T
0.1896920412580978	0.0069280611344808	0.5827882511688767	T	T	T
0.1947563432166451	0.8735935943578851	0.5643804091915892	T	T	T
0.9879996428762805	0.0396539540421495	0.7858435620444260	T	T	T
0.9858239734583872	0.8710936841923693	0.7844744286941655	T	T	T
0.1404685484468737	0.9323119657984328	0.2211250085439214	T	T	T
0.1831022966879933	0.9506673833970496	0.4056365533836123	T	T	T
0.2970788555816382	0.9499777068066785	0.5075011565572594	T	T	T
0.4074957886592355	0.9316851985092689	0.4016188135324671	T	T	T
0.3968236084341737	0.9358106927427238	0.2048262782469167	T	T	T
0.2702261941852473	0.9481391312988429	0.2582354688138822	T	T	T
0.1394560193808468	0.1743870684462770	0.2525015714594212	T	T	T

Structure files (CONTCAR) involved in this work:

0.1964572864175590	0.1384375889951662	0.4201613786810519	T	T	T
0.3101952718227096	0.1516025688763392	0.5174463720332684	T	T	T
0.4122309020325080	0.1689387113879763	0.3935133356437265	T	T	T
0.3960500524636960	0.1582384201345833	0.1978983853219085	T	T	T
0.2709793890999532	0.1542315228057164	0.2586355204689040	T	T	T
0.1863819234251018	0.0510974885852355	0.2711694968411759	T	T	T
0.4150179230329643	0.0485446587124041	0.3083939595458792	T	T	T
0.0654451385389682	0.8722548839063738	0.0846855020935497	T	T	T
0.0854960720019109	0.0027148300858752	0.0703769339953927	T	T	T
0.1113092863227756	0.1335041241691099	0.0687810612867358	T	T	T
0.3054716768717272	0.8623720780437454	0.1153707365637703	T	T	T
0.3120146367036052	0.9946367789689861	0.0821368578515575	T	T	T
0.2997615760277660	0.1276454866964186	0.0670169531200496	T	T	T
0.5131850363248655	0.9575132340943353	0.2876052455801550	T	T	T
0.5149318588570926	0.1342754963633544	0.2787864423031871	T	T	T
0.6388830618707088	0.5619454963427577	0.2801201534036685	T	T	T
0.7036210049667952	0.5740405044185424	0.1103546677738422	T	T	T
0.7948193855157694	0.5662630601429552	0.9624566707128235	T	T	T
0.8863381398928832	0.5782773250975870	0.1083519310755694	T	T	T
0.8898144446021101	0.5270269941101675	0.3217452501321146	T	T	T
0.7633382397027147	0.5210376710012052	0.2679705880169325	T	T	T
0.6384773176593818	0.3355793014510819	0.2640124570727227	T	T	T
0.6892719002272556	0.3363701020458914	0.0830715380040142	T	T	T
0.8071182001284636	0.3517452148610062	0.9918164340951287	T	T	T
0.9112943541380165	0.3201990273956532	0.1068155537922183	T	T	T
0.9053721162085481	0.3593563286080209	0.2977380923739926	T	T	T
0.7664498850462965	0.3661188927945287	0.2392567054230335	T	T	T
0.6703105563932831	0.4508765313366933	0.1785263188940189	T	T	T
0.9242796616269492	0.4489535221103133	0.1521836988361465	T	T	T
0.5670825318853094	0.6267422526001344	0.4143639998791793	T	T	T
0.5880122317327793	0.4970912539928082	0.4397215098428894	T	T	T
0.5845011454985248	0.3631707008987506	0.4428003155449893	T	T	T
0.8046596047875806	0.6293486320510544	0.3713544093292833	T	T	T
0.7978731404997510	0.5153957496325458	0.4632329137911927	T	T	T
0.8228013136621153	0.3864475904871460	0.4376334886728411	T	T	T
0.0200133522723481	0.3629967112565635	0.2036720849993622	T	T	T
0.8546645585908319	0.4352152078428672	0.7884647874677105	T	T	T
0.7874859804553729	0.4315397261624954	0.6176867836284690	T	T	T
0.6980192081902175	0.4264724733790825	0.4695411442615893	T	T	T
0.6040635429195480	0.4303054489956656	0.6106106919842890	T	T	T
0.6024330980502784	0.4472830074213868	0.8086957770604999	T	T	T
0.7282150816076153	0.4785452601002083	0.7766062169657867	T	T	T
0.8592351380067180	0.6800034495308649	0.7560895565471878	T	T	T
0.8102703713615302	0.6472826470999264	0.5655725580191459	T	T	T
0.6909349638047122	0.6474430725039458	0.4776322448788321	T	T	T
0.5878073607972834	0.6692663969133059	0.6000619385186660	T	T	T
0.5931612676573923	0.6613491017590062	0.7978450787455844	T	T	T
0.7184995596059099	0.6473642707448870	0.7429315673188392	T	T	T
0.8252396912689601	0.5494343221523211	0.6939725084297748	T	T	T
0.5813025604241225	0.5500583825246953	0.6853871023685574	T	T	T
0.9295803305488516	0.3771242664787039	0.9261539819745228	T	T	T
0.9115136514971928	0.5096170341726728	0.9354559582916284	T	T	T
0.9051881770517850	0.6403782146250262	0.9360098926260150	T	T	T

Structure files (CONTCAR) involved in this work:

0.6952823772258779	0.3735370557014992	0.8920640133712384	T	T	T
0.6783248717094115	0.5002165324943434	0.9540146768514007	T	T	T
0.6828744253807530	0.6342174224608289	0.9373360627502704	T	T	T
0.4903688570218672	0.4523108966351663	0.7110310688468781	T	T	T
0.4803035275855586	0.6344113125462485	0.7059329784560436	T	T	T
0.6439056548330798	0.9410544973910759	0.2885177129513354	T	T	T
0.6986054023434273	0.9335002545285488	0.1100010571740215	T	T	T
0.7996499805273117	0.9478785400266975	0.9804393882208670	T	T	T
0.8985210692320863	0.9295325787668028	0.1120816337623401	T	T	T
0.8976864698933696	0.9485225911265357	0.3098179793902612	T	T	T
0.7720281963778336	0.9685160791204196	0.2650476899529848	T	T	T
0.6403356351972210	0.1735581295772773	0.2545832887720300	T	T	T
0.6963932108942090	0.1591811201401150	0.0801375737677260	T	T	T
0.8090129009186746	0.1473297949691870	0.9783719847681259	T	T	T
0.9138070603295361	0.1685080133238981	0.0948344150908984	T	T	T
0.8976063754146789	0.1591890788882934	0.2922584267593805	T	T	T
0.7706606891104260	0.1464043798176554	0.2441706099230491	T	T	T
0.6806259589948256	0.0531549161952140	0.1969251781447519	T	T	T
0.9191092625681737	0.0501118192227071	0.1828328984857211	T	T	T
0.5696307621271546	0.8763201318137464	0.4199480843050007	T	T	T
0.5828008105587575	0.0079335963603739	0.4378370748383404	T	T	T
0.5977492751500911	0.1403087311356276	0.4364007975731237	T	T	T
0.8077767592094334	0.8704994636950968	0.3926911157230615	T	T	T
0.8155893070148251	0.9976376882474174	0.4481755633966411	T	T	T
0.8093037215964896	0.1315627848873232	0.4343220719089740	T	T	T
0.0104858345271830	0.9544947300053120	0.2160691761142731	T	T	T
0.0162802185903045	0.1387019310333389	0.2112394693907348	T	T	T
0.8573555219491238	0.0539961070933070	0.7847343478342231	T	T	T
0.8006350028262375	0.0714647318119651	0.6091500749741714	T	T	T
0.7008835073433578	0.0601524395703695	0.4769966100153222	T	T	T
0.6007010988193483	0.0759335456377942	0.6071623637977187	T	T	T
0.6026953156826304	0.0526038724411072	0.8043037788663213	T	T	T
0.7283630250415456	0.0297066674208775	0.7628262214150758	T	T	T
0.8607050510952760	0.8341755725979932	0.7605688825908155	T	T	T
0.8051965157950801	0.8322774576542650	0.5849308875935412	T	T	T
0.6923106403590182	0.8513227482223696	0.4850440300342245	T	T	T
0.5884494599692548	0.8295585423566026	0.6043350547180831	T	T	T
0.6030865970307884	0.8524749474515854	0.7987294200176968	T	T	T
0.7298525883306729	0.8542341562824963	0.7450766990389235	T	T	T
0.8157569110630136	0.9476055056848454	0.6815158691861027	T	T	T
0.5803800963076229	0.9536898224001957	0.6726319826137067	T	T	T
0.9309888175619077	0.1279501036420695	0.9066073451412717	T	T	T
0.9185800793882917	0.9981664125836823	0.9431940274475008	T	T	T
0.9023156574477386	0.8659412608073404	0.9421171149050221	T	T	T
0.6936048077425137	0.1303621605662220	0.8855854487856756	T	T	T
0.6822677975291707	0.0039437098990648	0.9455572946148529	T	T	T
0.6961800679055717	0.8702848485297974	0.9375249474902747	T	T	T
0.4895694281359843	0.0487204976131888	0.7126595080225800	T	T	T
0.4843189680542218	0.8663090589369713	0.7150739282629547	T	T	T
0.3594199269080760	0.4334226308199656	0.7128139098039499	T	T	T
0.3152942952310822	0.4449735088779292	0.8983640159909820	T	T	T
0.2023302308659274	0.4575035442373236	0.0029080493783840	T	T	T
0.0910491597743186	0.4350526735162716	0.9014824301790606	T	T	T

Structure files (CONTCAR) involved in this work:

0.1007264935023614	0.4393539368300928	0.7032507146251955	T	T	T
0.2291904341477299	0.4507079367270671	0.7513568071241121	T	T	T
0.3569916644591635	0.6750678275701615	0.7429400888718218	T	T	T
0.3044571479491265	0.6415888587247026	0.9149231549217512	T	T	T
0.1899600293277120	0.6480704892652220	0.0112511747502597	T	T	T
0.0865410231664719	0.6708455405224646	0.8916923825313937	T	T	T
0.1024782162857325	0.6586774572505261	0.6945847548891901	T	T	T
0.2270126297874472	0.6495750348406275	0.7548155206876861	T	T	T
0.3158356660016245	0.5505776030899846	0.7720742945931997	T	T	T
0.0785272423584792	0.5508418296690738	0.8064227562159431	T	T	T
0.4330710106503647	0.3786955397389626	0.5703006655770452	T	T	T
0.4182692129795356	0.5104684712255723	0.5713380737536102	T	T	T
0.3904596778049139	0.6409207042431442	0.5584913126792985	T	T	T
0.1901245040403554	0.3651227494766572	0.6105482215507156	T	T	T
0.1839075008554325	0.4975520992559465	0.5773449833507155	T	T	T
0.1972192872331184	0.6302993317665713	0.5612928897048030	T	T	T
0.9836882188073076	0.4567692593763120	0.7879981005683327	T	T	T
0.9837970978695256	0.6422619397881899	0.7710663632291298	T	T	T
0.1421689295299758	0.5717360825337291	0.2186442555495793	T	T	T
0.1895672397868925	0.5548336807239704	0.4007846102398199	T	T	T
0.2981703711902727	0.5482000345410020	0.5160593946333194	T	T	T
0.4014762648882582	0.5707093447357573	0.3956565472471409	T	T	T
0.3981906989649258	0.5648927806677179	0.1983406640322628	T	T	T
0.2723787228735122	0.5496018918507268	0.2493499928882474	T	T	T
0.1416187846401822	0.3270178010312636	0.2473587777150064	T	T	T
0.1967166875691475	0.3628750639378804	0.4160941023606876	T	T	T
0.3082644591045339	0.3530935636612725	0.5203446909531628	T	T	T
0.4051692472608130	0.3318679295935612	0.3876693473219467	T	T	T
0.3954250155609929	0.3447043879844002	0.1905365341261059	T	T	T
0.2719614723900685	0.3507513020255760	0.2538630291164108	T	T	T
0.1844077601552031	0.4516272243943026	0.2713197616087007	T	T	T
0.4094791577571895	0.4526375955237802	0.3064484018259143	T	T	T
0.0671175305696713	0.6250270883725364	0.0761261941897436	T	T	T
0.0857022047872887	0.4942220274041684	0.0795652529042199	T	T	T
0.1149487221888664	0.3643939676596214	0.0609382151572994	T	T	T
0.3052120742987935	0.6378542473333849	0.1099426820720891	T	T	T
0.3156993673277393	0.5057958637758833	0.0721466989114976	T	T	T
0.2977447019517733	0.3725236591694129	0.0604235023848085	T	T	T
0.5104155319190825	0.5393582033717392	0.2913185384804604	T	T	T
0.5107662042479257	0.3671467532590663	0.2778840324720058	T	T	T
0.4376850588557121	0.7524497709652141	0.6380771663324101	T	T	T
0.1903414952854329	0.7513607113955429	0.6355547381953803	T	T	T
0.2752380663434943	0.7512189125589402	0.0191175656035223	T	T	T
0.1067037904855214	0.7495589065642998	0.0470498873510402	T	T	T
0.0681297192011085	0.2496872479258189	0.1295280241574062	T	T	T
0.3093457197600429	0.2505740887731798	0.1322889669729893	T	T	T
0.2208324698700456	0.2515793788650796	0.5197466173968098	T	T	T
0.3952503489349668	0.2529291512267540	0.5447022716276265	T	T	T
0.5545460079320806	0.2510689706831155	0.3519415805459105	T	T	T
0.8114564496808486	0.2518397848185281	0.3542473412059687	T	T	T
0.7264240520537063	0.2505926006862602	0.9421460844277435	T	T	T
0.8901526310396093	0.2510311562360314	0.9434918885472634	T	T	T
0.9451897895135453	0.7548163227138663	0.8591338624087898	T	T	T

Structure files (CONTCAR) involved in this work:

0.6831766209035632	0.7525793405732593	0.8552009222003931	T	T	T
0.7744965181163428	0.7484646937078115	0.4408325923850397	T	T	T
0.6080684226189184	0.7507912878383709	0.4480914207110012	T	T	T
0.9199970350865364	0.4766708959415222	0.5397842115988950	T	T	T
0.9608072942808766	0.6205480685637720	0.5731521460283380	T	T	T
0.9275684563094124	0.5302928505944561	0.1978871115757761	T	T	T
0.8205722469177703	0.3351370256735677	0.3271647507134016	T	T	T
0.7971316923045036	0.6357211573336078	0.6975316929086068	T	T	T
0.9205700173572681	0.4243709807575753	0.4145883542251946	T	T	T
0.8762012381197630	0.5625421693342068	0.5633355041320240	T	T	T
0.0250204845391332	0.4036888524781432	0.4396003532322978	T	T	T
0.0563650624434389	0.4707388063884853	0.4325014301783470	T	T	T
0.9532318788063848	0.4635106287326943	0.5892488572759430	T	T	T
0.0330335932162156	0.3687690273988854	0.3775560763823814	T	T	T
0.0227593581626083	0.3796183969122293	0.5133277267395006	T	T	T
0.0450990684806007	0.5039490814869249	0.4956497856131017	T	T	T
0.0452361159977501	0.4971559969987005	0.3620233442688277	T	T	T
0.1112174859141473	0.4631354543507223	0.4324934413080492	T	T	T
0.9694748011757172	0.6357309534015457	0.6433965079003041	T	T	T
0.9641570195957105	0.6598430421930315	0.5300612308289180	T	T	T

Figure 7(a) ④

Si O Al Zn C H

1.0000000000000000

20.0219999999999985 0.0000000000000000 0.0000000000000000

0.0000000000000000 19.8990000000000009 0.0000000000000000

0.0000000000000000 0.0000000000000000 13.3829999999999991

93 194 3 2 2 8

Selective dynamics

Direct

0.4235691122555082	0.0596556776828219	0.6492226807511284	T	T	T
0.3057965016270808	0.0298232071921089	0.7936573845441569	T	T	T
0.2824954402833567	0.0577391467204689	0.0176925654913507	T	T	T
0.1226429114904860	0.0632247412182986	0.0135978740934264	T	T	T
0.0680519864168153	0.0306859664795397	0.8015640292149205	T	T	T
0.1810746854540796	0.0631662877969728	0.6662113647653610	T	T	T
0.4208395410600239	0.8276969319922051	0.6718993776476180	T	T	T
0.3024332898543677	0.8703523643229363	0.8045870176951122	T	T	T
0.2673181811855302	0.8326120570131769	0.0249547966476427	T	T	T
0.1127348337597117	0.8284288557442490	0.0145551986370155	T	T	T
0.0660020782518549	0.8741654009236297	0.8001651649055572	T	T	T
0.1803158551021112	0.8265416405364118	0.6698614919392231	T	T	T
0.0766397580964210	0.9413018681953766	0.1522674173823152	T	T	T
0.1947383156628294	0.9701422950609957	0.2957036713243094	T	T	T
0.2177642122517817	0.9411985485110536	0.5198449395803143	T	T	T
0.3781575507334741	0.9350338383143101	0.5154256946650541	T	T	T
0.4341031467950118	0.9689999188409422	0.3042935704158257	T	T	T
0.3202435963926882	0.9386853069329079	0.1681022219056972	T	T	T
0.0817546354732560	0.1728990045393658	0.1677788996711817	T	T	T
0.1979186800963377	0.1294251701883476	0.3039773131249317	T	T	T
0.2326002825708577	0.1703564017866504	0.5222891294058665	T	T	T
0.3876365435720303	0.1740411829869052	0.5103866296718282	T	T	T
0.4361332787987723	0.1272254702637055	0.2977728712872107	T	T	T

Structure files (CONTCAR) involved in this work:

0.3193690933935637	0.1714181569197751	0.1680059745003055	T	T	T
0.5777467500065373	0.5556634052519099	0.3578118226037208	T	T	T
0.6970318946123827	0.5240817099664153	0.2130500192803582	T	T	T
0.7164021878641910	0.5665954494088580	0.9943737335934949	T	T	T
0.8749707558034251	0.5716047876916442	0.9858658638121496	T	T	T
0.8174558083918272	0.5520697897441640	0.3518207633463333	T	T	T
0.5777771146339304	0.3274975719339884	0.3360048773428796	T	T	T
0.6965991576772150	0.3706152554096823	0.1948958108891607	T	T	T
0.7327491854241942	0.3275778657445224	0.9813871266332415	T	T	T
0.8877135596678799	0.3259138996281769	0.9964934790448516	T	T	T
0.9404657750092328	0.3699073724442320	0.2006089816978585	T	T	T
0.9209514397329277	0.4437741402125760	0.8597323401332613	T	T	T
0.8001258349741075	0.4710446482696198	0.7225765963772418	T	T	T
0.7775451356910342	0.4364374265055671	0.4978895986273800	T	T	T
0.6198638157443022	0.4320648147526379	0.4915669878134090	T	T	T
0.5710391630272132	0.4697329058219313	0.7044819260800990	T	T	T
0.6769428446615450	0.4480153229118918	0.8617353236052934	T	T	T
0.9195799842918756	0.6799107770285228	0.8334556339483473	T	T	T
0.7655871341081814	0.6676786766961311	0.4714487607715044	T	T	T
0.6110618931077269	0.6729232855123437	0.4914945481348406	T	T	T
0.5610785225815946	0.6278939791065574	0.7039677787577722	T	T	T
0.6744358509716362	0.6713516192670382	0.8354197352511045	T	T	T
0.5784427938730428	0.9442648740336769	0.3600367143889396	T	T	T
0.6979130801779324	0.9722150512810186	0.2149965261921568	T	T	T
0.7200857015517602	0.9377077665839193	0.9942029289587184	T	T	T
0.8798379921743489	0.9367099187277679	0.9962507482426771	T	T	T
0.9315173290430706	0.9706190387352688	0.2076207524934140	T	T	T
0.8212330630931363	0.9437411617505003	0.3546557541171695	T	T	T
0.5793994789975243	0.1727972192462134	0.3324206570823848	T	T	T
0.6985110759539490	0.1293458940868947	0.1951989687039983	T	T	T
0.7342883309615825	0.1714210096334967	0.9751679846323643	T	T	T
0.8890713649039079	0.1737573768155323	0.9830640549596367	T	T	T
0.9367628924075302	0.1291391414954431	0.1989444521411348	T	T	T
0.8200209645940673	0.1706009914100516	0.3319740893659688	T	T	T
0.9236557832194496	0.0549459531099795	0.8558493277206485	T	T	T
0.8016267579042354	0.0248055659758025	0.7118425930597231	T	T	T
0.7825304076584814	0.0628207017247642	0.4926271219742497	T	T	T
0.6222283146781930	0.0685726972514515	0.4919006889732325	T	T	T
0.5695263586641253	0.0322048801734994	0.7017684580643181	T	T	T
0.6787397642415075	0.0538559969676601	0.8523768039172479	T	T	T
0.9228763983726214	0.8317526004653769	0.8375024113985230	T	T	T
0.8027441808957562	0.8668833383829221	0.6946328253740833	T	T	T
0.7680575273699876	0.8252045538487623	0.4777057958372933	T	T	T
0.6136387410733745	0.8265277708295075	0.4926994784692668	T	T	T
0.5647589638922218	0.8747875792283391	0.7023283884766951	T	T	T
0.6801214542871551	0.8302868165650299	0.8345323998550616	T	T	T
0.4263825676240430	0.4440992315464239	0.6396949557527750	T	T	T
0.3058353110539436	0.4705893847184192	0.7842079960859694	T	T	T
0.2837843210350273	0.4395285174347289	0.0052490754558286	T	T	T
0.1245976091307434	0.4340537008596101	0.0074332701098727	T	T	T
0.0658515337295304	0.4699764563457927	0.7994690091848887	T	T	T
0.1787122056690390	0.4429568271178560	0.6526979422692847	T	T	T
0.4204228892692868	0.6736802449758625	0.6609419105705160	T	T	T

Structure files (CONTCAR) involved in this work:

0.3013503677739289	0.6291035967731486	0.7959951878893632	T	T	T
0.2697962768374422	0.6728415028696476	0.0156036340097307	T	T	T
0.1158185484319172	0.6747115295237585	0.0063526515877971	T	T	T
0.0642513083515107	0.6289587100406963	0.7975770693692631	T	T	T
0.1787669813718871	0.6680825039254241	0.6615703534123338	T	T	T
0.0815792236381924	0.5581331254565363	0.1387382542000217	T	T	T
0.2013594477624322	0.5280876452171919	0.2801679801458263	T	T	T
0.2222719418908169	0.5603235820757588	0.5083276857864316	T	T	T
0.3820530426931582	0.5678679441455476	0.5066007153238229	T	T	T
0.4331151619671377	0.5302071447773524	0.2945739959006265	T	T	T
0.3265102007580775	0.5586174602055441	0.1436702831093780	T	T	T
0.0846468795852526	0.3256622657265119	0.1626081311017945	T	T	T
0.1998943150420797	0.3702034001103935	0.2999831259987231	T	T	T
0.2314007563188819	0.3310009615577845	0.5206677572629268	T	T	T
0.3860710627853457	0.3280993966651431	0.5066855288242573	T	T	T
0.4348457046373186	0.3722984866826602	0.2938562704579255	T	T	T
0.3203954405364480	0.3291449731736641	0.1645519349399084	T	T	T
0.0143044173445474	0.5500545945961142	0.2137749125541090	T	T	T
0.3598195307531017	0.0678135584258862	0.7233321099538311	T	T	T
0.3170498645998576	0.0532477117446631	0.9082798789814380	T	T	T
0.2022813195598092	0.0492755202547386	0.0083949161534938	T	T	T
0.0919553661023628	0.0689002942070154	0.9022927207218548	T	T	T
0.1043943124578123	0.0641187975343415	0.7051973034059287	T	T	T
0.2302723591374768	0.0500207714899207	0.7610472635282043	T	T	T
0.3611714641474310	0.8260032762342989	0.7541701297483192	T	T	T
0.3041569960460567	0.8577965728719420	0.9239229586750036	T	T	T
0.1893149823887948	0.8556740842638452	0.0210509255971410	T	T	T
0.0866107744048398	0.8333560040186218	0.9005789197814790	T	T	T
0.1034844799533360	0.8393188868138620	0.7051086188885785	T	T	T
0.2299023144538562	0.8469003478628474	0.7615717305729169	T	T	T
0.3156654447980453	0.9490853378333676	0.7797835928250204	T	T	T
0.0897205685660459	0.9518553193109518	0.8098468581374551	T	T	T
0.4327247627105714	0.1281113083266843	0.5842297510628992	T	T	T
0.4136514237449974	0.9968441435224331	0.5734270530647980	T	T	T
0.3948119967614213	0.8646182955610003	0.5709738533267618	T	T	T
0.1973378370977412	0.1360691798643976	0.6182157049770033	T	T	T
0.1896671108680769	0.0037705235808778	0.5844593586465846	T	T	T
0.1969485307282371	0.8698616285111580	0.5703363187214618	T	T	T
0.9881275691995807	0.0383712546926815	0.7862917435253538	T	T	T
0.9856682325275825	0.8703993249969224	0.7846566646999049	T	T	T
0.1410966308500668	0.9320413652234408	0.2247473583965182	T	T	T
0.1841974045495788	0.9448750261280265	0.4096870797850279	T	T	T
0.2981831289914317	0.9471215994268956	0.5124365366909512	T	T	T
0.4073750804487527	0.9302694178755323	0.4031791113197190	T	T	T
0.3968460120706409	0.9380963489229420	0.2068378710435572	T	T	T
0.2706553998281716	0.9519766167515673	0.2624685098122679	T	T	T
0.1410267319051761	0.1742267794406739	0.2503920808592580	T	T	T
0.1948158967091518	0.1446127982103793	0.4224669837410667	T	T	T
0.3105632817625331	0.1480262628641837	0.5162408016833856	T	T	T
0.4140881285783237	0.1693159763306546	0.3964062440024762	T	T	T
0.3963823354640237	0.1573080836802696	0.2011574318653226	T	T	T
0.2713466903463326	0.1493955593084408	0.2609718554747123	T	T	T
0.1825886284562840	0.0505041473794606	0.2834933692685205	T	T	T

Structure files (CONTCAR) involved in this work:

0.4168213349522600	0.0486812456011600	0.3140488339312015	T	T	T
0.0660944754692465	0.8719062442875258	0.0894126473246789	T	T	T
0.0867948926618305	0.0021624961338424	0.0731324077299973	T	T	T
0.1075486253601783	0.1338223557325073	0.0687755605907825	T	T	T
0.3040983505157681	0.8656487498773514	0.1203813765320698	T	T	T
0.3115408104679731	0.9970093739430392	0.0850362922878946	T	T	T
0.3010361654947889	0.1297086289798536	0.0674944507950358	T	T	T
0.5135142485206822	0.9567762255845369	0.2897090226334564	T	T	T
0.5159590121701740	0.1350788950871336	0.2798642748807436	T	T	T
0.6437489333660616	0.5593995701267607	0.2881728081977601	T	T	T
0.7056169942898639	0.5712589115617815	0.1147495258460842	T	T	T
0.7953549929821701	0.5597558660446855	0.9660762871990649	T	T	T
0.8930258549774501	0.5758154839578056	0.1019456629931144	T	T	T
0.8944739608496716	0.5485313268469466	0.3178862846727533	T	T	T
0.7689839259642063	0.5175068630541392	0.2701002766265963	T	T	T
0.6423923826284380	0.3322324505642791	0.2652532846349809	T	T	T
0.6917961738252748	0.3358945532411537	0.0847959272686241	T	T	T
0.8102913871259673	0.3514958357535248	0.9953181374071659	T	T	T
0.9162461615501206	0.3203895460659009	0.1096331227496321	T	T	T
0.9065333188647606	0.3458697349739265	0.3056351689001983	T	T	T
0.7701611487802976	0.3651959046405251	0.2401279082661396	T	T	T
0.6724861430309031	0.4491437760933810	0.1837652315166741	T	T	T
0.9218682830108827	0.4452905986953811	0.1706257206575176	T	T	T
0.5670772599709292	0.6264026483597450	0.4163350086566562	T	T	T
0.5824514703117973	0.4959083724069826	0.4407363040566214	T	T	T
0.5914803367881073	0.3627387677170437	0.4442041250449189	T	T	T
0.7941708891358470	0.6286440119580557	0.3731625169879008	T	T	T
0.8113332619349488	0.5103940292437715	0.4616096961762488	T	T	T
0.8174447571381759	0.3758343473190473	0.4455609161093828	T	T	T
0.0221057420113454	0.3642921854990193	0.2129450807266914	T	T	T
0.8564537983194547	0.4314846737843783	0.7875411277204687	T	T	T
0.7873739260182968	0.4315252725782379	0.6178536092802916	T	T	T
0.6994296976303976	0.4385418710726612	0.4675607013179890	T	T	T
0.6065752379964994	0.4311018402771850	0.6110794763273304	T	T	T
0.6037516239734017	0.4448588700655652	0.8091838780311320	T	T	T
0.7299696592625108	0.4770484200861309	0.7802122097094500	T	T	T
0.8615259237864290	0.6795452630150290	0.7527756730099956	T	T	T
0.8093037580133794	0.6445148201157740	0.5668814528005377	T	T	T
0.6878562023038779	0.6463717449417394	0.4903790618721892	T	T	T
0.5818779627353607	0.6693210145389238	0.6041777761761097	T	T	T
0.5962533653245854	0.6597430560399040	0.8022658092625083	T	T	T
0.7220039286214772	0.6436722695443994	0.7478813970030826	T	T	T
0.8279787285571735	0.5465483524301489	0.6965357603577303	T	T	T
0.5821646126453385	0.5497743063741464	0.6893363626049137	T	T	T
0.9322585520408881	0.3780471784428208	0.9295944264404795	T	T	T
0.9143103283575914	0.5106357865366689	0.9277318621235575	T	T	T
0.9002486888630732	0.6417632661234735	0.9359457726835146	T	T	T
0.6979078512851941	0.3728034689914746	0.8948849462250971	T	T	T
0.6766811705974384	0.4995486655622974	0.9558322218096346	T	T	T
0.6863955303838111	0.6336040784457554	0.9423971573791075	T	T	T
0.4916731581634329	0.4523457102433314	0.7098747497884709	T	T	T
0.4801022470748504	0.6334900140739557	0.7177214853413101	T	T	T
0.6437404177746365	0.9381804808715123	0.2893748700914895	T	T	T

Structure files (CONTCAR) involved in this work:

0.6987242841176584	0.9305665973754211	0.1106413797998886	T	T	T
0.8002636179810393	0.9490903140010789	0.9833470520988339	T	T	T
0.9002445949910414	0.9299769871618226	0.1129688852352548	T	T	T
0.8968617772677143	0.9454054730245551	0.3106273599613542	T	T	T
0.7713385588060757	0.9679882738499265	0.2658950036759576	T	T	T
0.6421803560897014	0.1708299568860385	0.2565713795831693	T	T	T
0.6985376057352758	0.1579328305054165	0.0818968157474096	T	T	T
0.8120035420138447	0.1474260094230224	0.9811882386663788	T	T	T
0.9179117163871185	0.1667987736649336	0.0953741938547464	T	T	T
0.8971024703155175	0.1617841481933343	0.2924050246167193	T	T	T
0.7715986331865643	0.1380053256995194	0.2455019942168497	T	T	T
0.6781081309764257	0.0501108534815291	0.1945958719774063	T	T	T
0.9184907189608662	0.0499724290115203	0.1892079190093197	T	T	T
0.5685826912197445	0.8744769916330746	0.4214445360644051	T	T	T
0.5841610473208132	0.0052561841957121	0.4404050466636376	T	T	T
0.5982579044288244	0.1374897773210876	0.4381475317735823	T	T	T
0.8052013369664228	0.8674955693271396	0.3903963655536234	T	T	T
0.8152597414555811	0.9935075279257711	0.4503478512738179	T	T	T
0.8119338538903823	0.1274013209782126	0.4349380361039968	T	T	T
0.0109130385535835	0.9550904563639004	0.2194148031279650	T	T	T
0.0168479353211257	0.1372845580470825	0.2174166032151748	T	T	T
0.8575521536962968	0.0547432736917560	0.7867353333102809	T	T	T
0.8015126392451629	0.0692799451591507	0.6103200094570673	T	T	T
0.7019148681772807	0.0582245697639867	0.4783721300196729	T	T	T
0.6017215904758727	0.0740517806151358	0.6090139400857149	T	T	T
0.6036448572096261	0.0540683353721470	0.8067286483122781	T	T	T
0.7288537129989306	0.0285947879061165	0.7646092132096887	T	T	T
0.8604087489513722	0.8322877642941431	0.7615059849085900	T	T	T
0.8060383268637656	0.8338457618363013	0.5841253073218432	T	T	T
0.6911644716289910	0.8513868558886847	0.4884337013452642	T	T	T
0.5873235944332144	0.8295646332060680	0.6072120756193089	T	T	T
0.6040293348009211	0.8499325947915601	0.8019162724820874	T	T	T
0.7298362256701794	0.8530741432390327	0.7439464974775755	T	T	T
0.8175745680180396	0.9467946424058616	0.6863465906100402	T	T	T
0.5817647862329367	0.9528956760247788	0.6790401353328548	T	T	T
0.9330571647750402	0.1287538566242954	0.9058296121305464	T	T	T
0.9191889381245752	0.9995987915839764	0.9454361322671991	T	T	T
0.9023696919874445	0.8673492288282691	0.9421323028926474	T	T	T
0.6967057925900163	0.1294598079018975	0.8879335033973431	T	T	T
0.6821415299062831	0.0026803352155444	0.9470066726544142	T	T	T
0.6990561705496839	0.8691905769830890	0.9372080252478683	T	T	T
0.4904126203343531	0.0479371080842246	0.7147246413419822	T	T	T
0.4847222023316934	0.8661832245708635	0.7202932465307148	T	T	T
0.3599620982119593	0.4377936970123346	0.7089836598111272	T	T	T
0.3096922326963009	0.4320682357273523	0.8909424549101032	T	T	T
0.2034401629057239	0.4533158933117712	0.0089939289880085	T	T	T
0.0974129594867143	0.4295961324463518	0.8936092900071025	T	T	T
0.1026499831531802	0.4477455321172442	0.6958898655113853	T	T	T
0.2301901045202194	0.4621195733805569	0.7416774519648131	T	T	T
0.3535578596857393	0.6711122795981739	0.7292149299811654	T	T	T
0.3041284264633918	0.6576108404866801	0.9087640999380603	T	T	T
0.1922295521719830	0.6471238186305480	0.0135935349243925	T	T	T
0.0909924461392723	0.6729653238758470	0.8910248360434188	T	T	T

Structure files (CONTCAR) involved in this work:

0.1015890762843021	0.6521044010250846	0.6945978525841372	T	T	T
0.2264014490893808	0.6393948530482387	0.7505014212708844	T	T	T
0.3212573904097960	0.5501976411121406	0.7965713124142642	T	T	T
0.0776504600848951	0.5499097170194555	0.8188376496970758	T	T	T
0.4339324644575657	0.3759256155391952	0.5738270624979098	T	T	T
0.4214768879463571	0.5077547499985771	0.5635020459922566	T	T	T
0.4038144129044368	0.6398573052434940	0.5529157529814818	T	T	T
0.1927220811018188	0.3672252672275985	0.6130809496129199	T	T	T
0.1864138797250167	0.4956912298994316	0.5600460280287066	T	T	T
0.1936288288267310	0.6296041653208826	0.5565078535714235	T	T	T
0.9865994410138229	0.4531391644440043	0.7864396083978653	T	T	T
0.9846260020541447	0.6415129164540008	0.7793012955852152	T	T	T
0.1442175061350160	0.5666840840591367	0.2142755263390073	T	T	T
0.2013214857946905	0.5609038814906283	0.3910431478298407	T	T	T
0.3021968979900764	0.5554655451095999	0.5229702167550485	T	T	T
0.3997747278666178	0.5696368068997884	0.3887764342614677	T	T	T
0.4008791181050433	0.5584853674802158	0.1910955875723555	T	T	T
0.2740970539956806	0.5381259416846231	0.2315688249458064	T	T	T
0.1459007781921624	0.3245330451452739	0.2422214486813765	T	T	T
0.1952641323968969	0.3546476918616968	0.4180979132960712	T	T	T
0.3091978396354769	0.3546766471900787	0.5179688019582706	T	T	T
0.4084035077514575	0.3304582778798175	0.3904073033495744	T	T	T
0.3979772821523959	0.3429809918879773	0.1942677975297623	T	T	T
0.2744794078664851	0.3541918651350733	0.2586001486113766	T	T	T
0.1812895045663433	0.4492462199474812	0.2823336555827746	T	T	T
0.4155446493560266	0.4510049041104229	0.3081199190016281	T	T	T
0.0691896340647997	0.6255519094025944	0.0745223489900130	T	T	T
0.0844253978596571	0.4933605407887054	0.0673259066949028	T	T	T
0.1103461784661653	0.3628286246185192	0.0608258687952058	T	T	T
0.3097721486903277	0.6334338349377685	0.1029667931186078	T	T	T
0.3214640558895898	0.5041628166181842	0.0536462682077177	T	T	T
0.3007894252190508	0.3707171891302035	0.0643680580905720	T	T	T
0.5127896132310543	0.5426719940996508	0.2876967501656434	T	T	T
0.5148130556944557	0.3642005252150237	0.2808352242452963	T	T	T
0.4407926925813087	0.7513010350827580	0.6422831286953213	T	T	T
0.1898315199187035	0.7474834960808147	0.6424112072890511	T	T	T
0.2727031861698967	0.7521122341567146	0.0384343116324202	T	T	T
0.1094877115359105	0.7501448528512465	0.0495351011351915	T	T	T
0.0649683282617362	0.2492880837155054	0.1338628636876889	T	T	T
0.3082225996118861	0.2502666940278606	0.1419690085767846	T	T	T
0.2255757496402912	0.2508608726819149	0.5344416064695374	T	T	T
0.3921168192593694	0.2516199991588099	0.5472024860839888	T	T	T
0.5589479149173687	0.2497241917676231	0.3571408646503004	T	T	T
0.8029229051626910	0.2472656138637364	0.3533002235095726	T	T	T
0.7297063035441853	0.2500289664877471	0.9447021473890209	T	T	T
0.8935883684804365	0.2515143390800021	0.9466403415065655	T	T	T
0.9447938705814123	0.7550691487532131	0.8624079650837785	T	T	T
0.6862552750656553	0.7509473053261362	0.8562499332750998	T	T	T
0.7703630042314693	0.7469911121948709	0.4456933731784827	T	T	T
0.6066353905716021	0.7499726811748426	0.4525341974693129	T	T	T
0.9335377177461233	0.4604863899167289	0.5529053180479787	T	T	T
-0.0446276154903425	0.6143496778747495	0.5861613679305137	T	T	T
0.9230497050024438	0.5285650604279030	0.1983557326772651	T	T	T

Structure files (CONTCAR) involved in this work:

0.8203669412429695	0.3302903340017896	0.3307294273469515	T	T	T
0.7996206294654243	0.6331336538846158	0.6963501074104396	T	T	T
0.9293192887628811	0.3735645488171192	0.4694296509769432	T	T	T
0.8828224969765275	0.5449585456032965	0.5685764874191209	T	T	T
0.0444489374792830	0.5349039616644216	0.4296159169770360	T	T	T
0.0461225396234978	0.6015515838059999	0.4136621458348543	T	T	T
0.9591036924381370	0.4498216646683188	0.6133059439346962	T	T	T
0.0897036683016506	0.5055610438460796	0.4421299057108750	T	T	T
-0.0024475437900609	0.5069693116331894	0.4328969457260283	T	T	T
0.0001766752185303	0.6302209847342894	0.4016053029872453	T	T	T
0.0265622522964004	0.5562560164140149	0.2860926738731876	T	T	T
0.0930309606298795	0.6294256943288190	0.4119265987012636	T	T	T
-0.0373474318493473	0.6290005809818595	0.6567975694356106	T	T	T
-0.0011775074624634	0.5997284360332437	0.5600936480719672	T	T	T

Figure 7(b) TS1

Si O Al Zn C H

1.0000000000000000

20.0219999999999985 0.0000000000000000 0.0000000000000000

0.0000000000000000 19.8990000000000009 0.0000000000000000

0.0000000000000000 0.0000000000000000 13.3829999999999991

93 194 3 2 2 8

Selective dynamics

Direct

0.4230116472795291	0.0596417915470523	0.6485472724054061	T	T	T
0.3053620051790783	0.0316214035365329	0.7918577594079081	T	T	T
0.2828609424286840	0.0550914337097236	0.0171884798360987	T	T	T
0.1237745384929585	0.0625226730806294	0.0125567560668352	T	T	T
0.0681829931183086	0.0309653069970342	0.8014596023097774	T	T	T
0.1807970046619449	0.0651063930940855	0.6656142631396234	T	T	T
0.4191551701147482	0.8270573651905676	0.6692716699095713	T	T	T
0.3006337936466509	0.8728081935172028	0.7995318531187450	T	T	T
0.2678333334802185	0.8308681890667201	0.0189518258457579	T	T	T
0.1118727291905999	0.8271627595589545	0.0134214170165967	T	T	T
0.0660945800755922	0.8741825704233082	0.7992574506978124	T	T	T
0.1786031502539794	0.8280848078094911	0.6644315633653984	T	T	T
0.0759486715583015	0.9412545323803392	0.1501686838829568	T	T	T
0.1957108481564938	0.9692256631268967	0.2909702451138066	T	T	T
0.2170876354523226	0.9433680431180800	0.5171455758411093	T	T	T
0.3774684911267693	0.9347721840947436	0.5141842104817625	T	T	T
0.4335396926008299	0.9685701423069674	0.3019841216452603	T	T	T
0.3208545132544830	0.9343313999657161	0.1653225424521353	T	T	T
0.0825388407359351	0.1717337441518878	0.1664819018199567	T	T	T
0.1990965584498090	0.1279579139446404	0.3004855019074598	T	T	T
0.2318500549560894	0.1689755745161703	0.5182191381783708	T	T	T
0.3876587358208051	0.1733871803221630	0.5088791635206392	T	T	T
0.4346966322461980	0.1265069239517303	0.2950107080881563	T	T	T
0.3192346791953088	0.1722636012855642	0.1642975071381824	T	T	T
0.5768135840816778	0.5550338675236685	0.3603757301353531	T	T	T
0.6895670643013568	0.5264989463304921	0.2070553993406165	T	T	T
0.7135654941106605	0.5666532055717715	0.9918286007923686	T	T	T
0.8725558501942635	0.5730232880706423	0.9850708828110232	T	T	T
0.8109723127999934	0.5510586933343763	0.3442080829034778	T	T	T
0.5726848120303413	0.3279412910235666	0.3316810452544411	T	T	T

Structure files (CONTCAR) involved in this work:

0.6911199345887271	0.3728621510652627	0.1917477259219346	T	T	T
0.7307178869094799	0.3288841951689355	0.9783013161716343	T	T	T
0.8857513721372978	0.3260219201045300	0.9917123120329898	T	T	T
0.9417569878753633	0.3738587544756128	0.1895972688598147	T	T	T
0.9193166864777140	0.4461891163361474	0.8585011728047151	T	T	T
0.8013271229524329	0.4753308926959915	0.7175344121329715	T	T	T
0.7771761022109991	0.4379360628562903	0.4945355067950404	T	T	T
0.6198114986864568	0.4277355557157831	0.4904765624890026	T	T	T
0.5704843521099384	0.4685512246261793	0.7010985400868303	T	T	T
0.6779394420782042	0.4493560369883912	0.8556033868846419	T	T	T
0.9201718909371296	0.6784555168204632	0.8276794475343747	T	T	T
0.7667677099067522	0.6686884718988361	0.4628376623172044	T	T	T
0.6119811990339096	0.6735601642051647	0.4885009518085298	T	T	T
0.5620690349351785	0.6267057105377130	0.6989108280398114	T	T	T
0.6751402589453311	0.6732374457689099	0.8306180351282683	T	T	T
0.5781028539901989	0.9458250891654492	0.3590193145979673	T	T	T
0.6981165285668658	0.9738313509973029	0.2149419339650859	T	T	T
0.7194450459362328	0.9382474960924905	0.9937546151122787	T	T	T
0.8793097693707296	0.9345417661045158	0.9954651357394928	T	T	T
0.9308337576560305	0.9707124368389770	0.2052918124840132	T	T	T
0.8216842579216426	0.9465503668491332	0.3550710640384098	T	T	T
0.5771879797670377	0.1731697060438883	0.3304000105288671	T	T	T
0.6977668171195948	0.1315389187267768	0.1945760099173219	T	T	T
0.7317705172819422	0.1724235636335648	0.9731457185756798	T	T	T
0.8865976246645986	0.1738300875071525	0.9817292406103063	T	T	T
0.9354734446471974	0.1287285547293463	0.1957904965653141	T	T	T
0.8205870860286532	0.1731852934020850	0.3307762797718507	T	T	T
0.9231989713136524	0.0538040125022727	0.8559579371774433	T	T	T
0.8012922169737243	0.0254898773391334	0.7100039604599938	T	T	T
0.7816587031914524	0.0664567397238821	0.4920643867872382	T	T	T
0.6212031186912171	0.0704970604301987	0.4910178399530832	T	T	T
0.5685797653147112	0.0322010624065665	0.6998492627304568	T	T	T
0.6781791651478000	0.0542645903504517	0.8510211478767681	T	T	T
0.9227688902974162	0.8308424535204528	0.8371980073585346	T	T	T
0.8019278315220346	0.8675581829862038	0.6944914995728383	T	T	T
0.7683286038441972	0.8260705649753214	0.4769223760635504	T	T	T
0.6134971240423311	0.8269290501946522	0.4899558451430867	T	T	T
0.5636109542407156	0.8750946976887684	0.6985062803941913	T	T	T
0.6780781109451562	0.8320577417329919	0.8340624610137440	T	T	T
0.4237962868039227	0.4412114508510564	0.6469413320913695	T	T	T
0.3050290063828974	0.4683993912722298	0.7893726430536485	T	T	T
0.2792720750037758	0.4461059519855395	0.0164024528500972	T	T	T
0.1213186727978342	0.4372498878251332	0.0175074958770042	T	T	T
0.0647145452016398	0.4681511194649418	0.8043026495974714	T	T	T
0.1775485872252030	0.4348614743671723	0.6636652086907626	T	T	T
0.4170451114413462	0.6729410888994311	0.6683326439072850	T	T	T
0.3000678181435012	0.6270055812707725	0.7993314901498764	T	T	T
0.2687712366723454	0.6694714276149152	0.0198213531888593	T	T	T
0.1141301437134151	0.6735163648133183	0.0119639653815928	T	T	T
0.0659379013120135	0.6267650795827721	0.8001899556876422	T	T	T
0.1780045929294256	0.6705346694560900	0.6628390232805601	T	T	T
0.0782479859728776	0.5598165534313103	0.1493260788564744	T	T	T
0.1973860624285635	0.5285043968550912	0.2888138579032360	T	T	T

Structure files (CONTCAR) involved in this work:

0.2146375432947598	0.5551169406903781	0.5159502888822334	T	T	T
0.3745227823089201	0.5653010998654404	0.5152144293177462	T	T	T
0.4307342112299205	0.5305532112963142	0.3045997106731352	T	T	T
0.3225343432655264	0.5645983678566519	0.1627194890803823	T	T	T
0.0857144079694369	0.3243797648803167	0.1653901697296258	T	T	T
0.1994795848037191	0.3703384502313641	0.3006945086513950	T	T	T
0.2304583705674552	0.3303111182634230	0.5192461313262150	T	T	T
0.3856677053324389	0.3273259586771853	0.5075991479575425	T	T	T
0.4304282645749223	0.3737602203704283	0.2937704146616401	T	T	T
0.3174936943658527	0.3290006759487921	0.1623672144879006	T	T	T
0.0115390690316196	0.5580117267440108	0.2279681468735754	T	T	T
0.3596154165976516	0.0702797442717356	0.7226740867760411	T	T	T
0.3177311739779790	0.0513767512109038	0.9078058365199109	T	T	T
0.2027981632840985	0.0457402698861532	0.0063280760524604	T	T	T
0.0926121693416275	0.0695929566289103	0.9016397862022202	T	T	T
0.1040688267159937	0.0642135023297687	0.7045141683109574	T	T	T
0.2301121140799018	0.0541603833993546	0.7610442599769421	T	T	T
0.3599129075253070	0.8278212088363849	0.7521219523523464	T	T	T
0.3007921775219045	0.8627613661669021	0.9192581274023283	T	T	T
0.1892055780903703	0.8513884558235075	0.0232263899243701	T	T	T
0.0882926959884811	0.8321611466432353	0.8979776733630835	T	T	T
0.1021250637247867	0.8407243498023842	0.7019032210557210	T	T	T
0.2287362486599335	0.8486879905835495	0.7553263430746616	T	T	T
0.3139589831105526	0.9512117647054078	0.7727495680381365	T	T	T
0.0893886176614743	0.9519846076448540	0.8105101125108283	T	T	T
0.4332807274427840	0.1267244338128585	0.5809182431446478	T	T	T
0.4123176585947931	0.9955966681574345	0.5753135859816769	T	T	T
0.3936162535007521	0.8634153607388227	0.5675884930221652	T	T	T
0.1955360618125965	0.1380463221724706	0.6160708344873554	T	T	T
0.1910502422846932	0.0051649643693200	0.5851875071103845	T	T	T
0.1941398441174284	0.8717640919053151	0.5648037321060445	T	T	T
0.9882326357187663	0.0389025728087317	0.7868478814789145	T	T	T
0.9855528456040131	0.8701835681878923	0.7856443851211220	T	T	T
0.1399203274414616	0.9314399111163441	0.2233515206197376	T	T	T
0.1836683883194456	0.9501518508468234	0.4072015883716001	T	T	T
0.2975960215238133	0.9470170774675878	0.5092220193271030	T	T	T
0.4079769273987047	0.9313700701084735	0.4026803823955594	T	T	T
0.3970884058029360	0.9346365231293237	0.2059629004086428	T	T	T
0.2702138041332766	0.9449648533805322	0.2593333168890828	T	T	T
0.1388361780054224	0.1718185063368920	0.2536547331910311	T	T	T
0.1967071423664787	0.1364572364668875	0.4204902724015748	T	T	T
0.3103846923909350	0.1484760756337199	0.5177197216522674	T	T	T
0.4124298250826662	0.1680111645110964	0.3940671866590791	T	T	T
0.3960508866613075	0.1580691149531572	0.1985116949512854	T	T	T
0.2707709927063910	0.1543917321017757	0.2587519485333106	T	T	T
0.1884748728762152	0.0495340974486039	0.2708291592255578	T	T	T
0.4141321682812786	0.0479621824811257	0.3082420583016325	T	T	T
0.0653055371120066	0.8726635389101888	0.0856412381509588	T	T	T
0.0861137452606368	0.0026719948954284	0.0721290234190804	T	T	T
0.1114161199513898	0.1333327210680097	0.0687945514982554	T	T	T
0.3063729755613699	0.8615212712100926	0.1149123880117354	T	T	T
0.3119115444723343	0.9942971619608343	0.0846084313908107	T	T	T
0.3000887601141001	0.1272803618825923	0.0673622714278860	T	T	T

Structure files (CONTCAR) involved in this work:

0.5133088921052991	0.9581342762386765	0.2883364728326336	T	T	T
0.5148929102974108	0.1329316605394895	0.2788415222535506	T	T	T
0.6392005062466066	0.5627347232516346	0.2849420699157005	T	T	T
0.6940359997788889	0.5740983778894705	0.1090009972267491	T	T	T
0.7933088009070872	0.5554385555680414	0.9771171655710577	T	T	T
0.8971445279650633	0.5823733030020988	0.0983638523408463	T	T	T
0.8869721995028803	0.5393430673222867	0.3100161015362939	T	T	T
0.7629677451842338	0.5212579894491329	0.2580251627154576	T	T	T
0.6372112022655861	0.3326876934066313	0.2604505344085026	T	T	T
0.6889246925373860	0.3391493262092473	0.0806941449112883	T	T	T
0.8084004828427174	0.3509037318814211	0.9948513379682189	T	T	T
0.9151589212913411	0.3215440642246430	0.1048050542048134	T	T	T
0.9032137310238866	0.3576269101180687	0.2949475123067628	T	T	T
0.7640897524925025	0.3683035910602192	0.2400387962718248	T	T	T
0.6651814910548085	0.4508016375831461	0.1810980800322590	T	T	T
0.9308316748159322	0.4495402194439072	0.1532997112703584	T	T	T
0.5655993305468013	0.6259556125054587	0.4182891116645221	T	T	T
0.5894924465936640	0.4961925397731536	0.4423918824135391	T	T	T
0.5852555908182333	0.3622115254609720	0.4406741852302191	T	T	T
0.7956906130050050	0.6304999727595113	0.3642279327866177	T	T	T
0.7965047649433393	0.5135190463741131	0.4527023115970284	T	T	T
0.8246346838449362	0.3826127452735786	0.4396989494446588	T	T	T
0.0210918663415089	0.3615927547881467	0.2113534082758991	T	T	T
0.8550100727143658	0.4352137743753083	0.7860269127339415	T	T	T
0.7901851406852518	0.4347058217010540	0.6135930541972111	T	T	T
0.6995678834284246	0.4233343853497676	0.4683867790934400	T	T	T
0.6050029978783642	0.4273789970415498	0.6094475063108675	T	T	T
0.6043364105058832	0.4451457350607986	0.8052734767772828	T	T	T
0.7300197827140358	0.4805407309925624	0.7741099343299701	T	T	T
0.8700509632629910	0.6822153103290881	0.7335309878518708	T	T	T
0.8113229738704729	0.6451851684555350	0.5588052915617882	T	T	T
0.6891601964076388	0.6477965616220327	0.4832100544841989	T	T	T
0.5855889305054468	0.6701924399284649	0.6025920371567369	T	T	T
0.5978477611015967	0.6567908921163789	0.7980511429812513	T	T	T
0.7252730741880442	0.6516745018786362	0.7422733780574443	T	T	T
0.8290633864506236	0.5509814917181558	0.6930619298747488	T	T	T
0.5817655288912598	0.5483652133779668	0.6816961516215415	T	T	T
0.9292360177336314	0.3785183623572094	0.9250688118893607	T	T	T
0.9125656680459944	0.5120679719771218	0.9289446992903002	T	T	T
0.8869582222914407	0.6425109223612958	0.9238636508786044	T	T	T
0.6995778943227952	0.3742623913480628	0.8889464497031198	T	T	T
0.6749927059991297	0.5000615287113396	0.9504080597545230	T	T	T
0.6898485935661655	0.6341370230335359	0.9350106152465510	T	T	T
0.4914680572788112	0.4512823396469952	0.7109897701738226	T	T	T
0.4812849477378077	0.6326126695414146	0.7117663919810927	T	T	T
0.6436685699912545	0.9399700358181224	0.2889096139007024	T	T	T
0.6987216556331100	0.9324131292893837	0.1104954740483367	T	T	T
0.7998412795758257	0.9466280536356375	0.9810523260208953	T	T	T
0.8988042821858995	0.9285287318048039	0.1126816525912457	T	T	T
0.8970613299479290	0.9480054481273298	0.3101891093550002	T	T	T
0.7714690133506937	0.9687477725307779	0.2656577927310610	T	T	T
0.6404924397780665	0.1720875905003818	0.2553662843986705	T	T	T
0.6971013983232592	0.1590592372220949	0.0807369365895678	T	T	T

Structure files (CONTCAR) involved in this work:

0.8094490425576030	0.1479626500760304	0.9777172352263099	T	T	T
0.9135948311266980	0.1686834808043230	0.0954497935278555	T	T	T
0.8972149815142823	0.1588406098314975	0.2926055550896560	T	T	T
0.7706504757003332	0.1426349406193003	0.2446750889122433	T	T	T
0.6790976956033062	0.0519387360625020	0.1953611226958219	T	T	T
0.9177687717268490	0.0496375049047383	0.1826344798051422	T	T	T
0.5685084460146118	0.8757738173430791	0.4199954748297174	T	T	T
0.5836571290367798	0.0069303203492908	0.4392228179681544	T	T	T
0.5970440950764012	0.1394014920970954	0.4370811758579868	T	T	T
0.8066307358686711	0.8707833666872243	0.3936959483842465	T	T	T
0.8156823000701937	0.9982316843141995	0.4483093676407075	T	T	T
0.8093441779083553	0.1324068264680505	0.4353925617239716	T	T	T
0.0100819925506108	0.9548095166558295	0.2170879233262463	T	T	T
0.0157987574200150	0.1366373128817352	0.2110841873842986	T	T	T
0.8577370856511214	0.0536855099007988	0.7854845327232550	T	T	T
0.8011422716610063	0.0714631526471666	0.6098073261001256	T	T	T
0.7010857715429758	0.0606462592085747	0.4781584941885482	T	T	T
0.6006503970733886	0.0754142214144163	0.6082579316754099	T	T	T
0.6031650543534439	0.0519376908123966	0.8053729693211545	T	T	T
0.7288050216566355	0.0297337676597426	0.7634834870684977	T	T	T
0.8600481185355261	0.8336990095340711	0.7614908239645268	T	T	T
0.8043549760640815	0.8320843325210657	0.5854049788817847	T	T	T
0.6911610435787244	0.8514974965620254	0.4857796615490653	T	T	T
0.5875441344475220	0.8293040635453338	0.6047101538129634	T	T	T
0.6026588655605429	0.8522057347395893	0.7992353585411492	T	T	T
0.7294578421987356	0.8547642567110634	0.7455690065154461	T	T	T
0.8161340651025195	0.9474487043202805	0.6820482628752196	T	T	T
0.5796588867459127	0.9532014403023977	0.6734633137972706	T	T	T
0.9315283983668154	0.1271616821457120	0.9080255771109910	T	T	T
0.9187432121481623	0.9969918249642985	0.9435153262872062	T	T	T
0.9024278948496917	0.8646309190908503	0.9432321060734932	T	T	T
0.6937749342622972	0.1305172616647648	0.8861514892117291	T	T	T
0.6832528935620823	0.0041704617270063	0.9466530591554454	T	T	T
0.6956006982309403	0.8702894037710811	0.9377878987063518	T	T	T
0.4896732797878343	0.0481570310667043	0.7145658444576318	T	T	T
0.4838394377392210	0.8649691096482830	0.7161370173132793	T	T	T
0.3612914990372305	0.4301910839751176	0.7231942165346681	T	T	T
0.3116783066722829	0.4463631183863032	0.9054377053860310	T	T	T
0.1990438733965929	0.4608577052416939	0.0128908716438402	T	T	T
0.0901015592559333	0.4328257580741729	0.9067472622964666	T	T	T
0.1024730365711588	0.4348234311254159	0.7090482671669979	T	T	T
0.2302379723003657	0.4481563880490914	0.7536767247166057	T	T	T
0.3584121291961214	0.6734210046651219	0.7524921966991587	T	T	T
0.2996489598162529	0.6372777869799423	0.9189602655689366	T	T	T
0.1903953245346543	0.6480157436605002	0.0272370535672657	T	T	T
0.0939814016912662	0.6684327596158754	0.8952640071467693	T	T	T
0.1007089085633260	0.6562264077113367	0.6982077405786123	T	T	T
0.2274742452971752	0.6481392365964458	0.7535941910682629	T	T	T
0.3156011031790020	0.5488393509876648	0.7737776375573404	T	T	T
0.0838293643785081	0.5477525118903523	0.8114484409990882	T	T	T
0.4324853186427919	0.3755318280878545	0.5757467073503462	T	T	T
0.4127363658632041	0.5064597636671521	0.5760047238512431	T	T	T
0.3879591627226603	0.6375482768455942	0.5675935020085303	T	T	T

Structure files (CONTCAR) involved in this work:

0.1915888338463464	0.3615023954928086	0.6149637289464230	T	T	T
0.1831038844268234	0.4940852638996549	0.5804237136218033	T	T	T
0.1924381867661488	0.6273757461920942	0.5620455968548695	T	T	T
0.9854744642905650	0.4564347604118612	0.7888756456918437	T	T	T
0.9861041566693105	0.6363403068148569	0.7891429279958472	T	T	T
0.1433301574688728	0.5685303005166691	0.2193630492197557	T	T	T
0.1839168497400039	0.5505332360353717	0.4035160201907351	T	T	T
0.2950776252147160	0.5483405552843930	0.5134868987435843	T	T	T
0.4027892748620340	0.5697301830175794	0.4023405480085600	T	T	T
0.3981860551223654	0.5643236751298920	0.2051727501190123	T	T	T
0.2719475514353776	0.5504892021801310	0.2563006734547967	T	T	T
0.1428588970161399	0.3231860048696951	0.2514100159790726	T	T	T
0.1962868357305010	0.3628084316576543	0.4205317498197763	T	T	T
0.3086130970804961	0.3521219791847304	0.5218169025994864	T	T	T
0.4063930308753868	0.3306087176107472	0.3905657860501693	T	T	T
0.3943765538259253	0.3455301833286532	0.1928972445075105	T	T	T
0.2723893657808397	0.3475486769020720	0.2603236053029589	T	T	T
0.1850489164339830	0.4487039262481833	0.2711372135358723	T	T	T
0.4092887373762981	0.4518004111602412	0.3118440651262092	T	T	T
0.0665274849936799	0.6252602521224822	0.0800914158224772	T	T	T
0.0787464252596462	0.4920708090617842	0.0839825563909225	T	T	T
0.1146455904034946	0.3638129384815698	0.0679010809307017	T	T	T
0.3077507550269726	0.6381713712012387	0.1151682139547653	T	T	T
0.3140482902324831	0.5059804102726400	0.0797004266049861	T	T	T
0.2936581893662630	0.3733734562640152	0.0669108805518161	T	T	T
0.5107767796201151	0.5377622417919933	0.2953386950256166	T	T	T
0.5102579034810965	0.3662866300324847	0.2778717280676442	T	T	T
0.4372316544814449	0.7497538276963918	0.6419750208935192	T	T	T
0.1879582702444826	0.7492003540485823	0.6357914367807017	T	T	T
0.2764645187297351	0.7500677754825311	0.0193196393984884	T	T	T
0.1045841314822603	0.7497388684326790	0.0505264100911341	T	T	T
0.0675445532577933	0.2484520473623695	0.1324064861302682	T	T	T
0.3096351517801853	0.2504808368353464	0.1326388074625172	T	T	T
0.2224199846453050	0.2496824598724766	0.5190933090021747	T	T	T
0.3940348906865683	0.2506277618782150	0.5461948199069583	T	T	T
0.5540873351230957	0.2498442348815003	0.3516150942248852	T	T	T
0.8083435257158991	0.2512703170547833	0.3490975785646210	T	T	T
0.7264660628071828	0.2510150634348648	0.9431101713019188	T	T	T
0.8916628421249512	0.2511872170015922	0.9433291669305420	T	T	T
0.9445634403759954	0.7536202480747055	0.8590439692167017	T	T	T
0.6827580802752553	0.7526825565125448	0.8555014940624300	T	T	T
0.7721837033674946	0.7485341312848843	0.4410531167295753	T	T	T
0.6064989629981312	0.7504858547516411	0.4489076136009267	T	T	T
0.9325043450558911	0.4876269348801763	0.5214022851141302	T	T	T
0.9510758788580954	0.6480378661107511	0.5725947112567538	T	T	T
0.9230662450810915	0.5305172690153066	0.1932076571846673	T	T	T
0.8189266820090392	0.3350359509298624	0.3253599095912261	T	T	T
0.8013740027323782	0.6365308286937512	0.6902612701053815	T	T	T
0.9264588275212543	0.4070153127621574	0.4275326182269286	T	T	T
0.8888613134391739	0.5641726019889467	0.5635732263863726	T	T	T
0.0261869077572510	0.4145774275540089	0.4610002113826177	T	T	T
0.0148417621855353	0.6008532967341783	0.3190669914415065	T	T	T
0.9905493013095314	0.4611573351955521	0.5076314018834431	T	T	T

Structure files (CONTCAR) involved in this work:

0.0595134505186471	0.4336690282121025	0.4023015910729143	T	T	T
0.0519671571270144	0.3773425948616511	0.5074768900411568	T	T	T
0.0027364047387004	0.5686142804607232	0.3828882042176469	T	T	T
0.9779269096626612	0.6411635971401259	0.3115721445857748	T	T	T
0.0653050403265101	0.6214621206069444	0.3257534347003199	T	T	T
0.9950789976660110	0.6399662362823323	0.6020925752951332	T	T	T
0.9266707574503819	0.6756577251596432	0.6229500573912988	T	T	T

Figure 7(b) TS2

Si O Al Zn C H

1.0000000000000000

20.0219999999999985 0.0000000000000000 0.0000000000000000

0.0000000000000000 19.8990000000000009 0.0000000000000000

0.0000000000000000 0.0000000000000000 13.3829999999999991

93 194 3 2 2 8

Selective dynamics

Direct

0.4225605148920058	0.0593457292963918	0.6483130706896634	T	T	T
0.3042543032970933	0.0316087563719407	0.7910327208742578	T	T	T
0.2823426323670456	0.0540087803717226	0.0168622656472412	T	T	T
0.1231506130371967	0.0623404687271209	0.0123870187699169	T	T	T
0.0677831133977095	0.0307857788994782	0.8018983129210503	T	T	T
0.1800147665836376	0.0662279843870204	0.6656400789587844	T	T	T
0.4190066490323228	0.8282676468662532	0.6713301125128084	T	T	T
0.2987411391772305	0.8730161734912075	0.7981749476623792	T	T	T
0.2672248286415294	0.8305064666903179	0.0183213297228231	T	T	T
0.1108342028366011	0.8256043821724216	0.0159509411383895	T	T	T
0.0661691333978034	0.8741267178605980	0.8014824510623879	T	T	T
0.1766686934455178	0.8278826531449445	0.6621227818586664	T	T	T
0.0751430578074859	0.9413555900526268	0.1501377693608220	T	T	T
0.1957526127291371	0.9698567007450728	0.2901153555306141	T	T	T
0.2160148986337845	0.9442458819183656	0.5168605128775571	T	T	T
0.3764606038278191	0.9344149054557853	0.5143000635838010	T	T	T
0.4327737882941475	0.9680938865531974	0.3026363312133611	T	T	T
0.3203700871386199	0.9331743081324910	0.1654601164851889	T	T	T
0.0821276048369170	0.1721021922858994	0.1667647965128831	T	T	T
0.1999389223144780	0.1285110030369042	0.2983547093063290	T	T	T
0.2311176838093450	0.1691681089265278	0.5172738668775182	T	T	T
0.3872869588215960	0.1736933134032816	0.5100635216215601	T	T	T
0.4336918311175389	0.1259607714806047	0.2961652491635497	T	T	T
0.3201638479890961	0.1722532532714295	0.1615684781253033	T	T	T
0.5768463457859490	0.5554733858777082	0.3606742648521233	T	T	T
0.6903694373990654	0.5268401183703907	0.2100354565401313	T	T	T
0.7149809339634902	0.5656572347143636	0.9929675388653977	T	T	T
0.8736275117123603	0.5719940531315999	0.9889260706711359	T	T	T
0.8127326102805157	0.5523355359670165	0.3479465502017661	T	T	T
0.5731331161657397	0.3286047473922064	0.3327726995786063	T	T	T
0.6930804315974625	0.3727152379722540	0.1955192640422415	T	T	T
0.7308850197424206	0.3293112553195814	0.9786063444421383	T	T	T
0.8855915412552666	0.3255496617906520	0.9875066067283806	T	T	T
0.9391919673258030	0.3725261573701918	0.1855783705754303	T	T	T
0.9203528021382745	0.4469170790742466	0.8595659742316537	T	T	T
0.7996958464817022	0.4758744218960138	0.7208200113399063	T	T	T
0.7806394300029011	0.4397653948799798	0.4969960734197486	T	T	T

Structure files (CONTCAR) involved in this work:

0.6235511398953717	0.4285183030388566	0.4901408224896881	T	T	T
0.5715663888182013	0.4690735673052890	0.6997141289994280	T	T	T
0.6757952330979227	0.4488883369588599	0.8580709370034446	T	T	T
0.9200149896176830	0.6783826057441993	0.8311919751742037	T	T	T
0.7658583731792271	0.6702685437863379	0.4635782631733611	T	T	T
0.6112456267508936	0.6740000000447076	0.4889141272045873	T	T	T
0.5622303742111816	0.6271213262308253	0.6999201246307485	T	T	T
0.6731430527308889	0.6740115961263641	0.8351216570246170	T	T	T
0.5775057094426344	0.9468190138000130	0.3601178835131516	T	T	T
0.6981655953840635	0.9751271508667747	0.2172150937275818	T	T	T
0.7185538123578082	0.9396876463877994	0.9954188073366369	T	T	T
0.8781729106647096	0.9353533300468592	0.9968829884954157	T	T	T
0.9300048712815701	0.9721059779594566	0.2066076421921683	T	T	T
0.8218542557766720	0.9470503614335023	0.3569888369329859	T	T	T
0.5761679894230480	0.1741050036232548	0.3320541139769604	T	T	T
0.6974578173691091	0.1335547193123344	0.1971779793838500	T	T	T
0.7311822148735108	0.1727381092293102	0.9745101676756800	T	T	T
0.8859196073177016	0.1736544226527376	0.9803176908579005	T	T	T
0.9343817838478379	0.1305781409198789	0.1961884750773543	T	T	T
0.8205310359488367	0.1758202851934595	0.3346482653991129	T	T	T
0.9228253725920724	0.0530407583054776	0.8561307222002872	T	T	T
0.7997727472818411	0.0251962150454876	0.7113762449134153	T	T	T
0.7815461810119284	0.0668130559572864	0.4934046289870010	T	T	T
0.6211171985859331	0.0714747446251132	0.4917235200686846	T	T	T
0.5685872862679195	0.0325816721484526	0.7001600755730705	T	T	T
0.6767735182602596	0.0551793592948120	0.8526283362454696	T	T	T
0.9221402435293665	0.8312424728424668	0.8395661779570338	T	T	T
0.8007742030036397	0.8668424652177973	0.6964929536566724	T	T	T
0.7674649631963811	0.8269210250491342	0.4783266658564298	T	T	T
0.6125877646950392	0.8275603746494125	0.4910285597609893	T	T	T
0.5635320102393259	0.8759847282793882	0.6995337756670628	T	T	T
0.6767411010052853	0.8320981023974784	0.8376192975162075	T	T	T
0.4251854549195161	0.4426606428998606	0.6405929190107222	T	T	T
0.3060593909562025	0.4682471920700765	0.7844333158886745	T	T	T
0.2825491950669459	0.4452815232827149	0.0098203456037907	T	T	T
0.1246869021968502	0.4362897431906849	0.0129182182406999	T	T	T
0.0649240387964990	0.4683201219581886	0.8025484622402449	T	T	T
0.1778378334164402	0.4343469241553667	0.6617249749172744	T	T	T
0.4177168473402852	0.6738909378373412	0.6675679897601481	T	T	T
0.2985590396999818	0.6270316813843724	0.7949563865285151	T	T	T
0.2685690461319389	0.6695846577669063	0.0169381499831323	T	T	T
0.1128769952589653	0.6716442931452473	0.0152204592380093	T	T	T
0.0657504383125261	0.6271012891929596	0.8010702740425973	T	T	T
0.1757201439283410	0.6708424416647253	0.6589426196395931	T	T	T
0.0769823285055707	0.5566323490624183	0.1529155904624593	T	T	T
0.1998213271425948	0.5289447144385770	0.2847502607486791	T	T	T
0.2157985419226870	0.5552365896520584	0.5153317548846860	T	T	T
0.3756661864303008	0.5676503838230451	0.5131305065996735	T	T	T
0.4297160424112220	0.5304816124184930	0.3031961157334893	T	T	T
0.3245532151631497	0.5644918399701362	0.1570269972613226	T	T	T
0.0861542805592658	0.3253985889828588	0.1592603558210085	T	T	T
0.2001693963814510	0.3704637520049683	0.2959106983084845	T	T	T
0.2298985099322044	0.3302376365624573	0.5159798195568935	T	T	T

Structure files (CONTCAR) involved in this work:

0.3853292254757469	0.3271198275544923	0.5055924050009087	T	T	T
0.4298832610847362	0.3740077917245276	0.2934390272738201	T	T	T
0.3192784065333488	0.3283228807171197	0.1574326131078505	T	T	T
0.0127925856384927	0.5472088494594577	0.2275930030914609	T	T	T
0.3596699065996849	0.0698180017615065	0.7233440662444134	T	T	T
0.3173164267631817	0.0487643460258946	0.9076811352849943	T	T	T
0.2022082470176180	0.0459690564333351	0.0053464083393797	T	T	T
0.0916467162666910	0.0701954264971724	0.9017241215713718	T	T	T
0.1033894887976730	0.0641758050585674	0.7048324429479117	T	T	T
0.2298039971802361	0.0571625566994160	0.7610085932996702	T	T	T
0.3602590546212248	0.8289383403108049	0.7550058419600901	T	T	T
0.2967335968821788	0.8654048735110782	0.9182600623922800	T	T	T
0.1883618941188134	0.8487514239898730	0.0282606742043098	T	T	T
0.0892569366323253	0.8320531454438548	0.8995911083421090	T	T	T
0.1010075373031955	0.8407375926669486	0.7030409872761162	T	T	T
0.2285858764030952	0.8459785490590188	0.7518279803833616	T	T	T
0.3102282492970185	0.9513033931080074	0.7685716060246447	T	T	T
0.0896877545100348	0.9520053992104398	0.8116908530518405	T	T	T
0.4331271926364185	0.1267305572878069	0.5813572139826699	T	T	T
0.4110876119982272	0.9958970094925313	0.5742602700717073	T	T	T
0.3926330930893372	0.8636036073637542	0.5693018201964890	T	T	T
0.1931111325130422	0.1389509420321773	0.6142182135115390	T	T	T
0.1914405906760478	0.0057979476406211	0.5864844803000958	T	T	T
0.1913103613261998	0.8728864446942987	0.5634437309068941	T	T	T
0.9877423692525602	0.0378349183732475	0.7869520135206045	T	T	T
0.9854651503687450	0.8705445347285513	0.7896773439328311	T	T	T
0.1388798873745385	0.9326604168533462	0.2239666248706903	T	T	T
0.1829392696141519	0.9531830495689418	0.4070184883338837	T	T	T
0.2965696264882187	0.9460466789493603	0.5086623624001433	T	T	T
0.4072838103874002	0.930311077729360	0.4029572791495810	T	T	T
0.3966098016471245	0.9343637556917945	0.2062448357213605	T	T	T
0.2694366775804752	0.9424202597359322	0.2595382793963918	T	T	T
0.1380000751549830	0.1715572628883220	0.2546761326715572	T	T	T
0.1988661470160515	0.1348834526885950	0.4187044351324965	T	T	T
0.3098841303136814	0.1499018654205609	0.5219807783270870	T	T	T
0.4099958470987666	0.1674926261951586	0.3944032606531537	T	T	T
0.3962285580404037	0.1568652758194450	0.1982705037890233	T	T	T
0.2701835934474816	0.1578446461080481	0.2555238841811066	T	T	T
0.1914595848603301	0.0500943615964759	0.2666995973782264	T	T	T
0.4131777324361594	0.0474143334397838	0.3095144144025314	T	T	T
0.0644691998190920	0.8720804558614049	0.0873116427179448	T	T	T
0.0856649208920885	0.0018151797905147	0.0705769006248604	T	T	T
0.1107495473112762	0.1325415130588954	0.0700140427304201	T	T	T
0.3072347113307163	0.8606054334852613	0.1134695071894445	T	T	T
0.3103866319602981	0.9936027112066522	0.0858577738572155	T	T	T
0.3007584155364778	0.1262289373399688	0.0659132302251672	T	T	T
0.5126992541658062	0.9584900975225995	0.2892615548406480	T	T	T
0.5139859164917929	0.1329788891215295	0.2819801141661571	T	T	T
0.6375427738992319	0.5649177742148861	0.2823090552446473	T	T	T
0.6984796422797975	0.5729911427485016	0.1111660973563035	T	T	T
0.7944259138951043	0.5543084793487001	0.9745087131248524	T	T	T
0.8953574171127464	0.5805161457490153	0.1034499823631089	T	T	T
0.8886403072409266	0.5361879648084908	0.3163343296947894	T	T	T

Structure files (CONTCAR) involved in this work:

0.7619444618934047	0.5217614310107332	0.2671565065179427	T	T	T
0.6367691861213770	0.3322314805983994	0.2595729707448972	T	T	T
0.6928472200694193	0.3400431181631858	0.0838540540989650	T	T	T
0.8087916690811490	0.3523409167048468	0.9870758795777815	T	T	T
0.9127843976284180	0.3196941717173349	0.1011493219068968	T	T	T
0.9064896644574837	0.3527240784675298	0.2933378988758908	T	T	T
0.7649143919853416	0.3678591193890259	0.2470776280803767	T	T	T
0.6669886392759637	0.4507779828536243	0.1853081296591404	T	T	T
0.9215005317581487	0.4477458215691549	0.1538068043726006	T	T	T
0.5645389229223741	0.6258273091030561	0.4199501593723832	T	T	T
0.5935222184954960	0.4967965414667436	0.4413763234512950	T	T	T
0.5889264305363926	0.3628188305945033	0.4410854956615104	T	T	T
0.7991550637026897	0.6320021814722763	0.3677264886023251	T	T	T
0.8002603155792588	0.5176647263148224	0.4608738450293295	T	T	T
0.8320332013535637	0.3900331172503919	0.4382148378521773	T	T	T
0.0202041871463010	0.3644302656814634	0.1958769731160336	T	T	T
0.8554142127363710	0.4376454291634553	0.7876429954547249	T	T	T
0.7910155722566342	0.4347211284817679	0.6164362200820325	T	T	T
0.7037483247780829	0.4244744318570277	0.4676227099893471	T	T	T
0.6091019951361228	0.4289122854870581	0.6094041975755119	T	T	T
0.6026437590840789	0.4461754148727289	0.8061921759507062	T	T	T
0.7283887036332324	0.4789586300532803	0.7763803535879676	T	T	T
0.8690882819483595	0.6819505492266246	0.7376985090137741	T	T	T
0.8080981306971146	0.6477392663274434	0.5627051045971839	T	T	T
0.6883534577536788	0.6479667671850921	0.4796753360270496	T	T	T
0.5869425788962345	0.6707249511770607	0.6041418364837098	T	T	T
0.5964509945262824	0.6564539668727075	0.8008743816471574	T	T	T
0.7231307768552291	0.6552693428513211	0.7452382425010528	T	T	T
0.8246355926121410	0.5524619638837429	0.6960644193267074	T	T	T
0.5824552961203940	0.5490489367960000	0.6815426687283326	T	T	T
0.9308124852264502	0.3777554320509479	0.9222641085180383	T	T	T
0.9151392058947048	0.5118394213267834	0.9319056599682333	T	T	T
0.8885682015722564	0.6417831721778262	0.9281299418816271	T	T	T
0.6957470372999855	0.3734268878643359	0.8911357505859498	T	T	T
0.6746580243222533	0.4996276478566438	0.9528886466484289	T	T	T
0.6896565641291471	0.6330929624521286	0.9373160470210341	T	T	T
0.4927102157522890	0.4508203502925909	0.7054562041481383	T	T	T
0.4814016294198371	0.6328732565194786	0.7115161877437909	T	T	T
0.6432215645747431	0.9411979843631326	0.2903101688634397	T	T	T
0.6984436780552146	0.9341417884758065	0.1123858392634544	T	T	T
0.7988531479791475	0.9484238636276393	0.9815922311829616	T	T	T
0.8971364581015565	0.9301721487028106	0.1143226609456561	T	T	T
0.8970933956583336	0.9484408195449682	0.3117718335512439	T	T	T
0.7714253303478593	0.9689870640613978	0.2678165726651999	T	T	T
0.6387033501651468	0.1733668044081427	0.2557165762156161	T	T	T
0.6972825063221036	0.1596440310995326	0.0826233880561632	T	T	T
0.8087240874541213	0.1477677377842737	0.9772586446083822	T	T	T
0.9130266945430610	0.1688172243497605	0.0940391583166588	T	T	T
0.8962964338191028	0.1624652250965058	0.2919520665912905	T	T	T
0.7694015411688782	0.1474516992868520	0.2484681718935176	T	T	T
0.6802939299723061	0.0536271761221572	0.1991710269256921	T	T	T
0.9164770691688131	0.0512368884935586	0.1859744361220023	T	T	T
0.5678709928284279	0.8768142421912061	0.4213773818225527	T	T	T

Structure files (CONTCAR) involved in this work:

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0.5971295271020823	0.1407073290291088	0.4385306684737046	T	T	T
0.8067195030415479	0.8714318618241664	0.3961507810891362	T	T	T
0.8157155281348614	0.9984989685764727	0.4503678990898191	T	T	T
0.8105462366835336	0.1322188354604105	0.4370246198101001	T	T	T
0.0092898469263470	0.9561544505330584	0.2165344191307063	T	T	T
0.0147058962689285	0.1384671413003773	0.2114589024065955	T	T	T
0.8571431947442938	0.0520008243020603	0.7862169198575780	T	T	T
0.7999849113368411	0.0715206046705009	0.6115569598395039	T	T	T
0.7009889767222919	0.0614621436999721	0.4780721802851501	T	T	T
0.6008979240985750	0.0761218009611693	0.6091222969374643	T	T	T
0.6019610347876948	0.0529529503977595	0.8062963252718067	T	T	T
0.7276490692050567	0.0305559362486828	0.7655563245685666	T	T	T
0.8604550724492667	0.8344148000438957	0.7618872508473421	T	T	T
0.8028180873905068	0.8312334858776751	0.5874045737677435	T	T	T
0.690267557794177	0.8521513747726454	0.4866178149896555	T	T	T
0.5869339113620110	0.8296638069625427	0.6059470529544425	T	T	T
0.6019498656968415	0.8527475839205835	0.8005935982137189	T	T	T
0.7292271629845732	0.8520200840133286	0.7491919422598899	T	T	T
0.8127046855027116	0.9469309046851054	0.6828174395006495	T	T	T
0.5812041206753896	0.9537047595726558	0.6742191056873672	T	T	T
0.9307962548374212	0.1267596247311925	0.9069272985447497	T	T	T
0.9187123358900718	0.9969744790734024	0.9447329400442217	T	T	T
0.9004099870605936	0.8649543643866885	0.9451319284657247	T	T	T
0.6920841667440644	0.1313964596809601	0.8880421400898887	T	T	T
0.6815776650311599	0.0051626520761627	0.9483675908271232	T	T	T
0.6945514524174221	0.8715730869859347	0.9400935987365806	T	T	T
0.4893989852520074	0.0472190833637916	0.7135717469146585	T	T	T
0.4835442946106268	0.8673373080435842	0.7166968727282739	T	T	T
0.3618923657923682	0.4320417499708268	0.7151708053528287	T	T	T
0.3166099584053032	0.4459162439101975	0.8997136417554525	T	T	T
0.2024956034078221	0.4582264972853435	0.0009156717249894	T	T	T
0.0894644708984156	0.4319503011876032	0.9041084942046537	T	T	T
0.1022391907823914	0.4355691730613457	0.7061396067017900	T	T	T
0.2310565290278595	0.4457341557700694	0.7515912962114608	T	T	T
0.3578011401615792	0.6730298362101568	0.7495730222795858	T	T	T
0.2962061455320353	0.6366361719310252	0.9144240694006134	T	T	T
0.1903654681274451	0.6494488469796961	0.0307079721972035	T	T	T
0.0945860821591107	0.6668462668023448	0.8971314134401828	T	T	T
0.0993067543016350	0.6568010952007357	0.6982841420970171	T	T	T
0.2268264230996475	0.6489056187734283	0.7475665784678457	T	T	T
0.3138782777363354	0.5489194975032197	0.7689525310646158	T	T	T
0.0835245627102711	0.5477992033830725	0.8094876421182352	T	T	T
0.4331163387811678	0.3771258359094804	0.5690867231807482	T	T	T
0.4162500309344894	0.5087220975870744	0.5705133102968051	T	T	T
0.3911987564339400	0.6399291127910923	0.5641137148947591	T	T	T
0.1897564054152787	0.3613639185480603	0.6107168007759768	T	T	T
0.1837472493014298	0.4939850517883340	0.5791259773591335	T	T	T
0.1888518880062640	0.6268638106759246	0.5582686829409523	T	T	T
0.9850595379951707	0.4573110910698142	0.7853748561640289	T	T	T
0.9857911017547648	0.6369448460036810	0.7903971389517936	T	T	T
0.1432889008761370	0.5689619590495372	0.2213115752974245	T	T	T
0.1890784963480803	0.5482228115291378	0.4013984627786691	T	T	T

Structure files (CONTCAR) involved in this work:

0.2962762845153846	0.5510977783660320	0.5197977963877088	T	T	T
0.3992096424366468	0.5714912006547445	0.3977265782442139	T	T	T
0.4001254411506210	0.5627123387733329	0.2005716090677243	T	T	T
0.2737242303241917	0.5519871863985770	0.2505724563728919	T	T	T
0.1395881496141575	0.3263320258191527	0.2508944738742396	T	T	T
0.1982895940975059	0.3638739218108513	0.4161961023454176	T	T	T
0.3082443489267468	0.3509154611370416	0.5227727212296113	T	T	T
0.4037105269525582	0.3295283118841371	0.3876372710228345	T	T	T
0.3953477952918273	0.3462779653327402	0.1911680772196324	T	T	T
0.2712246057476189	0.3439637476992745	0.2532813323216833	T	T	T
0.1893875909002576	0.4490080759928673	0.2653397705636344	T	T	T
0.4079258238646425	0.4518331451909745	0.3123588440321636	T	T	T
0.0659794538761235	0.6222920820961007	0.0817134393139624	T	T	T
0.0858684137362005	0.4912323341276635	0.0815452012665778	T	T	T
0.1195665450795346	0.3621594000027962	0.0626069529757869	T	T	T
0.3110068658401590	0.6381499631515245	0.1089982885923003	T	T	T
0.3152357000715647	0.5058115043455244	0.0742989350034723	T	T	T
0.2972565781342417	0.3730541551139721	0.0615389048801455	T	T	T
0.5100531722425033	0.5366019003749116	0.2987895856971631	T	T	T
0.5101837371811702	0.3677513660748732	0.2815265524127780	T	T	T
0.4382639052566007	0.7511007916557738	0.6448469604952600	T	T	T
0.1845302313768092	0.7493597955521415	0.6300931451789996	T	T	T
0.2781676625793744	0.7500523952178434	0.0143435795179262	T	T	T
0.1013183143482481	0.7482780654473765	0.0518448431868676	T	T	T
0.0686612692978175	0.2485791460130743	0.1305305976394394	T	T	T
0.3134789831729751	0.2499613212773610	0.1260618622527330	T	T	T
0.2205204478690276	0.2497555222991761	0.5146298433058322	T	T	T
0.3957045917766382	0.2510869620325574	0.5460053534648409	T	T	T
0.5529624392977316	0.2508668346561863	0.3532439331991699	T	T	T
0.8089666352394494	0.2533005501249934	0.3596067681654341	T	T	T
0.7261909848803770	0.2513220620197328	0.9447245434230280	T	T	T
0.8908949255866793	0.2505367944493165	0.9394950161530756	T	T	T
0.9434489332004309	0.7539526447047898	0.8618870618709394	T	T	T
0.6791587230635935	0.7530691012497420	0.8631686575829013	T	T	T
0.7708325483413011	0.7496757176929809	0.4407775149109938	T	T	T
0.6052007884718138	0.7510461642360285	0.4499278397960175	T	T	T
0.9296049851917818	0.4858412888530783	0.5447642608143252	T	T	T
0.9462810123224616	0.6448297295598218	0.5729231794036201	T	T	T
0.9267513622686472	0.5289963360910220	0.1969291089788725	T	T	T
0.8230336253692596	0.3358932255106133	0.3292796987006872	T	T	T
0.7990459896636685	0.6388887537148643	0.6947804529972506	T	T	T
0.9314491290396182	0.4232557012159722	0.4179672722135497	T	T	T
0.8780465354135158	0.5655357233063190	0.5639347322023816	T	T	T
0.0278205078449325	0.4362958227450337	0.3981066588375088	T	T	T
0.0250545438334463	0.5751119244009602	0.3831757281997632	T	T	T
0.9487158518970046	0.4675813697308189	0.6061402666038720	T	T	T
0.0620724731620804	0.4404848494134715	0.4621423817624439	T	T	T
0.0541102853094934	0.4344540857251812	0.3266821962294364	T	T	T
0.0116193859232480	0.5369874906142725	0.4385054702337017	T	T	T
0.9867012717449621	0.6115000637474238	0.3647275098589000	T	T	T
0.0773633777673297	0.5876434061548780	0.3730751105993169	T	T	T
0.9237970134723459	0.6736309556471003	0.6238510699237761	T	T	T
0.9900465550503266	0.6347616887668309	0.6018534509679180	T	T	T

Structure files (CONTCAR) involved in this work:**Figure 7(b) TS3**

Si O Al Zn C H

1.0000000000000000

20.0219999999999985 0.0000000000000000 0.0000000000000000

0.0000000000000000 19.8990000000000009 0.0000000000000000

0.0000000000000000 0.0000000000000000 13.3829999999999991

93 194 3 2 2 8

Selective dynamics

Direct

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0.1226905105873939 0.0619156301864935 0.0122289576811252 T T T

0.0679617327684517 0.0313766461963070 0.8001360386895475 T T T

0.1807549915323337 0.0642749908327867 0.6644696257796269 T T T

0.4195654030049073 0.8281586733587004 0.6702402031014180 T T T

0.3020702252112413 0.8708314863085569 0.8029859212378264 T T T

0.2668374084289212 0.8329973490727620 0.0230093616854204 T T T

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0.1803544789065917 0.8275685722178530 0.6674348684482607 T T T

0.0762893902609707 0.9401484943888552 0.1501170776863607 T T T

0.1944344537057198 0.9705917883271028 0.2930963906184031 T T T

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0.0818932108305722 0.1724374244566778 0.1665705709215775 T T T

0.1974557009928098 0.1296424783209209 0.3027147370197816 T T T

0.2323513116523947 0.1710815244805558 0.5207623412928554 T T T

0.3875143909439481 0.1754204329259011 0.5090399376121408 T T T

0.4353604444451279 0.1274968398738137 0.2965062468035081 T T T

0.3187273720146381 0.1708937812578724 0.1656570903905566 T T T

0.5763270497901957 0.5570355186370317 0.3533670091094779 T T T

0.6960368038917087 0.5255800909097750 0.2118143852522776 T T T

0.7163881470876365 0.5669631148351576 0.9912607165524104 T T T

0.8745238565004712 0.5722583618978357 0.9840680779083155 T T T

0.8172598548088998 0.5535879071772165 0.3529529678189968 T T T

0.5779131123789638 0.3282039002387682 0.3344424409291851 T T T

0.6959945741003960 0.3716407416768214 0.1927584481350085 T T T

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0.7786593092836579 0.4384986460010130 0.4958282098354030 T T T

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0.7642526268144574 0.6716285873553526 0.4688247107528378 T T T

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Structure files (CONTCAR) involved in this work:

0.6714219745638620	0.6715952500917742	0.8352429730249564	T	T	T
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0.6975999384277821	0.9731980162485819	0.2143337044151580	T	T	T
0.7196645289144986	0.9378312691263169	0.9933130512459979	T	T	T
0.8794444842477502	0.9358808155333509	0.9942283126324496	T	T	T
0.9312523735441768	0.9704249251682822	0.2053309680512154	T	T	T
0.8212375597951515	0.9460205889527655	0.3536176385143235	T	T	T
0.5785735037598628	0.1734540318064561	0.3321996210505818	T	T	T
0.6977820788068515	0.1302444290948421	0.1951308660109531	T	T	T
0.7329111092103073	0.1716756701202753	0.9746127872307646	T	T	T
0.8876253853675469	0.1732771444550336	0.9815613063312851	T	T	T
0.9361648408543457	0.1290268669616240	0.1969334569102896	T	T	T
0.8199766559248075	0.1719378828906479	0.3311556983871676	T	T	T
0.9232778222800094	0.0542787098104737	0.8543655822976058	T	T	T
0.8005560129308972	0.0249463610026826	0.7102513592590640	T	T	T
0.7822809648712479	0.0647700654807211	0.4917923853681725	T	T	T
0.6219848228139874	0.0688834432870722	0.4910294985722954	T	T	T
0.5690077632076868	0.0320349271075718	0.7007731883427200	T	T	T
0.6778455701618343	0.0540872936562504	0.8517654475570039	T	T	T
0.9228325491902647	0.8318741431097229	0.8345601722410537	T	T	T
0.8015506645035572	0.8667884221450316	0.6926358513861518	T	T	T
0.7657807161050272	0.8273351188729287	0.4752795693584694	T	T	T
0.6120906404859945	0.8272676890370124	0.4908399899952984	T	T	T
0.5636959926581268	0.8744203491844653	0.7011839820787779	T	T	T
0.6792503467864011	0.8300213653409299	0.8344043893148941	T	T	T
0.4258750690236391	0.4459794385559680	0.6359161376228932	T	T	T
0.3046636719297396	0.4711026552985237	0.7809588740503116	T	T	T
0.2838761199040384	0.4385526965187616	0.0014632142174432	T	T	T
0.1240786005397806	0.4349046323154098	0.0053132707964497	T	T	T
0.0654193528225962	0.4710640492037609	0.7955940183415454	T	T	T
0.1778069627721426	0.4436878798648087	0.6484498626239217	T	T	T
0.4194391591393691	0.6741852578121714	0.6534814677609970	T	T	T
0.2999010290357709	0.6297048687377799	0.7896969864836233	T	T	T
0.2695253049941650	0.6737864998540158	0.0076120440081557	T	T	T
0.1152546044747435	0.6737908479252070	0.0004914595323139	T	T	T
0.0628867002920580	0.6303589502121021	0.7904032453062545	T	T	T
0.1779999167173659	0.6693436920881595	0.6557529863758422	T	T	T
0.0788684890928359	0.5585405855737904	0.1388221502173391	T	T	T
0.2020429329920886	0.5294743132209625	0.2745534452610710	T	T	T
0.2214527347310496	0.5615468693442526	0.5043759970115780	T	T	T
0.3808814461394951	0.5687450859133930	0.5017417008937980	T	T	T
0.4311165489717343	0.5300086668788118	0.2893497924581678	T	T	T
0.3267211232437024	0.5593769291699288	0.1365799055571035	T	T	T
0.0853813256631322	0.3252669637061107	0.1566862640338072	T	T	T
0.2018006466501759	0.3706744152791746	0.2934024884360437	T	T	T
0.2308143672697457	0.3318776298971640	0.5151758759270255	T	T	T
0.3858263501421339	0.3293608316371951	0.5031985298405477	T	T	T
0.4349504630400164	0.3720822117509387	0.2896003827253728	T	T	T
0.3219612773797442	0.3280730555053972	0.1597504278081897	T	T	T
0.0124985891850911	0.5528649138863813	0.2119034991002548	T	T	T
0.3595030114041750	0.0686174388893195	0.7210797133842578	T	T	T
0.3168424637087117	0.0532005392461514	0.9059656830764894	T	T	T
0.2021079686239519	0.0469505355057007	0.0058478065264709	T	T	T

Structure files (CONTCAR) involved in this work:

0.0915106110302061	0.0693553923246714	0.9013465722965348	T	T	T
0.1042283565501853	0.0654770345122438	0.7042163683427927	T	T	T
0.2301658301577790	0.0499723691662131	0.7586469612079351	T	T	T
0.3603205737681183	0.8254287023414961	0.7530994540327990	T	T	T
0.3037053124915567	0.8593492132440052	0.9225326733686299	T	T	T
0.1888913362926574	0.8562734097957556	0.0195722426363790	T	T	T
0.0865786321606483	0.8341640144787531	0.8983339362112457	T	T	T
0.1033646531337951	0.8400416486885627	0.7025634613064555	T	T	T
0.2293943282363192	0.8479237093766684	0.7599517761862586	T	T	T
0.3162152494171606	0.9493396869419801	0.7769954645785845	T	T	T
0.0896895900037442	0.9525667129001371	0.8074025223828550	T	T	T
0.4328473225723573	0.1298089354013714	0.5831173103376306	T	T	T
0.4136265063076929	0.9987687743532905	0.5701684912937879	T	T	T
0.3933108442974361	0.8667225064070265	0.5709470530745103	T	T	T
0.1972489467683671	0.1375280376442050	0.6175043008024117	T	T	T
0.1885738734773934	0.0054608119221382	0.5816203049499670	T	T	T
0.1972287503758833	0.8716235138483163	0.5686943471504378	T	T	T
0.9879763665073833	0.0389591107753700	0.7847630993828525	T	T	T
0.9856355842456751	0.8710627180231180	0.7827409382829766	T	T	T
0.1408076229793816	0.9320438853247278	0.2227094973041474	T	T	T
0.1838654193278733	0.9459158648576779	0.4073307880391863	T	T	T
0.2977375863820098	0.9497196376333779	0.5100272543882305	T	T	T
0.4072288136168398	0.9303929878869993	0.4018119328062110	T	T	T
0.3966845226240606	0.9380351908797572	0.2055983322677383	T	T	T
0.2703900365456779	0.9525137153258392	0.2599807961973261	T	T	T
0.1397785715518760	0.1747920446536451	0.2513874417476651	T	T	T
0.1951153292921599	0.1432677101074548	0.4216555597101444	T	T	T
0.3105161901133431	0.1494592046175730	0.5160289087767258	T	T	T
0.4132180618671801	0.1699142970251412	0.3947336464494448	T	T	T
0.3956108358285190	0.1566062054859702	0.1993109093012959	T	T	T
0.2705130962587818	0.1505236032860167	0.2592559897423318	T	T	T
0.1822695178992316	0.0509455841206531	0.2800617595421375	T	T	T
0.4163135535789092	0.0489403548185409	0.3131909107674857	T	T	T
0.0658459533303680	0.8703569410717746	0.0883122837099167	T	T	T
0.0860993679376692	0.0006135556701815	0.0701096825352186	T	T	T
0.1090816403722394	0.1320421575640300	0.0696408641359329	T	T	T
0.3038313665396467	0.8650957384059994	0.1191448187449706	T	T	T
0.3121676644367058	0.9960130844802946	0.0820410142476297	T	T	T
0.2997399059711588	0.1284551430655501	0.0661968758378016	T	T	T
0.5133166854357610	0.9579868349269985	0.2880988753826011	T	T	T
0.5152087989080750	0.1360886578847319	0.2789843319249380	T	T	T
0.6404212550806923	0.5631801928444945	0.2802608250119646	T	T	T
0.7087509972648960	0.5703894705803445	0.1121832902943811	T	T	T
0.7949125159187668	0.5641674327031796	0.9583041440226422	T	T	T
0.8885068624764274	0.5758379691208408	0.1012577508979971	T	T	T
0.8928049989717803	0.5444187646554537	0.3157271580214189	T	T	T
0.7650132782586134	0.5197459403125679	0.2762169945780394	T	T	T
0.6426888045918059	0.3322464748177296	0.2635350614928163	T	T	T
0.6904048308493066	0.3383591217502263	0.0817255477023811	T	T	T
0.8092436633730991	0.3516155898245338	0.9926123633428265	T	T	T
0.9157745521314726	0.3206469234850297	0.1053640709508254	T	T	T
0.9076323508211338	0.3485013646152284	0.3003114024845218	T	T	T
0.7702005852255547	0.3656357864917714	0.2359920763669226	T	T	T

Structure files (CONTCAR) involved in this work:

0.6717187512578233	0.4502093034624237	0.1844217528744163	T	T	T
0.9233107000604185	0.4465612682174914	0.1642135467773628	T	T	T
0.5654845489851844	0.6273480881043529	0.4131791952933023	T	T	T
0.5845426994796948	0.4972690110107616	0.4356759806692036	T	T	T
0.5920052388158439	0.3639873366220362	0.4421814032254213	T	T	T
0.7984432522027151	0.6312873255486112	0.3756922298335538	T	T	T
0.8117744014121653	0.5140573590528135	0.4652388422089498	T	T	T
0.8216627117044878	0.3823834045786262	0.4377896122657474	T	T	T
0.0227195414371311	0.3633038628629423	0.2081803546748792	T	T	T
0.8560002870371555	0.4341078721414428	0.7844041656370591	T	T	T
0.7877846572602983	0.4304378197092765	0.6155554355813031	T	T	T
0.7006381445744562	0.4385262110712290	0.4651948045166568	T	T	T
0.6069377176494670	0.4336565037698771	0.6079152724088340	T	T	T
0.6030787067294709	0.4452467488688403	0.8067047216234662	T	T	T
0.7287552103338821	0.4775708083067388	0.7762642836358484	T	T	T
0.8584966169499419	0.6791936040040687	0.7551180906249019	T	T	T
0.8063122104802669	0.6568604717314536	0.5695285295225194	T	T	T
0.6873412719561814	0.6463858005089684	0.4839343813743216	T	T	T
0.5827115169679455	0.6694489387156412	0.6010466760028076	T	T	T
0.5933606097204578	0.6625124579453459	0.7998550830136945	T	T	T
0.7187865120881719	0.6425669298651455	0.7483015808412271	T	T	T
0.8250385071038145	0.5479436032103794	0.6897214002967675	T	T	T
0.5819279575696242	0.5511534581297397	0.6894477806184305	T	T	T
0.9308647155641920	0.3769778083453201	0.9243836191662520	T	T	T
0.9131510615789834	0.5095939263431878	0.9284251911630820	T	T	T
0.9047468538299988	0.6405294828679218	0.9339527383591706	T	T	T
0.6975595040448190	0.3725680177326103	0.8905577707618277	T	T	T
0.6780693306528434	0.4986807943787734	0.9538346772759463	T	T	T
0.6817995895608387	0.6326713218659510	0.9416992900137878	T	T	T
0.4913938507452066	0.4534640523401656	0.7059779445584993	T	T	T
0.4788961966592755	0.6343485502485745	0.7113930112328833	T	T	T
0.6435977326403211	0.9385691187496589	0.2884635751475773	T	T	T
0.6989783753399730	0.9314801128931638	0.1100925792187431	T	T	T
0.7998748315541098	0.9483909024638998	0.9809663588340973	T	T	T
0.8995533741483220	0.9294854718632934	0.1111666399756178	T	T	T
0.8966655342880494	0.9461814400387082	0.3089264215042709	T	T	T
0.7711200226366743	0.9700992493222420	0.2650998866722429	T	T	T
0.6415519644736556	0.1715935209690374	0.2567094795764843	T	T	T
0.6977084580387654	0.1588380360425360	0.0818718800826427	T	T	T
0.8105156376451553	0.1471551231144531	0.9799583659610902	T	T	T
0.9164755198104246	0.1671928150198125	0.0940281717845002	T	T	T
0.8967091716660240	0.1613247617570202	0.2910329468176549	T	T	T
0.7708185618955262	0.1394968891353425	0.2455696590588019	T	T	T
0.6773946397415878	0.0510294104560144	0.1942180697075861	T	T	T
0.9183198376779587	0.0498158863073467	0.1863028523199555	T	T	T
0.5669036622734869	0.8748530234309615	0.4192716219626282	T	T	T
0.5843012037333046	0.0053405821397842	0.4396164579341371	T	T	T
0.5971394974530345	0.1377431647620314	0.4378253561196429	T	T	T
0.8041338792453114	0.8703907548800026	0.3903787390761574	T	T	T
0.8162949723599527	0.9963582762207618	0.4486909811004047	T	T	T
0.8113121335837816	0.1300799804216216	0.4352446321945929	T	T	T
0.0105117538908205	0.9544928851589699	0.2170521979637203	T	T	T
0.0162046482963365	0.1375048001258116	0.2150178589239871	T	T	T

Structure files (CONTCAR) involved in this work:

0.8572231886519952	0.0532389326205245	0.7852140215993170	T	T	T
0.8007209986740500	0.0705399946867328	0.6097504456669821	T	T	T
0.7017807879765601	0.0594177646993470	0.4765671660769337	T	T	T
0.6021037454283016	0.0736501223163429	0.6084191715275283	T	T	T
0.6027573749187105	0.0535866711710146	0.8061706139966198	T	T	T
0.7281498805943372	0.0295333749686780	0.7638596678144840	T	T	T
0.8607260116584282	0.8332232985141016	0.7577018978688657	T	T	T
0.8036892395949696	0.8329098208414158	0.5823864258412219	T	T	T
0.6891646522220553	0.8538233653570113	0.4873728597714685	T	T	T
0.5857663143962624	0.8295737541495564	0.6053433124868448	T	T	T
0.6033542473284145	0.8491740016505351	0.8002245792669196	T	T	T
0.7295861388626232	0.8524661030127545	0.7444564210432705	T	T	T
0.8148721323118150	0.9469139383042839	0.6824488328931952	T	T	T
0.5807575670828219	0.9526112882853304	0.6784263707957768	T	T	T
0.9317283179492212	0.1280777209098229	0.9048681657590304	T	T	T
0.9191581030087504	0.9986018151891906	0.9435014782163426	T	T	T
0.9017248877317204	0.8665131896083047	0.9397566261486111	T	T	T
0.6948799409984409	0.1298145872694371	0.8877792458872377	T	T	T
0.6819369863809788	0.0029757238353866	0.9463386091479425	T	T	T
0.6974156432892026	0.8693943894552225	0.9370344646971730	T	T	T
0.4900371338592751	0.0485873392001285	0.7128150520160009	T	T	T
0.4837571477896128	0.8657310521490144	0.7194569396595180	T	T	T
0.3595321581680464	0.4400431130519540	0.7052215230758959	T	T	T
0.3086311844696802	0.4312102377245978	0.8865633098350062	T	T	T
0.2035466314104459	0.4516003318971755	0.0079150971199103	T	T	T
0.0976307496937531	0.4327439227506731	0.8907950821948649	T	T	T
0.1017328525098729	0.4470288418266777	0.6924548916568817	T	T	T
0.2293798586191923	0.4616407616711215	0.7377865593068647	T	T	T
0.3516540105919884	0.6692127221188376	0.7189281405800930	T	T	T
0.3042422053971715	0.6623104568694412	0.8999078306765960	T	T	T
0.1923124657479469	0.6471330486615773	0.0036834325844518	T	T	T
0.0878759497207094	0.6733133822112154	0.8860938035334025	T	T	T
0.1007599348613614	0.6549167872074102	0.6890872694606169	T	T	T
0.2247779355614583	0.6390060559669276	0.7447471214329894	T	T	T
0.3189166623942111	0.5506762238949544	0.7963487772538506	T	T	T
0.0762372094546726	0.5512809050308117	0.8109915539673496	T	T	T
0.4332007618662274	0.3778007975106605	0.5700140542711708	T	T	T
0.4214513438547145	0.5096177531543904	0.5596311990948917	T	T	T
0.4048181073592353	0.6412799333792419	0.5441442097461644	T	T	T
0.1913664940096673	0.3683436237893190	0.6065505310038775	T	T	T
0.1856462636238526	0.4975576751329114	0.5577647670453463	T	T	T
0.1929303791920410	0.6315585062199179	0.5503315152668651	T	T	T
0.9859241583848314	0.4535432360983639	0.7842740027539205	T	T	T
0.9831104106861972	0.6424650616046542	0.7695286678398284	T	T	T
0.1433517736863341	0.5673611237010224	0.2118077562859665	T	T	T
0.2031949733067294	0.5602847358593132	0.3864802407790202	T	T	T
0.3014641640535661	0.5568354251887787	0.5219993878993483	T	T	T
0.3963273665012339	0.5683092088296552	0.3832157985270996	T	T	T
0.4008545544936345	0.5593195546080464	0.1852253272726988	T	T	T
0.2740600889940917	0.5415481580888997	0.2248919206894165	T	T	T
0.1475219605295331	0.3257327734248884	0.2346667159767609	T	T	T
0.1955149334854638	0.3551348988291969	0.4115865449783802	T	T	T
0.3086894297743688	0.3553107592333959	0.5136309342234125	T	T	T

Structure files (CONTCAR) involved in this work:

0.4085757686124327	0.3312173409237746	0.3870946238765065	T	T	T
0.3997270771910888	0.3405772830481023	0.1901017311502821	T	T	T
0.2765204344663028	0.3533196795936634	0.2541746842455164	T	T	T
0.1848664064997070	0.4497331908740606	0.2746640141521660	T	T	T
0.4138651924416608	0.4505490317960629	0.3003562975237874	T	T	T
0.0698119492619812	0.6246139598389097	0.0694563579465218	T	T	T
0.0845474255595600	0.4927509920248027	0.0681097693949220	T	T	T
0.1083543664922388	0.3620493820203160	0.0535319746813000	T	T	T
0.3107687892293824	0.6333615803706409	0.0924754121702796	T	T	T
0.3218717312659671	0.5032383111239150	0.0489413310057178	T	T	T
0.3027520886629623	0.3698259211744386	0.0597189954342537	T	T	T
0.5108073111472357	0.5425406366403074	0.2857159675363974	T	T	T
0.5152556774607241	0.3651334367495678	0.2788973679788030	T	T	T
0.4392678026927704	0.7522477010069666	0.6376804791992264	T	T	T
0.1906282981408232	0.7488663360994299	0.6390972544277125	T	T	T
0.2718776448037301	0.7524781140319139	0.0348788452502181	T	T	T
0.1100958704265145	0.7492614672740452	0.0446586204116129	T	T	T
0.0656962428451699	0.2484710749431538	0.1303337772854657	T	T	T
0.3085443886916588	0.2494259708334408	0.1371673507628703	T	T	T
0.2245354590463007	0.2517270661430101	0.5297281048846116	T	T	T
0.3923830424693637	0.2531691074438760	0.5447910430218685	T	T	T
0.5588137752664296	0.2506058570404002	0.3569117106419598	T	T	T
0.8047326488001356	0.2492811407306213	0.3517325108092427	T	T	T
0.7281921479752987	0.2502446309079979	0.9440353016411815	T	T	T
0.8916968336123172	0.2508365084863091	0.9439330153345395	T	T	T
0.9447277840522386	0.7549937193157992	0.8578921540183089	T	T	T
0.6855450990888248	0.7507343526240392	0.8569992297506123	T	T	T
0.7664832979834396	0.7501390097127233	0.4378017240126240	T	T	T
0.6062741098843533	0.7507309367571177	0.4500600681299304	T	T	T
0.9335871775438285	0.4578848026403811	0.5559530348341435	T	T	T
0.9393684162419137	0.6284883096587515	0.5753967042332877	T	T	T
0.9248187419045065	0.5300806429329779	0.1954624496097682	T	T	T
0.8206997017391328	0.3322325422477075	0.3273368623085712	T	T	T
0.7962711035397946	0.6346669236291175	0.6960467029091945	T	T	T
0.9337603468582181	0.4078430763733157	0.4236241398893074	T	T	T
0.8878882398515339	0.5418868401316393	0.5719626556449723	T	T	T
0.0574323599680262	0.4928337688954921	0.4277074726737408	T	T	T
0.0425617380546250	0.5587570185664567	0.4037766497303072	T	T	T
0.9539314008767095	0.4390094509668720	0.6162618563297511	T	T	T
0.0988112299691945	0.4664813177093249	0.3923594146061657	T	T	T
0.0322505399614007	0.4667190938983571	0.4880294298435637	T	T	T
1.0029459455590033	0.5849300226009569	0.4438058235943926	T	T	T
0.0241960125943194	0.5543641586773408	0.3007280385577671	T	T	T
0.0829223494427664	0.5910756619286596	0.3759099869627969	T	T	T
0.9602139377132646	0.6354197334373102	0.6427266062602408	T	T	T
0.9028033012583585	0.6620497634989013	0.5709771134076862	T	T	T

Figure S15(b) CH₄+Zn-CH₃+O_M-H

Si O Al Zn C H

1.0000000000000000

20.0219999999999985 0.0000000000000000 0.0000000000000000

0.0000000000000000 19.8990000000000009 0.0000000000000000

0.0000000000000000 0.0000000000000000 13.3829999999999991

94 193 2 2 2 8

Structure files (CONTCAR) involved in this work:

Selective dynamics

Direct

0.4218098986542517	0.0600811471805169	0.6485167191610147	T	T	T
0.3043939877075508	0.0319646086030197	0.7921227775613494	T	T	T
0.2814707586683062	0.0570457728531062	0.0170433553340960	T	T	T
0.1215794195678927	0.0643283931631171	0.0121189870688750	T	T	T
0.0672961285024456	0.0310945235641922	0.8005894725645185	T	T	T
0.1798952829573534	0.0646849197814894	0.6643796803821900	T	T	T
0.4182930937242437	0.8274659466442223	0.6691818519865922	T	T	T
0.3005146622455517	0.8732073713450739	0.8012677128084515	T	T	T
0.2668343810392522	0.8306336480618057	0.0204119192241828	T	T	T
0.1110164229480253	0.8264367330995471	0.0139047697901381	T	T	T
0.0655653026733187	0.8739341139112811	0.7997703603719112	T	T	T
0.1787067191396036	0.8290173741221986	0.6655148325274679	T	T	T
0.0752318433304149	0.9417612174988468	0.1486519770046319	T	T	T
0.1940299619889110	0.9703235798425820	0.2906617565975342	T	T	T
0.2162988671483732	0.9433972263711534	0.5160245088730320	T	T	T
0.3766762117052543	0.9354029005460173	0.5136459394207689	T	T	T
0.4327995563305437	0.9689591124860463	0.3015030076239626	T	T	T
0.3193160436630367	0.9359292067389221	0.1643215128016293	T	T	T
0.0804732924423608	0.1739539022694516	0.1668502807131843	T	T	T
0.1973391272574737	0.1292451330251270	0.3010906684533329	T	T	T
0.2309243278313176	0.1698128864374011	0.5188806306715723	T	T	T
0.3864243577367141	0.1738497125322333	0.5092823084559874	T	T	T
0.4348035434404521	0.1274111681250151	0.2961552535285221	T	T	T
0.3186366845732991	0.1725565477391663	0.1664864322228512	T	T	T
0.5769092349485825	0.5559392284799094	0.3542539003440869	T	T	T
0.6907572907527398	0.5276150379618149	0.2024207257465252	T	T	T
0.7146979178075392	0.5678348829432824	0.9861655030965459	T	T	T
0.8742825108891124	0.5693479812423748	0.9866530482608228	T	T	T
0.9251545747389420	0.5280636830270208	0.1947444686960111	T	T	T
0.8126409926787906	0.5531797568693595	0.3417963764714514	T	T	T
0.5733179950303401	0.3292530685228597	0.3320913452259259	T	T	T
0.6947659664093608	0.3732680900199322	0.1949626028007582	T	T	T
0.7320043221988902	0.3277254775206712	0.9786286698657112	T	T	T
0.8866263133310734	0.3256038518695182	0.9841124401465647	T	T	T
0.9392786706612603	0.3720100499299174	0.1896975194363531	T	T	T
0.9205891744278248	0.4447545850038598	0.8554452888929847	T	T	T
0.7993113720959214	0.4737657688963910	0.7182665218184001	T	T	T
0.7802512068526812	0.4370277639494933	0.4925223244771574	T	T	T
0.6226602484363118	0.4298937678834538	0.4876522039084561	T	T	T
0.5710019892719245	0.4696272521523893	0.6995319648494173	T	T	T
0.6753275690257391	0.4468246824655160	0.8567751431938334	T	T	T
0.9211490872483979	0.6768883575609138	0.8346965877382132	T	T	T
0.7668947559256498	0.6698340050965218	0.4659818608235834	T	T	T
0.6121370605745394	0.6733452648149458	0.4868208804836471	T	T	T
0.5598096102294511	0.6277990333426465	0.6977552512682039	T	T	T
0.6705358129978011	0.6751516745717103	0.8283427890135630	T	T	T
0.5771075509639774	0.9454683809113865	0.3581931385471868	T	T	T
0.6975851076914849	0.9741916613694641	0.2156956328600354	T	T	T
0.7189158811109286	0.9393228122900512	0.9936505920883227	T	T	T
0.8785639327586778	0.9348650049843112	0.9950082860069496	T	T	T
0.9304298559127901	0.9718998427822795	0.2053075419563934	T	T	T

Structure files (CONTCAR) involved in this work:

0.8215845490564594	0.9460525454620698	0.3547841586630768	T	T	T
0.5779494883954955	0.1742795931609318	0.3298696586188355	T	T	T
0.6970957128053321	0.1320828172411307	0.1937912950037163	T	T	T
0.7323410249571771	0.1711349836466667	0.9725969265120163	T	T	T
0.8869096794523175	0.1729400790761136	0.9830739086413317	T	T	T
0.9347255050325326	0.1304133858792996	0.1985209101563695	T	T	T
0.8185215616265561	0.1734600664837852	0.3324864283155220	T	T	T
0.9229952669269404	0.0538257559998063	0.8557646863054874	T	T	T
0.8013705194020997	0.0252467810415685	0.7112414580593126	T	T	T
0.7806548884005929	0.0643597810847101	0.4928223991549555	T	T	T
0.6204502808718545	0.0698328397783677	0.4900667235100810	T	T	T
0.5672407544324037	0.0326977983698827	0.6988813735059854	T	T	T
0.6777151361826130	0.0541503501646514	0.8496697737950084	T	T	T
0.9224312521534018	0.8295508134630663	0.8389374272001427	T	T	T
0.8027469344092236	0.8674651289921554	0.6962026753380008	T	T	T
0.7683844186109623	0.8273162832277309	0.4779794865964900	T	T	T
0.6135496937935626	0.8272099627592459	0.4902535650953898	T	T	T
0.5630370896208472	0.8755628744157834	0.6981611505690893	T	T	T
0.6778026696606962	0.8331462551608466	0.8341718968124395	T	T	T
0.4238511887823649	0.4423039990099150	0.6426325317336471	T	T	T
0.3060181625736143	0.4693985509168186	0.7874709114886154	T	T	T
0.2806250122417080	0.4448908577455103	0.0120908715564247	T	T	T
0.1228021276885353	0.4363893175838526	0.0115443987491457	T	T	T
0.0647494579019921	0.4703266698287814	0.8016394227144574	T	T	T
0.1781372450291857	0.4366261556114766	0.6627306563436586	T	T	T
0.4148193159651642	0.6736521943373091	0.6665243481613041	T	T	T
0.3000260688622685	0.6277811893024767	0.8001912372047361	T	T	T
0.2668522087980830	0.6693474469201531	0.0194586460063368	T	T	T
0.1113416377494277	0.6726993714726104	0.0106746444292448	T	T	T
0.0642135787794649	0.6288819257305274	0.7965963794303043	T	T	T
0.1790623073722847	0.6717352943708886	0.6640041358439983	T	T	T
0.0717963349152102	0.5576968942074001	0.1472805501588509	T	T	T
0.1909394661806361	0.5310086564993731	0.2889933844830767	T	T	T
0.2146220441956620	0.5567914582729961	0.5147769280425081	T	T	T
0.3735087622871729	0.5663733353197052	0.5130398885037744	T	T	T
0.4291758369805723	0.5306090321453343	0.3042596355582038	T	T	T
0.3184795131526247	0.5637505244681901	0.1622661714369058	T	T	T
0.0846302847870799	0.3271115606117023	0.1606117994645997	T	T	T
0.1966657521832541	0.3723416059106509	0.2998264461081511	T	T	T
0.2298620386274258	0.3311189029139039	0.5188654556220813	T	T	T
0.3844685927353610	0.3274886171069066	0.5064178795625961	T	T	T
0.4297262618234144	0.3736417251437785	0.2944596035593031	T	T	T
0.3163731950256429	0.3301631428525828	0.1618836862560663	T	T	T
0.3581503305634258	0.0706026478450066	0.7220183613869635	T	T	T
0.3155993167310367	0.0543947029266743	0.9071427450551350	T	T	T
0.2011052396209048	0.0498204349617292	0.0081814997863052	T	T	T
0.0916925247205587	0.0703880327775002	0.9002339380669671	T	T	T
0.1031883299355744	0.0637913377793648	0.7032525698782749	T	T	T
0.2288242565123521	0.0520030094144674	0.7596696129894405	T	T	T
0.3592896984320591	0.8280920470149495	0.7523247429574854	T	T	T
0.3005944457198762	0.8619307975115361	0.9207248973464152	T	T	T
0.1882511478931127	0.8510927170419802	0.0241093055789520	T	T	T
0.0883212385013709	0.8320756958422980	0.8981063435306607	T	T	T

Structure files (CONTCAR) involved in this work:

0.1019558827489229	0.8413102935378957	0.7020991422538877	T	T	T
0.2282467611699702	0.8509941601940068	0.7565257555375502	T	T	T
0.3153537161319950	0.9516164450159581	0.7763547763412749	T	T	T
0.0877912860557019	0.9521125546747419	0.8110412473580103	T	T	T
0.4321207572421550	0.1275285236065830	0.5817880639253900	T	T	T
0.4116544164416985	0.9963580569424610	0.5744437824303570	T	T	T
0.3929474250963215	0.8643101600653011	0.5678001450975375	T	T	T
0.1953488343977013	0.1380059577002051	0.6167087635975432	T	T	T
0.1896535148326639	0.0059687692717850	0.5819576125930968	T	T	T
0.1940398885379947	0.8723142507601052	0.5654692091685054	T	T	T
0.9873377192388795	0.0394851646237163	0.7851572620314461	T	T	T
0.9849599277552503	0.8690385760354635	0.7870767230539457	T	T	T
0.1394282811453445	0.9322614360800954	0.2214177985306580	T	T	T
0.1828254152657941	0.9484042754623523	0.4059659122452056	T	T	T
0.2968612913534908	0.9478306056026550	0.5084938937693878	T	T	T
0.4071159904799175	0.9315318598298711	0.4020264474591336	T	T	T
0.3956353942668761	0.9367752282986352	0.2048608112274100	T	T	T
0.2692675261242403	0.9489007033021931	0.2583017018050571	T	T	T
0.1393166765563781	0.1742267695044543	0.2502380362414263	T	T	T
0.1940608496727654	0.1397627227130715	0.4207462285626979	T	T	T
0.3092627304819399	0.1482380150690386	0.5157202752101824	T	T	T
0.4126511147543747	0.1687547741540955	0.3952434903522827	T	T	T
0.3956630801361771	0.1587323707684524	0.2000382631185836	T	T	T
0.2704037340692271	0.1524864872366868	0.2602835776424151	T	T	T
0.1841454952314567	0.0507420879319953	0.2743306362399333	T	T	T
0.4153198425698906	0.0486699653646920	0.3096139132849349	T	T	T
0.0643956083128208	0.8728397806958993	0.0851267548400824	T	T	T
0.0850231974533908	0.0032228056464958	0.0704894386080060	T	T	T
0.1060961722761109	0.1348236089554957	0.0677283959284340	T	T	T
0.3047306777866154	0.8623295206229916	0.1164682107350027	T	T	T
0.3101061046542448	0.9945584131756499	0.0814889772560752	T	T	T
0.3005789660390278	0.1282752494632470	0.0684604931473814	T	T	T
0.5123795869201317	0.9566998826007379	0.2871095821208864	T	T	T
0.5149019028475798	0.1348020751542428	0.2794909992325634	T	T	T
0.6371072186209478	0.5641397333207637	0.2745765611941673	T	T	T
0.6997265338254697	0.5748272627271591	0.1048060213211491	T	T	T
0.7947348229449285	0.5608917441670522	0.9654346069533816	T	T	T
0.8892396048944589	0.5713209012793894	0.1064742317555201	T	T	T
0.8886846755694983	0.5430572231286509	0.3026110179297519	T	T	T
0.7622901316303293	0.5242823876771905	0.2601476016869463	T	T	T
0.6373360807512904	0.3356133990972171	0.2600305871976842	T	T	T
0.6968588550431800	0.3360921073621574	0.0865732549847910	T	T	T
0.8097233409878932	0.3525781987045871	0.9829501216294783	T	T	T
0.9146175387582917	0.3254011261879195	0.0973167550494769	T	T	T
0.9057027441535052	0.3465201783076097	0.2918038111101405	T	T	T
0.7656181695864726	0.3707245809888790	0.2500890762374742	T	T	T
0.6699076759075048	0.4511381819403119	0.1763012691549706	T	T	T
0.9180634750129213	0.4496290596124946	0.1657153754131524	T	T	T
0.5672153714967720	0.6266623260851021	0.4133532563997532	T	T	T
0.5939975746124607	0.4977457860882757	0.4357649336042375	T	T	T
0.5870937366109886	0.3641317931868600	0.4406606823178947	T	T	T
0.7998396993673758	0.6315201351254908	0.3698309326638650	T	T	T
0.8024546001761428	0.5135171285323006	0.4509688308163560	T	T	T

Structure files (CONTCAR) involved in this work:

0.8316022675500105	0.3837366118161792	0.4414720124581816	T	T	T
0.0029044760315169	0.5492114559248077	0.2106212053907246	T	T	T
0.0202320321909923	0.3693424473035038	0.1981069790372707	T	T	T
0.8554304628584148	0.4360037149905710	0.7842867197287704	T	T	T
0.7917989636086921	0.4352570836118415	0.6116634919065016	T	T	T
0.7029600017427686	0.4242328696414737	0.4646191958768781	T	T	T
0.6088260809531554	0.4319991944893727	0.6069008830427274	T	T	T
0.6022458645088637	0.4443679701132774	0.8049472036400679	T	T	T
0.7279210263863999	0.4736283111308297	0.7730027559362116	T	T	T
0.8596692194785475	0.6789991555616759	0.7589155425044913	T	T	T
0.8110477378108755	0.6464148444170845	0.5645274004592736	T	T	T
0.6897623383069230	0.6469894000551896	0.4827698699130615	T	T	T
0.5842943007705181	0.6691150682018168	0.5997610679893557	T	T	T
0.5925500013044426	0.6612865371031971	0.7971657220933467	T	T	T
0.7174123845898129	0.6526493421077026	0.7363202950474357	T	T	T
0.8221352346677407	0.5510484387916608	0.6953307973999915	T	T	T
0.5822709587082937	0.5498535971118218	0.6855227480592883	T	T	T
0.9322779564258846	0.3745372404663450	0.9145584460868764	T	T	T
0.9123298622569671	0.5056543572357872	0.9354709058140471	T	T	T
0.9024856361521102	0.6386349561496756	0.9392895698852087	T	T	T
0.6935306127560081	0.3720362832794599	0.8946802423126754	T	T	T
0.6766594540133455	0.5000138963053040	0.9486664704229949	T	T	T
0.6865373103125425	0.6338235120412631	0.9305747173679275	T	T	T
0.4923469468628201	0.4512331740455569	0.7052057149847971	T	T	T
0.4789607086278871	0.6316747975627208	0.7070084944975564	T	T	T
0.6430798824627446	0.9395088972760723	0.2888037929429667	T	T	T
0.6983549464267064	0.9336624350224217	0.1104725810414848	T	T	T
0.7991979403819343	0.9483784232337950	0.9805719617631925	T	T	T
0.8978239585400931	0.9304246929158531	0.1124296115601137	T	T	T
0.8968112765966793	0.9480030377583843	0.3098664940306508	T	T	T
0.7709879316329662	0.9688181211369445	0.2662254366597202	T	T	T
0.6398809565783462	0.1740939507075566	0.2523101116241420	T	T	T
0.6960726872166038	0.1569666017822010	0.0786390907755362	T	T	T
0.8098772060745922	0.1466835012742331	0.9796751128349934	T	T	T
0.9137132349789967	0.1699089863342682	0.0970627634825645	T	T	T
0.8954005450301101	0.1610129055064349	0.2941132088071978	T	T	T
0.7698702639448741	0.1447334309255333	0.2433528232703718	T	T	T
0.6784374118375317	0.0525256484233786	0.1985290627841701	T	T	T
0.9172566555162187	0.0512002287433173	0.1853270910273666	T	T	T
0.5682883722983363	0.8756187567982954	0.4201962501792681	T	T	T
0.5817293751773392	0.0073086754656020	0.4373433872799040	T	T	T
0.5996997589969437	0.1393662248424323	0.4348588939480234	T	T	T
0.8064565337114443	0.8699342254165733	0.3923718443580766	T	T	T
0.8154617472609238	0.9964038909296653	0.4495732798137156	T	T	T
0.8069114699992362	0.1300876236254709	0.4345203065073081	T	T	T
0.0096133720700833	0.9558486236251608	0.2161018001892841	T	T	T
0.0148078068090839	0.1389972406555050	0.2156664568825853	T	T	T
0.8566515176115573	0.0555486645219765	0.7868968636780507	T	T	T
0.8008708160216226	0.0703434389808924	0.6101723052878489	T	T	T
0.7001249193978241	0.0569575867209703	0.4804189947235070	T	T	T
0.5982213133000408	0.0759169791076071	0.6064737770983645	T	T	T
0.6028186910467505	0.0528862004891586	0.8035540388170762	T	T	T
0.7281978730602745	0.0279995100519744	0.7629494435052063	T	T	T

Structure files (CONTCAR) involved in this work:

0.8601467647185197	0.8316483207634172	0.7619992496617364	T	T	T
0.8047476126556918	0.8337788400682393	0.5857690015990719	T	T	T
0.6911457655895306	0.8521501804146439	0.4863062957402466	T	T	T
0.5874710802398776	0.8292801646160431	0.6049256583150863	T	T	T
0.6026212626452871	0.8536353307968485	0.7989304781616099	T	T	T
0.7297274459815837	0.8549275026993741	0.7459145245972342	T	T	T
0.8182301658217691	0.9472128663526520	0.6860451291341213	T	T	T
0.5785144876602142	0.9536816373708277	0.6723505810331551	T	T	T
0.9323027494033140	0.1261476798193110	0.9105093285328334	T	T	T
0.9189152214987863	0.9960866600352213	0.9417971649278727	T	T	T
0.9005074111732243	0.8642582137839162	0.9439024663596353	T	T	T
0.6951561694278884	0.1302811287792685	0.8837079476819745	T	T	T
0.6817605193250152	0.0046474573998091	0.9461849932873594	T	T	T
0.6955462325802994	0.8709836315361660	0.9380724584786110	T	T	T
0.4883973926486967	0.0483902150482563	0.7148913424195251	T	T	T
0.4834542087711424	0.8647722661620509	0.7159819358897156	T	T	T
0.3614455564948696	0.4317362673992620	0.7188765654373203	T	T	T
0.3156925181651841	0.4465872123642620	0.9027638292652485	T	T	T
0.2007296178261279	0.4576773052568718	0.0015019708337982	T	T	T
0.0886091610362839	0.4322092497622417	0.9021871032283819	T	T	T
0.1021948330103187	0.4375437015251278	0.7056942222361100	T	T	T
0.2306067838610059	0.4493959955320604	0.7534806635899139	T	T	T
0.3578263661291789	0.6748418003795698	0.7528074277927768	T	T	T
0.3002355802042445	0.6376911745680351	0.9197836225319809	T	T	T
0.1884118324376500	0.6479885022526621	0.0230402993428781	T	T	T
0.0897734888380004	0.6699007818028757	0.8940347210168337	T	T	T
0.1019163564061746	0.6581057266905339	0.6976978844843698	T	T	T
0.2272414578575944	0.6489276363085124	0.7561550483824754	T	T	T
0.3163224474783968	0.5499499674927346	0.7728970575528243	T	T	T
0.0827559906755248	0.5497799741609977	0.8098711834251328	T	T	T
0.4322655886405860	0.3764422039510619	0.5718276121360851	T	T	T
0.4135655852668931	0.5082129248124909	0.5729142930348741	T	T	T
0.3842078520493740	0.6387752494581656	0.5664934370067377	T	T	T
0.1917001968063899	0.3631312717358379	0.6145225101910617	T	T	T
0.1835479852531871	0.4957047993340527	0.5797410566796405	T	T	T
0.1959674436843285	0.6289936293618287	0.5638487485869655	T	T	T
0.9849002501588519	0.4600013282903535	0.7843515988591266	T	T	T
0.9842601279485761	0.6377487142648985	0.7816350089953240	T	T	T
0.1339111924389619	0.5688843344926401	0.2235807157454212	T	T	T
0.1817624632981298	0.5539362131416550	0.4042315853668066	T	T	T
0.2948773893711166	0.5471295046503606	0.5092432375643221	T	T	T
0.4030834562403810	0.5720219644656991	0.4009834625788659	T	T	T
0.3941854821746594	0.5621555136044006	0.2054676849829615	T	T	T
0.2655936057553436	0.5515963526899473	0.2529571787434991	T	T	T
0.1396189189457849	0.3258354795466422	0.2496680176227514	T	T	T
0.1953626089866121	0.3610564750456597	0.4190636502258350	T	T	T
0.3079344047541690	0.3535557548412616	0.5200549370183916	T	T	T
0.4053082305689875	0.3288994777451689	0.3893098965131249	T	T	T
0.3932845926632265	0.3468257337235217	0.1932064998224537	T	T	T
0.2696377082320639	0.3515452244153699	0.2565211385988323	T	T	T
0.1807802598227076	0.4505761747622524	0.2742625389152719	T	T	T
0.4094710650527450	0.4516146055708279	0.3158127713648796	T	T	T
0.0638454931337056	0.6237420238316651	0.0766953409635367	T	T	T

Structure files (CONTCAR) involved in this work:

0.0831755455069312	0.4918918147233098	0.0778109099465563	T	T	T
0.1168282523047337	0.3625346767315885	0.0620412279339534	T	T	T
0.3053790084681040	0.6376408750873392	0.1148656082173253	T	T	T
0.3115730477236003	0.5051202519425451	0.0788901131737305	T	T	T
0.2954423498510417	0.3722034745574903	0.0626530386701623	T	T	T
0.5094444506439184	0.5381262542777246	0.2932364226494465	T	T	T
0.5097805565655388	0.3661731008652745	0.2790936896976804	T	T	T
0.4363202734163300	0.7502329508185798	0.6407831975889527	T	T	T
0.1898812167465588	0.7504286628910478	0.6376984741807423	T	T	T
0.2754682949073324	0.7499268813000907	0.0213619860882813	T	T	T
0.1030991523188145	0.7491224514868832	0.0506452223002220	T	T	T
0.0639596544965170	0.2506037748558643	0.1336042447380539	T	T	T
0.3079814085160301	0.2509194299758449	0.1369314597974310	T	T	T
0.2228979293059939	0.2504736417691550	0.5230830592614979	T	T	T
0.3919501019292916	0.2511209482917717	0.5470077163573033	T	T	T
0.5562113764960740	0.2510641311230150	0.3535426046037535	T	T	T
0.8046715610909222	0.2507708894849598	0.3561669553105067	T	T	T
0.7278823620195715	0.2499907185100030	0.9435630315183744	T	T	T
0.8913354048765106	0.2495114023670952	0.9412975670056470	T	T	T
0.9445023860679549	0.7529043573057067	0.8634452198532506	T	T	T
0.6814888825895350	0.7536361255980379	0.8560468693388202	T	T	T
0.7723355991358073	0.7490297884673219	0.4444787566374839	T	T	T
0.6079670144396421	0.7506182059672831	0.4488244800784073	T	T	T
0.9290747404086755	0.4934436213496829	0.5346299968637888	T	T	T
0.8227506430552306	0.3329381880767541	0.3286608727729763	T	T	T
0.7971415330342607	0.6374979374582606	0.6982724847933293	T	T	T
0.9334996138885856	0.4025593215563750	0.4515429696085360	T	T	T
0.8697846281361048	0.5635994192444970	0.5594670005990838	T	T	T
0.9742174821268226	0.6521941541608920	0.4872831725960142	T	T	T
0.0303317202366335	0.3925392312574426	0.4443957800601685	T	T	T
0.0541224868764624	0.4098203615964481	0.5137291792309083	T	T	T
0.0468183920070241	0.4251456151812223	0.3826818915647399	T	T	T
0.0461020548933864	0.3409276732212285	0.4283383641836525	T	T	T
0.9717900125736595	0.4953329077554143	0.5693344627602069	T	T	T
0.9921318520777178	0.6203695094867672	0.5488182584382741	T	T	T
0.9685191132535952	0.6224628410588210	0.4187897148159364	T	T	T
0.9269907268946174	0.6769099981937013	0.5074273353229521	T	T	T
1.0114136391445843	0.6918684426041968	0.4754342458783595	T	T	T

Figure S15(b) TSI

Si O Al Zn C H

1.0000000000000000

20.0219999999999985 0.0000000000000000 0.0000000000000000

0.0000000000000000 19.8990000000000009 0.0000000000000000

0.0000000000000000 0.0000000000000000 13.3829999999999991

94 193 2 2 2 8

Selective dynamics

Direct

0.4215068136431224 0.0603524799730895 0.6484371054547392 T T T

0.3038455058465166 0.0325407394245451 0.7916075308670764 T T T

0.2810766224408792 0.0569160813189011 0.0169043534535128 T T T

0.1211014396932224 0.0649826651089821 0.0122822542689097 T T T

0.0670808910925934 0.0315782511431409 0.8004781772637842 T T T

0.1795614194778122 0.0659292559367922 0.6644433237387252 T T T

Structure files (CONTCAR) involved in this work:

0.4174626086290680	0.8278095154742339	0.6683992064740645	T	T	T
0.2989455577394753	0.8737926710806548	0.7992337516118048	T	T	T
0.2664523615653023	0.8306743645928183	0.0183939536877704	T	T	T
0.1104980692210622	0.8267027239548577	0.0127466296844277	T	T	T
0.0651022856761485	0.8747968412522771	0.7989711256097727	T	T	T
0.1772005288986711	0.8293996337616434	0.6637776185388994	T	T	T
0.0746231194016571	0.9418893894971314	0.1483708440710827	T	T	T
0.1937271672105148	0.9702050362692490	0.2898307629190603	T	T	T
0.2157210748522760	0.9442836814441614	0.5159029652752106	T	T	T
0.3762082868262577	0.9359235047656628	0.5129315681804136	T	T	T
0.4318659007701247	0.9697924749876543	0.3002201188160827	T	T	T
0.3185423465182271	0.9350796078259911	0.1638238810586307	T	T	T
0.0797966726103365	0.1740485284356107	0.1673273586882049	T	T	T
0.1976915852659906	0.1288368955982478	0.2992513392828650	T	T	T
0.2304198854052237	0.1698691812300157	0.5171142239085237	T	T	T
0.3864141484362472	0.1743089009074372	0.5095800229561823	T	T	T
0.4342018544286089	0.1281490571752304	0.2956820822812528	T	T	T
0.3188116324916588	0.1732573469815437	0.1649126827598826	T	T	T
0.5753997348075678	0.5575722746120831	0.3519891499103063	T	T	T
0.6901745720719271	0.5279895854710424	0.2051989660667951	T	T	T
0.7152726291592705	0.5675201396480208	0.9864522839812071	T	T	T
0.8740884170891429	0.5706392273791646	0.9840122492667933	T	T	T
0.9234902751493925	0.5283358707477680	0.1919832243617127	T	T	T
0.8128694528781164	0.5542301813379167	0.3449757270673336	T	T	T
0.5736621706598850	0.3297286894346942	0.3303628540885500	T	T	T
0.6928630149029145	0.3737972545934881	0.1916433520730639	T	T	T
0.7324515960164006	0.3290668175484802	0.9752674344941655	T	T	T
0.8873263982278990	0.3255756963416898	0.9829611054818178	T	T	T
0.9393160241811621	0.3725088283221680	0.1883271553459192	T	T	T
0.9205671148081159	0.4455958081806249	0.8543100786598203	T	T	T
0.8005456100630727	0.4758441841234960	0.7148591332655353	T	T	T
0.7828499121697484	0.4386153312432123	0.4924720734749483	T	T	T
0.6247118463718059	0.4323483712972666	0.4845458021571956	T	T	T
0.5721390102768293	0.4705159337420191	0.6969993857168788	T	T	T
0.6777098541803601	0.4483680471102550	0.8533698525215173	T	T	T
0.9209527505607362	0.6774807825291104	0.8331440852866147	T	T	T
0.7645278718037608	0.6721651707051371	0.4652457176242416	T	T	T
0.6100451941831394	0.6744473491678129	0.4846763449608082	T	T	T
0.5594053263155275	0.6286515078566272	0.6965174874131498	T	T	T
0.6691477590964914	0.6736865836359656	0.8311295731759917	T	T	T
0.5760123887100198	0.9466336460244630	0.3573570914901073	T	T	T
0.6963859580940994	0.9747497224595257	0.2145746097966710	T	T	T
0.7180377651497917	0.9388945465138229	0.9932511244193913	T	T	T
0.8775312399711215	0.9343822606923888	0.9938627353871204	T	T	T
0.9294407451024640	0.9717158032760885	0.2036625155822921	T	T	T
0.8204993111634189	0.9477430621828371	0.3539098202024774	T	T	T
0.5773515423100939	0.1749327844906008	0.3312082339037266	T	T	T
0.6961511439819744	0.1321365157998234	0.1938676522148939	T	T	T
0.7316418862708040	0.1721573653662640	0.9729659356706678	T	T	T
0.8864452499411517	0.1730194115042340	0.9822456118062397	T	T	T
0.9340276872410963	0.1301071262337358	0.1973754339191139	T	T	T
0.8178195594973844	0.1733873738190642	0.3317675500118529	T	T	T
0.9225099903912208	0.0532246518756845	0.8551690283273131	T	T	T

Structure files (CONTCAR) involved in this work:

0.8002874498520436	0.0252067040639325	0.7107198150870988	T	T	T
0.7801861564603119	0.0656815070820139	0.4926902059886058	T	T	T
0.6199969979817492	0.0704577376168711	0.4902511154212705	T	T	T
0.5668941182468440	0.0324680655057258	0.6994591646273176	T	T	T
0.6769041131407372	0.0543914316123418	0.8505418166745586	T	T	T
0.9218101030283958	0.8302445054349787	0.8366728408832846	T	T	T
0.8014944588836164	0.8671212110572097	0.6941480260283370	T	T	T
0.7659234119861019	0.8284705256083030	0.4756543931934736	T	T	T
0.6114468492037414	0.8282546095311081	0.4892523217307593	T	T	T
0.5621166353947736	0.8750532839128536	0.6986750449004067	T	T	T
0.6773253554047842	0.8318946311340004	0.8342223944453050	T	T	T
0.4245910766448954	0.4428463977369017	0.6422623852457355	T	T	T
0.3060395482196149	0.4696350392405437	0.7862349701012846	T	T	T
0.2800682071183049	0.4455298644944186	0.0111894436360636	T	T	T
0.1219730871856878	0.4363622506903932	0.0116941462387530	T	T	T
0.0646028927003855	0.4702216799939992	0.8011535731105153	T	T	T
0.1779960744587297	0.4355399763417936	0.6624857734833737	T	T	T
0.4139562874586318	0.6738840764896701	0.6658791879787203	T	T	T
0.2988995983662043	0.6278791189447426	0.7985291908410718	T	T	T
0.2661642830042997	0.6693729277204359	0.0175032043041159	T	T	T
0.1105537774983355	0.6728943532989775	0.0091152596630106	T	T	T
0.0635278122599024	0.6287933377381211	0.7948090693354826	T	T	T
0.1781865597837361	0.6721524768443569	0.6622399042964338	T	T	T
0.0707246062841165	0.5583210099976028	0.1467658860610838	T	T	T
0.1895754066456984	0.5316450407123685	0.2886694777206815	T	T	T
0.2139582910302123	0.5561491552766133	0.5150364251479443	T	T	T
0.3726380278214913	0.5664036186607090	0.5131860547879930	T	T	T
0.4276797965640136	0.5308032806879704	0.3038939954381410	T	T	T
0.3169038008434513	0.5647939319121354	0.1622227696148232	T	T	T
0.0841233449993282	0.3275138853026833	0.1618795411975091	T	T	T
0.1971291951245062	0.3733428694161882	0.2979910369993355	T	T	T
0.2294577377867080	0.3311398356905738	0.5171330186284300	T	T	T
0.3843880796834367	0.3276821682399054	0.5065243242878806	T	T	T
0.4289717913988503	0.3739211141873235	0.2943221768932462	T	T	T
0.3167070182992308	0.3305380040414776	0.1596519982770386	T	T	T
0.3581312890338585	0.0711571236979432	0.7223844037174785	T	T	T
0.3155596967828539	0.0530768419067273	0.9073038917398575	T	T	T
0.2006688591913433	0.0509519850799030	0.0074039886886083	T	T	T
0.0907893133609119	0.0707321854435935	0.9006136372675089	T	T	T
0.1028875212662162	0.0648751696036836	0.7035170682795401	T	T	T
0.2286868250020767	0.0546779309887717	0.7599526163458153	T	T	T
0.3577126082723510	0.8287083609596371	0.7503066964654234	T	T	T
0.2993719765811088	0.8630304544075703	0.9188171757808822	T	T	T
0.1878393777489238	0.8508788451179686	0.0238060842429626	T	T	T
0.0880845869690890	0.8325874859207517	0.8968689731886041	T	T	T
0.1005359423545164	0.8417617054624910	0.7007768513327299	T	T	T
0.2267394687621148	0.8510489919251539	0.7549941344340017	T	T	T
0.3132234113939943	0.9522026393441444	0.7734405089125356	T	T	T
0.0882817633519116	0.9527243904806694	0.8101811247826719	T	T	T
0.4320926345425037	0.1277425309049848	0.5816987362136961	T	T	T
0.4107816891813070	0.9969062948540249	0.5741262666286545	T	T	T
0.3933065876577553	0.8648746444675044	0.5665482547594732	T	T	T
0.1942326533791563	0.1389822121764694	0.6151366442974584	T	T	T

Structure files (CONTCAR) involved in this work:

0.1898932404181087	0.0064106781751119	0.5834660344084988	T	T	T
0.1927159762990795	0.8730043668375651	0.5640539812605820	T	T	T
0.9870781789625523	0.0392981104634144	0.7848689522339031	T	T	T
0.9843923162991609	0.8710447667208883	0.7873164350777434	T	T	T
0.1382626841414972	0.9321523734642270	0.2221366913042611	T	T	T
0.1821807620312329	0.9510016914920498	0.4060748943553040	T	T	T
0.2963071209637569	0.9477169981886370	0.5081383498714171	T	T	T
0.4064352665536299	0.9327895827288843	0.4011686613028269	T	T	T
0.3949108849641587	0.9366759189425291	0.2041022885495787	T	T	T
0.2683982917566811	0.9463906738111825	0.2581982018167263	T	T	T
0.1386177396421885	0.1737124971596941	0.2508089484238550	T	T	T
0.1951586866981339	0.1374594790117843	0.4193014949682748	T	T	T
0.3090672537360922	0.1494689506450567	0.5171618139863977	T	T	T
0.4116615984654652	0.1688715592058634	0.3951194459525810	T	T	T
0.3957691905142453	0.1603076752464463	0.1995305259266373	T	T	T
0.2701491086196876	0.1538152403141778	0.2584667559935890	T	T	T
0.1856608515779540	0.0505401243729078	0.2699313460701835	T	T	T
0.4139508373771031	0.0494747405528651	0.3072133062384546	T	T	T
0.0640661521877731	0.8733247899732953	0.0838899416065281	T	T	T
0.0849944941414432	0.0038479468709243	0.0712093123533520	T	T	T
0.1055585186199808	0.1356368681763810	0.0676162115077741	T	T	T
0.3049137838446987	0.8617585890187159	0.1144205935008005	T	T	T
0.3084039511686568	0.9943770311579232	0.0823628904162548	T	T	T
0.3013154843653230	0.1280981040833487	0.0675693182627627	T	T	T
0.5115368995541444	0.9582714864292849	0.2859122594163222	T	T	T
0.5144183600288804	0.1354177349982865	0.2805537000481173	T	T	T
0.6342963852209494	0.5673101719894822	0.2702245692380467	T	T	T
0.7050591564794223	0.5724744553633936	0.1064039809566958	T	T	T
0.7948171441037962	0.5635548470979062	0.9594705342902240	T	T	T
0.8869048615976100	0.5713249104059164	0.1042893794214778	T	T	T
0.8870751628823511	0.5433831841879622	0.2993537579534512	T	T	T
0.7586274312407415	0.5232065716899148	0.2706948769939145	T	T	T
0.6357075918847425	0.3335782342543839	0.2539448613505120	T	T	T
0.6945873504821215	0.3405946461910626	0.0804387204707479	T	T	T
0.8104545481163146	0.3523275228327223	0.9841169702359513	T	T	T
0.9170065992918456	0.3254130951413390	0.0951941533472657	T	T	T
0.9042133993186929	0.3470365260519915	0.2893332931889917	T	T	T
0.7640205901383903	0.3700664489288175	0.2458221951254530	T	T	T
0.6674115108094719	0.4519670694556082	0.1798033909294465	T	T	T
0.9175571764961127	0.4497585137878277	0.1629543741744789	T	T	T
0.5642919971196187	0.6276744517473863	0.4123110567937868	T	T	T
0.5945243973602170	0.4993962775624811	0.4324999906310791	T	T	T
0.5914167951087698	0.3656081683723210	0.4368027340247390	T	T	T
0.8002726096906289	0.6326081183814621	0.3719157678898354	T	T	T
0.8093580084811912	0.5148429588941809	0.4554179693348644	T	T	T
0.8311784295094033	0.3832416859876522	0.4393450831924163	T	T	T
0.0010577418994367	0.5499822408558852	0.2081662366988943	T	T	T
0.0201428326436593	0.3702284174785930	0.2004241160875262	T	T	T
0.8556240265884664	0.4380910118486661	0.7828843310795305	T	T	T
0.7927857472125853	0.4336642650766487	0.6116743792754821	T	T	T
0.7052620136034522	0.4295924266312275	0.4627039849513668	T	T	T
0.6098344772022721	0.4335890979766509	0.6036113760094166	T	T	T
0.6045108850663865	0.4454989268258158	0.8018760861085369	T	T	T

Structure files (CONTCAR) involved in this work:

0.7294392315366008	0.4786312043834436	0.7706616732386229	T	T	T
0.8584431155552067	0.6788138488788596	0.7594940926834309	T	T	T
0.8060693620611171	0.6526974366871293	0.5662730097369256	T	T	T
0.6873260858783476	0.6478357163543231	0.4773879086164420	T	T	T
0.5840728634016301	0.6702844994075159	0.5988180195310344	T	T	T
0.5913633140488196	0.6616697717331821	0.7969130005824858	T	T	T
0.7167500008838579	0.6481832136802829	0.7419894526190021	T	T	T
0.8245823940863932	0.5523500317036666	0.6874763442946774	T	T	T
0.5821429706004162	0.5508643365104412	0.6833459698525409	T	T	T
0.9319002631188450	0.3750927871870410	0.9125653723000570	T	T	T
0.9128521673669576	0.5068148068121825	0.9337482964452519	T	T	T
0.9038426502707730	0.6399161130779047	0.9390089166678238	T	T	T
0.6978229364682007	0.3730235084413790	0.8870855924809605	T	T	T
0.6784402747791035	0.4989597352523135	0.9486590232069724	T	T	T
0.6825053830832173	0.6331521794911339	0.9352441776953559	T	T	T
0.4936836725601420	0.4511512219558469	0.7035873588791917	T	T	T
0.4784738613974088	0.6321096303832691	0.7053288608490650	T	T	T
0.6419843239364834	0.9401971844371537	0.2880277002762260	T	T	T
0.6979679110203111	0.9331033786322078	0.1102996130438494	T	T	T
0.7982388964130011	0.9484960515687978	0.9795393557557717	T	T	T
0.8968622177528587	0.9296766103625748	0.1112724425541516	T	T	T
0.8955756111392537	0.9487332853664781	0.3084042708838517	T	T	T
0.7696621916810810	0.9710544840056279	0.2659286388975124	T	T	T
0.6394706400831589	0.1738273044450315	0.2539992139701033	T	T	T
0.6958734040866575	0.1593376194681015	0.0798055491181193	T	T	T
0.8091658831089584	0.1475091335342021	0.9793576921194134	T	T	T
0.9133276575333533	0.1702473284766872	0.0962609631690766	T	T	T
0.8945527255975855	0.1601576679986709	0.2932401312129431	T	T	T
0.7689880241903585	0.1428530421966082	0.2442662834374887	T	T	T
0.6765548068804834	0.0527230964616092	0.1950219455846378	T	T	T
0.9166845205189972	0.0509982661957303	0.1825548650104220	T	T	T
0.5662009280696538	0.8770621697921192	0.4197091822090134	T	T	T
0.5811632565595093	0.0084659243917871	0.4364345873169415	T	T	T
0.5986016935548270	0.1404657380420523	0.4367915574754344	T	T	T
0.8045033719275770	0.8719430693551518	0.3915787491204341	T	T	T
0.8155935908695041	0.9983248266261718	0.4485870397952755	T	T	T
0.8065506406877048	0.1319807861896869	0.4357257063683103	T	T	T
0.0085407047262982	0.9555146839506138	0.2149711211146424	T	T	T
0.0140716365133309	0.1386594096112521	0.2152662644349832	T	T	T
0.8564024737428384	0.0544403324351686	0.7858993434281114	T	T	T
0.7997835589346285	0.0709923389800642	0.6103148920041391	T	T	T
0.6996970063600414	0.0580340299800310	0.4793209839903710	T	T	T
0.5983740759113282	0.0752442975486412	0.6069977699447997	T	T	T
0.6021013040250465	0.0532519772372011	0.8041220544099931	T	T	T
0.7276265822891463	0.0288500252640410	0.7638102425207088	T	T	T
0.8603561985545779	0.8322236837341512	0.7582533155527579	T	T	T
0.8024139808608785	0.8334301937042069	0.5836649932988603	T	T	T
0.6888597711655889	0.8537888078994341	0.4852539529384132	T	T	T
0.5857633735429671	0.8296326807820893	0.6041371295080746	T	T	T
0.6020663619173641	0.8519215630298658	0.7985351923274850	T	T	T
0.7293690786615078	0.8534368499174403	0.7460506077681240	T	T	T
0.8156813712434750	0.9471478316388328	0.6837396459892433	T	T	T
0.5780606668695047	0.9532878415219468	0.6742446204101519	T	T	T

Structure files (CONTCAR) involved in this work:

0.9313024805792316	0.1256324631867606	0.9098768974821383	T	T	T
0.9184143562320125	0.9954619729517709	0.9411352249552837	T	T	T
0.8985776537309782	0.8637193823910559	0.9419878566854777	T	T	T
0.6939325638757728	0.1304446184155666	0.8855185641304154	T	T	T
0.6805699168092820	0.0042169834733837	0.9463015393281117	T	T	T
0.6947209742782053	0.8704917379897478	0.9377293973134525	T	T	T
0.4880429302507813	0.0482680168791205	0.7146643202445391	T	T	T
0.4824699676533150	0.8645780165927867	0.7167992041295623	T	T	T
0.3627261400219210	0.4322715015634573	0.7195914697621337	T	T	T
0.3158085935023397	0.4492210068072819	0.9024863327749189	T	T	T
0.1999768207948269	0.4565904955805044	-0.0006523139470449	T	T	T
0.0865089148631421	0.4326434853754841	0.9030492674264011	T	T	T
0.1023654624470169	0.4360782842318667	0.7067616876730165	T	T	T
0.2312752755865345	0.4469846030702061	0.7525664708829898	T	T	T
0.3574479260128659	0.6748117347915705	0.7529558167183044	T	T	T
0.2988931888335535	0.6361925844645893	0.9184056189965655	T	T	T
0.1876431643894004	0.6484104164365484	0.0222363226231398	T	T	T
0.0892385889356525	0.6696846490803312	0.8923358472599369	T	T	T
0.1010635707686117	0.6578418346256930	0.6956616458253465	T	T	T
0.2264397155771968	0.6504138277459263	0.7548638952245819	T	T	T
0.3141746427693407	0.5502016290371000	0.7688443185020524	T	T	T
0.0823723592412947	0.5496705598832330	0.8082493291586494	T	T	T
0.4322945728940848	0.3772690146639694	0.5706545290250292	T	T	T
0.4136215500117899	0.5089999187072133	0.5733461283572741	T	T	T
0.3826474799923035	0.6390192985131543	0.5662653672149712	T	T	T
0.1903784815179318	0.3623626514617796	0.6125774958828661	T	T	T
0.1828337058525101	0.4957222137416797	0.5812973258971237	T	T	T
0.1956187742137312	0.6288577957583515	0.5627850477347092	T	T	T
0.9846410277118344	0.4599244491832006	0.7814580458837103	T	T	T
0.9835867494087313	0.6375979803771551	0.7797700713863415	T	T	T
0.1316161742547150	0.5696865500188658	0.2251784733656410	T	T	T
0.1805826604352626	0.5521915615262755	0.4048890330338510	T	T	T
0.2941873488712812	0.5462261958493517	0.5094652345221586	T	T	T
0.4018495101746720	0.5720019304649566	0.4009464431500617	T	T	T
0.3925071609480151	0.5626811871028869	0.2055223524688226	T	T	T
0.2636758870846073	0.5542475233461611	0.2529299084752110	T	T	T
0.1397381233838013	0.3261595685906644	0.2500372339723530	T	T	T
0.1970909019621481	0.3636188198478087	0.4174971135008366	T	T	T
0.3076923101501370	0.3526243730150910	0.5222749271573492	T	T	T
0.4038456083626460	0.3292252680218370	0.3888591455497650	T	T	T
0.3934842335004232	0.3466976633264668	0.1924446952619102	T	T	T
0.2696452845735354	0.3521794729223235	0.2537545211207509	T	T	T
0.1806312111928375	0.4512605333079557	0.2709186295402895	T	T	T
0.4078937336546025	0.4517686565733066	0.3149800152089479	T	T	T
0.0631974702811650	0.6239121351411751	0.0752881525212079	T	T	T
0.0833710704099007	0.4922709738465284	0.0783761502005943	T	T	T
0.1156826775398793	0.3626231092387224	0.0625095695438580	T	T	T
0.3048109902260713	0.6384020932376901	0.1133279704524830	T	T	T
0.3092549667073671	0.5054609135944720	0.0801455834193881	T	T	T
0.2962408773961430	0.3726592844491438	0.0602764392076421	T	T	T
0.5078159726009488	0.5382291203695068	0.2923780264728438	T	T	T
0.5092078033885222	0.3671039426662302	0.2807012538664739	T	T	T
0.4350856349108864	0.7505161243967704	0.6399437011071993	T	T	T

Structure files (CONTCAR) involved in this work:

0.1881691820221381	0.7508482205760554	0.6352944617696461	T	T	T
0.2752737427185870	0.7499415372618180	0.0171904108376471	T	T	T
0.1020132099871486	0.7493120404504329	0.0488609015203164	T	T	T
0.0630642986700840	0.2509856822992301	0.1356325823070916	T	T	T
0.3079793839133905	0.2513988828874582	0.1341017985252754	T	T	T
0.2210615913746136	0.2505307678334481	0.5173949178589204	T	T	T
0.3932166479156146	0.2514914292545490	0.5472108967649904	T	T	T
0.5558952140975529	0.2519339463172253	0.3543118994180938	T	T	T
0.8039593007899406	0.2510509536126984	0.3526749074473573	T	T	T
0.7274609918539835	0.2508554759774271	0.9426859869316042	T	T	T
0.8916850963497280	0.2495121408347399	0.9399102178530728	T	T	T
0.9448376061481958	0.7536623382469638	0.8597947595921257	T	T	T
0.6815627102815124	0.7524123933467524	0.8566461637882595	T	T	T
0.7684688527525706	0.7509475108391679	0.4386431324943541	T	T	T
0.6052459352525520	0.7518595219306174	0.4472213281210712	T	T	T
0.9362538740909885	0.4806578327785176	0.5494840344679631	T	T	T
0.8209774076231956	0.3334368710399851	0.3254632978779015	T	T	T
0.7957170688694032	0.6383343161686452	0.6973254701345565	T	T	T
0.9339888281948537	0.3908160277725851	0.4527403910173742	T	T	T
0.8762038085082245	0.5714262552488557	0.5601002951833710	T	T	T
0.9652467788931980	0.6070188228046319	0.4928669102357835	T	T	T
0.0300051584495786	0.3752583712672699	0.4520946937076269	T	T	T
0.0506057455518678	0.3828756813532894	0.5272732766779495	T	T	T
0.0508562777741561	0.4140456201613696	0.4023049843138541	T	T	T
0.0443954533805766	0.3257008266186675	0.4236580909295288	T	T	T
0.9609354995443958	0.4680527661905405	0.6100011366283312	T	T	T
0.9566794001871228	0.5386727631262587	0.5202538379507106	T	T	T
0.9781577666389800	0.5954498203330859	0.4149895313439807	T	T	T
0.9383401884563860	0.6555780440135665	0.4893679311539620	T	T	T
1.0102580719840075	0.6170026703012625	0.5373070844052409	T	T	T

Figure S15(b) 2Zn-CH₃+2O_M-H

Si O Al Zn C H

1.0000000000000000

20.0219999999999985 0.0000000000000000 0.0000000000000000

0.0000000000000000 19.8990000000000009 0.0000000000000000

0.0000000000000000 0.0000000000000000 13.3829999999999991

94 193 2 2 2 8

Selective dynamics

Direct

0.4210640364222109	0.0606200832736915	0.6488092265656240	T	T	T
0.3031589089698952	0.0325684118006305	0.7916610375789085	T	T	T
0.2805219331145434	0.0567626981463537	0.0170914384979637	T	T	T
0.1204822300955242	0.0653165553804472	0.0125477481859381	T	T	T
0.0662204505159662	0.0318275270709309	0.8005317960057403	T	T	T
0.1789410948564356	0.0662392893412971	0.6647614273571013	T	T	T
0.4171243572713701	0.8279973635301709	0.6681879345579392	T	T	T
0.2982753226748213	0.8737938239618566	0.7987013337087598	T	T	T
0.2664107664828246	0.8307862533535246	0.0177258942779801	T	T	T
0.1104972198128584	0.8272502000361002	0.0120931657880388	T	T	T
0.0644505206706330	0.8750187069195058	0.7983895376830512	T	T	T
0.1766216871568833	0.8293565541390323	0.6636549762270008	T	T	T
0.0741364479509862	0.9420206244323824	0.1487761754566725	T	T	T
0.1934761074377261	0.9699229243679561	0.2901157293594102	T	T	T

Structure files (CONTCAR) involved in this work:

0.2154557456809537	0.9445101325067042	0.5163732731959713	T	T	T
0.3759744802562939	0.9364446714328476	0.5128072706847798	T	T	T
0.4312358728200865	0.9704934770933513	0.2998562620894100	T	T	T
0.3180404568970861	0.9346920049333141	0.1638947998882745	T	T	T
0.0792188283711811	0.1737054422141941	0.1677322628346926	T	T	T
0.1976129983158453	0.1285796416013554	0.2991866181921840	T	T	T
0.2298824980961437	0.1700483176425287	0.5171146964593794	T	T	T
0.3860453823480693	0.1746740192453382	0.5100439000313470	T	T	T
0.4337269078927470	0.1285879018117449	0.2959426982163446	T	T	T
0.3185995808839374	0.1733341685601318	0.1648237559939804	T	T	T
0.5752818828638249	0.5582676284319663	0.3524320370032360	T	T	T
0.6914370927379916	0.5293703639889235	0.2088495256090153	T	T	T
0.7157238287688913	0.5683429098694870	0.9879965838849781	T	T	T
0.8744657029067381	0.5724562275261140	0.9864277460805405	T	T	T
0.9238296627249163	0.5297213902976743	0.1950407829971712	T	T	T
0.8145506152118879	0.5544999896000053	0.3502747424338394	T	T	T
0.5735680999838614	0.3298314083920709	0.3290338021102246	T	T	T
0.6902662767994642	0.3750997037127564	0.1875517675213269	T	T	T
0.7309696388014321	0.3304972549778179	0.9722171834100389	T	T	T
0.8860962966280296	0.3256395373592170	0.9834875332454162	T	T	T
0.9384721168413229	0.3728728148505439	0.1888027785026875	T	T	T
0.9195917948772052	0.4466721747338595	0.8570654186083514	T	T	T
0.8029503176575427	0.4775366268127120	0.7094767643697186	T	T	T
0.7839806540869843	0.4371378031397244	0.4914290962341658	T	T	T
0.6250877120614776	0.4325652081486209	0.4838621992839266	T	T	T
0.5725221368686818	0.4714186054415946	0.6956603275722884	T	T	T
0.6806555105358816	0.4502271269486774	0.8489051649103596	T	T	T
0.9206116833392793	0.6770144057236280	0.8341563296699104	T	T	T
0.7619678581553264	0.6742928801581646	0.4668115282043011	T	T	T
0.6081362038063516	0.6751400120915884	0.4829970265640960	T	T	T
0.5595120191131142	0.6293609553460187	0.6953006649479712	T	T	T
0.6687350103346469	0.6714638530430186	0.8336286908096279	T	T	T
0.5751623711670858	0.9473553899710044	0.3570946461646995	T	T	T
0.6949843303082567	0.9744298170694583	0.2127884515394773	T	T	T
0.7174923029071922	0.9376437825887426	0.9926922236829602	T	T	T
0.8769080381822304	0.9336500094338210	0.9926244308606206	T	T	T
0.9286956115435295	0.9708416965255723	0.2022538592486288	T	T	T
0.8187611971011680	0.9484361661285670	0.3520831742010038	T	T	T
0.5768774763862722	0.1748317420720614	0.3325995638434064	T	T	T
0.6948296918623593	0.1306849900083167	0.1934651348853430	T	T	T
0.7301486493967427	0.1731286427673028	0.9737439289652469	T	T	T
0.8853732224662595	0.1731131460505214	0.9823288214396255	T	T	T
0.9335116611783543	0.1290342950995441	0.1962574938120452	T	T	T
0.8165207968489845	0.1706438495272331	0.3299677412822364	T	T	T
0.9214969734429546	0.0528880259461308	0.8550264531292993	T	T	T
0.7990951881506958	0.0244875962510168	0.7107786902351262	T	T	T
0.7794102000726724	0.0655656715799797	0.4928362265466953	T	T	T
0.6192094553731490	0.0708243338189092	0.4911961320885568	T	T	T
0.5663113718814360	0.0322262255055165	0.7006445924015131	T	T	T
0.6760235161143699	0.0540757718328035	0.8516278802141642	T	T	T
0.9209849684327673	0.8299170960592414	0.8338461739391050	T	T	T
0.8007224195522318	0.8661047665180418	0.6910125399529872	T	T	T
0.7635614260713689	0.8284501793577105	0.4721043229273015	T	T	T

Structure files (CONTCAR) involved in this work:

0.6095037742321960	0.8287130939761190	0.4883230730939666	T	T	T
0.5615825369836597	0.8745673948789064	0.6991702649058845	T	T	T
0.6775256777180263	0.8302325956911419	0.8329802854734547	T	T	T
0.4250350122874700	0.4431576846917396	0.6427518715884939	T	T	T
0.3059995422788192	0.4698643529940809	0.7859962163537697	T	T	T
0.2803018942964516	0.4456074544648851	0.0115537432017782	T	T	T
0.1220134963218653	0.4362464459964273	0.0133643089438893	T	T	T
0.0657998815368062	0.4706970813518257	0.8036694736282272	T	T	T
0.1778369882459479	0.4358247241099837	0.6623335607080907	T	T	T
0.4137995163940024	0.6740461143855555	0.6648869526366452	T	T	T
0.2986443827737741	0.6281122420782709	0.7979161301483836	T	T	T
0.2658829219623760	0.6694308969183913	0.0164957101141008	T	T	T
0.1102904444580845	0.6735905335400948	0.0082958649344633	T	T	T
0.0630390435750053	0.6290990844707258	0.7949701626285512	T	T	T
0.1778011205454530	0.6720931728013873	0.6622202274001754	T	T	T
0.0711153591880269	0.5590986234253511	0.1465439335995870	T	T	T
0.1900276547807623	0.5320958262820424	0.2883461161366455	T	T	T
0.2142004520376431	0.5562650995153228	0.5147538219069556	T	T	T
0.3729078331387581	0.5662406970941509	0.5125627406148237	T	T	T
0.4282072544938738	0.5310258114293098	0.3028153764007561	T	T	T
0.3171385267981620	0.5651928388405874	0.1622140569584603	T	T	T
0.0832079598007100	0.3273540756584082	0.1643392892439908	T	T	T
0.1970347925880508	0.3738212792604926	0.2982607381778232	T	T	T
0.2290033061427937	0.3313451843949602	0.5173759540242442	T	T	T
0.3840521032064942	0.3281250661484418	0.5069979698966943	T	T	T
0.4285785421003493	0.3741077769389306	0.2941364646359076	T	T	T
0.3164818596312510	0.3302957553058836	0.1594531976237725	T	T	T
0.3575981061208660	0.0711675515508642	0.7227011794603929	T	T	T
0.3150370139495146	0.0524734152066800	0.9075759808193887	T	T	T
0.2000661222488928	0.0516856456857961	0.0073259229059388	T	T	T
0.0897627218383450	0.0705986628054126	0.9011246572747980	T	T	T
0.1022781450691811	0.0654284046422876	0.7039368435507163	T	T	T
0.2281615012314533	0.0555064835290717	0.7603132682697379	T	T	T
0.3569018338404405	0.8288318914402204	0.7493464164622491	T	T	T
0.2994768594263564	0.8632479072792799	0.9183507195583709	T	T	T
0.1878862360184290	0.8513887742827004	0.0229804991099645	T	T	T
0.0877283707145544	0.8330116599662227	0.8963823162375706	T	T	T
0.0999697405023075	0.8419902752943338	0.7002812494638678	T	T	T
0.2259459215213631	0.8506646151392410	0.7553552669435510	T	T	T
0.3119198044142502	0.9522819139211481	0.7725498328454455	T	T	T
0.0875233942900504	0.9530137199143170	0.8096208322688099	T	T	T
0.4315863446932440	0.1282303978655512	0.5824451598444763	T	T	T
0.4104671531257076	0.9975661370783816	0.5738384503960700	T	T	T
0.3934975835656351	0.8655924391353407	0.5664621959044013	T	T	T
0.1933928133150078	0.1392548419365432	0.6149065987990302	T	T	T
0.1894449808386549	0.0064669784712742	0.5842857335797371	T	T	T
0.1926963273614917	0.8730796418066535	0.5642260932999270	T	T	T
0.9862780637596144	0.0399275371548648	0.7847296320042417	T	T	T
0.9838316562086462	0.8713930949679319	0.7864663595413628	T	T	T
0.1376355152282608	0.9321692805308714	0.2228163779872056	T	T	T
0.1818636938743425	0.9515477640339189	0.4066066001816215	T	T	T
0.2960206161061672	0.9481733693793835	0.5085298710904528	T	T	T
0.4058943956483227	0.9334760644582819	0.4008288397366440	T	T	T

Structure files (CONTCAR) involved in this work:

0.3944466542424516	0.9370684815201812	0.2038110425231038	T	T	T
0.2678834313267235	0.9452762184505039	0.2584841767843497	T	T	T
0.1380805326506929	0.1731402244215509	0.2511077216081296	T	T	T
0.1950039990185860	0.1373640801899133	0.4192210121298903	T	T	T
0.3085892605103037	0.1501375334664948	0.5178168480448465	T	T	T
0.4111536932484045	0.1691561671546783	0.3955388480572256	T	T	T
0.3956064710367753	0.1613301538194393	0.1998524886480889	T	T	T
0.2698512634101917	0.1541262358358284	0.2583813915633075	T	T	T
0.1861851909007080	0.0503132893400691	0.2695725235818622	T	T	T
0.4126904947944832	0.0500924342307948	0.3066310169493068	T	T	T
0.0641143450129316	0.8739098970675167	0.0831600986711621	T	T	T
0.0846228740505418	0.0046473217240770	0.0727595896288823	T	T	T
0.1049219378387616	0.1363409597392050	0.0672090922312727	T	T	T
0.3049715974942556	0.8613919450006007	0.1140413207446534	T	T	T
0.3070240749196264	0.9940362746943916	0.0827747285720544	T	T	T
0.3014585418509422	0.1277627186680410	0.0678074122848871	T	T	T
0.5109287581757626	0.9598261591419781	0.2853202406436015	T	T	T
0.5140008728731968	0.1355099442132480	0.2813679882601445	T	T	T
0.6351228306003024	0.5693839407335106	0.2724976828567139	T	T	T
0.7060242876063011	0.5714941155866999	0.1078972280618378	T	T	T
0.7954010037832346	0.5677750458214048	0.9606760440399049	T	T	T
0.8871805535720577	0.5716147256104978	0.1064798087767129	T	T	T
0.8887786321290641	0.5458894093247325	0.3020641400325825	T	T	T
0.7602692076210507	0.5246439522551307	0.2730568849924311	T	T	T
0.6345878548238278	0.3330582199503022	0.2503583303960921	T	T	T
0.6900199138397948	0.3454827462328108	0.0739820846925335	T	T	T
0.8092923849498894	0.3518420352829986	0.9863042374841036	T	T	T
0.9165723798331981	0.3264152464210227	0.0954960493244479	T	T	T
0.9016576951775128	0.3446863879340948	0.2888467400811018	T	T	T
0.7628257909443996	0.3685490387868394	0.2374944686706633	T	T	T
0.6662815685276752	0.4537004635494215	0.1843473223951976	T	T	T
0.9170695837834488	0.4503448815956985	0.1682410987612800	T	T	T
0.5608349506879797	0.6275407915745967	0.4134437116465164	T	T	T
0.5946624506621359	0.4995457968187262	0.4321224511845688	T	T	T
0.5924839772422534	0.3658032613388938	0.4347494698542680	T	T	T
0.8006562297347294	0.6318858796614533	0.3791085938648913	T	T	T
0.8133675323142514	0.5098918526690663	0.4540364488128118	T	T	T
0.8278158072471853	0.3776918321400591	0.4365032015382286	T	T	T
0.0019953418209979	0.5499644717845119	0.2084186446113064	T	T	T
0.0188662169999780	0.3691997645185245	0.2050397799193348	T	T	T
0.8569615546170384	0.4408695477010178	0.7816874553216695	T	T	T
0.7968641135886861	0.4308557071478724	0.6102134842966528	T	T	T
0.7056974265694095	0.4293677938551222	0.4641386069349862	T	T	T
0.6091612586300561	0.4331167064267126	0.6026592475499768	T	T	T
0.6064644812579187	0.4481903371380829	0.8003476787657172	T	T	T
0.7314289198476793	0.4807942902571179	0.7648539978616524	T	T	T
0.8568441118668658	0.6759770015466332	0.7638586410145520	T	T	T
0.7964909974390412	0.6646381654485489	0.5732725001326264	T	T	T
0.6843960722382267	0.6481720657671285	0.4707235243905353	T	T	T
0.5842139493640321	0.6718643994173964	0.5985852486793887	T	T	T
0.5910968093933324	0.6609204831884726	0.7969294770711398	T	T	T
0.7171667901391399	0.6407397019473713	0.7500744963332390	T	T	T
0.8283963254754856	0.5530981206737020	0.6791500995455607	T	T	T

Structure files (CONTCAR) involved in this work:

0.5815479516317432	0.5515401401270561	0.6794804254659637	T	T	T
0.9303930763279341	0.3755373309912917	0.9132597188727292	T	T	T
0.9121461410444668	0.5074241271076867	0.9365103493763829	T	T	T
0.9068484797677764	0.6407076805143231	0.9422155622736526	T	T	T
0.7009716612905132	0.3741184596215221	0.8799625095198136	T	T	T
0.6826871168307327	0.4986760034839651	0.9465689457213353	T	T	T
0.6791375798210553	0.6333698877392668	0.9407924493432722	T	T	T
0.4941154521367743	0.4513564190790547	0.7041297425952365	T	T	T
0.4784394054549418	0.6327270936853894	0.7044804345620445	T	T	T
0.6411250311314468	0.9404740057721137	0.2877308496670656	T	T	T
0.6972021169610304	0.9313630916647588	0.1097417721744734	T	T	T
0.7976234323157965	0.9484595355838672	0.9797376669933238	T	T	T
0.8970015617838873	0.9282162260013036	0.1097691410933178	T	T	T
0.8939925954197816	0.9491563751169091	0.3068571949539462	T	T	T
0.7683392982177873	0.9732821641882926	0.2642615319598318	T	T	T
0.6396645745920563	0.1723522351669838	0.2566420582552466	T	T	T
0.6949656228291146	0.1615313713031528	0.0813904649794440	T	T	T
0.8077859013899285	0.1488042512925714	0.9801348179002438	T	T	T
0.9128823618237805	0.1703363690903636	0.0960751051200474	T	T	T
0.8936385103617777	0.1584869128124475	0.2923805415166433	T	T	T
0.7681661627064518	0.1376993201485084	0.2441171045466402	T	T	T
0.6737406141877933	0.0517741814446265	0.1899319940159752	T	T	T
0.9165534953244481	0.0501381406767035	0.1794728524090901	T	T	T
0.5642379978921361	0.8780715426126111	0.4193846446816702	T	T	T
0.5806162604894253	0.0092146628415925	0.4362009647796452	T	T	T
0.5970828776095152	0.1411746065601919	0.4391956672568015	T	T	T
0.8016831044147504	0.8729081535790970	0.3884139217111881	T	T	T
0.8145030570440793	0.9985413467628943	0.4475302434011182	T	T	T
0.8064031723784498	0.1320289501709147	0.4363965042664249	T	T	T
0.0077664689084581	0.9548589874597569	0.2150369395568625	T	T	T
0.0134455447427529	0.1381159369378201	0.2151702511938731	T	T	T
0.8553791333152347	0.0535528287663710	0.7859572617851297	T	T	T
0.7989969906769876	0.0704673968714575	0.6104433278514242	T	T	T
0.6989111557103139	0.0590482437812141	0.4791027599317322	T	T	T
0.5981235034514147	0.0747702771086881	0.6081869173285548	T	T	T
0.6011316426768623	0.0532585321287712	0.8054836826897995	T	T	T
0.7265964163521590	0.0292118684227888	0.7642513394966276	T	T	T
0.8605115528358149	0.8314289336600120	0.7538177673230323	T	T	T
0.8009352635886703	0.8339117063253257	0.5797153278451425	T	T	T
0.6867091933393199	0.8545949262658613	0.4843816915264275	T	T	T
0.5840362539182874	0.8300028448801894	0.6033668562668681	T	T	T
0.6020927306457498	0.8505042755567405	0.7980117017451953	T	T	T
0.7292163127556468	0.8519790907099887	0.7445679790374522	T	T	T
0.8141521764907226	0.9465547412789699	0.6833892042003800	T	T	T
0.5774426526600204	0.9530412083627603	0.6761143885844451	T	T	T
0.9295349615376065	0.1254651601679365	0.9096186198807029	T	T	T
0.9180669306386227	0.9950100810051410	0.9408264016647107	T	T	T
0.8968495517305016	0.8633475089841831	0.9388644279820955	T	T	T
0.6926613177765903	0.1301177812107563	0.8875617585450313	T	T	T
0.6798644601589039	0.0031920397802409	0.9464589824932939	T	T	T
0.6950249832216595	0.8692826539832016	0.9363199365390105	T	T	T
0.4874442841127792	0.0483789678251814	0.7151848233478960	T	T	T
0.4818972803685717	0.8642709395431663	0.7180572532564907	T	T	T

Structure files (CONTCAR) involved in this work:

0.3630264525833540	0.4325993108450790	0.7200601028054467	T	T	T
0.3153086246783997	0.4498282730939334	0.9024614948026554	T	T	T
0.2000108242218818	0.4557212606631022	0.0008026629874533	T	T	T
0.0873068919207535	0.4317035053499421	0.9040485066564957	T	T	T
0.1020007116378626	0.4372574906724894	0.7071700650258095	T	T	T
0.2312963686723191	0.4466331653287476	0.7521181995170118	T	T	T
0.3570118936427142	0.6748188622741685	0.7516904754235922	T	T	T
0.2992297071468774	0.6361686672557961	0.9178803517673785	T	T	T
0.1873160118544499	0.6485211158199760	0.0198280552239923	T	T	T
0.0881525161197181	0.6709431274108901	0.8918192537797774	T	T	T
0.1007898709439607	0.6570473765023526	0.6954849642994014	T	T	T
0.2259472763901128	0.6506972844521615	0.7551874387410771	T	T	T
0.3133745134354132	0.5503411575721368	0.7679774055233306	T	T	T
0.0826853128272418	0.5500607970767141	0.8109368764764757	T	T	T
0.4321125270898706	0.3774851093311826	0.5711319617660069	T	T	T
0.4137209504687028	0.5090586683286402	0.5734550183305880	T	T	T
0.3825421899021041	0.6389435872948738	0.5653422371393925	T	T	T
0.1890080599449254	0.3624592012100976	0.6122909806977762	T	T	T
0.1824451559891810	0.4958046602426072	0.5808331066029627	T	T	T
0.1959531290207271	0.6287530642026610	0.5630112600409957	T	T	T
0.9852048740578455	0.4601949380450686	0.7851902032991276	T	T	T
0.9829493236075354	0.6364264118592640	0.7798376623899753	T	T	T
0.1327183914562611	0.5703169120863218	0.2238695023203863	T	T	T
0.1804800383537111	0.5521656743124956	0.4047322680716887	T	T	T
0.2943216705473345	0.5458550219210422	0.5089756786228490	T	T	T
0.4021207472632904	0.5715455231573807	0.4003657953086731	T	T	T
0.3929020257994137	0.5636865769946849	0.2048926475760453	T	T	T
0.2644130166781786	0.5542376374721324	0.2536005570966950	T	T	T
0.1388382025525110	0.3265353192653913	0.2523810603146224	T	T	T
0.1967138947893514	0.3645212969911215	0.4179469906521660	T	T	T
0.3071630832524604	0.3527571182371589	0.5233642799656233	T	T	T
0.4030430830714020	0.3301142246153451	0.3892066124049396	T	T	T
0.3931478573318276	0.3460021933214635	0.1927224496304978	T	T	T
0.2690547590656817	0.3520174089600901	0.2533131105310910	T	T	T
0.1805408217916604	0.4516255096454156	0.2706153085662640	T	T	T
0.4074846408861195	0.4521031971669277	0.3128676897863825	T	T	T
0.0633179201194087	0.6244368450159312	0.0748008493391997	T	T	T
0.0832902849820747	0.4928332549678719	0.0781138817009671	T	T	T
0.1139641644574898	0.3629441578945634	0.0649855650622454	T	T	T
0.3038860665296004	0.6384695908070095	0.1129352810115368	T	T	T
0.3092599984540531	0.5055231328715400	0.0805888221705966	T	T	T
0.2966617414926109	0.3726347376666848	0.0600263104920570	T	T	T
0.5083684677363177	0.5376859459712960	0.2912676042823614	T	T	T
0.5087032509196013	0.3671361164153001	0.2806246386853595	T	T	T
0.4342914345654412	0.7507993568395878	0.6388383401130896	T	T	T
0.1873331174731411	0.7507753659019476	0.6350323709073801	T	T	T
0.2748572425751607	0.7499999597879723	0.0161024249110765	T	T	T
0.1022961404564125	0.7498822807961782	0.0486203908247706	T	T	T
0.0621975729305615	0.2510029855608080	0.1377725358958779	T	T	T
0.3071439280773090	0.2513332238629342	0.1334657662304131	T	T	T
0.2200811063592802	0.2507881993235671	0.5168184385695400	T	T	T
0.3929095046803938	0.2519152497374575	0.5473452030309062	T	T	T
0.5557612096207086	0.2521510920642593	0.3537969880761553	T	T	T

Structure files (CONTCAR) involved in this work:

0.8009789423282642	0.2485357844046862	0.3464438547846597	T	T	T
0.7254983784542961	0.2517244789981423	0.9424523062597244	T	T	T
0.8914189674984326	0.2497731166497624	0.9404592782432897	T	T	T
0.9447822060888010	0.7536184196561182	0.8573385330368098	T	T	T
0.6823048141287238	0.7507387812379186	0.8548507262525966	T	T	T
0.7644240364936655	0.7521551271640358	0.4309214044835507	T	T	T
0.6020341770206707	0.7526446276717289	0.4458111121219029	T	T	T
0.9497655658714503	0.4855868080995607	0.5929686578244667	T	T	T
0.8158475764148547	0.3310021101098793	0.3203987399509418	T	T	T
0.7944868301163952	0.6378241458680398	0.6960405607233969	T	T	T
0.9284117133834833	0.3769194176556692	0.4329507580929973	T	T	T
0.9032532313715138	0.5814446234553806	0.5823368788897426	T	T	T
0.9539615577910773	0.6465278467990543	0.5047236899891789	T	T	T
0.0232911512312381	0.3811983638101067	0.4606857072199790	T	T	T
0.0362652701776069	0.3832258717910477	0.5402810312308359	T	T	T
0.0450558471425230	0.4246649525562605	0.4213195897699625	T	T	T
0.0461198621491847	0.3359293784719066	0.4282893662276879	T	T	T
0.9631072639010594	0.4713932130074495	0.6615685753488240	T	T	T
0.9900881723135376	0.4825774160540360	0.5522147954762600	T	T	T
0.9526984475340743	0.6332093951593371	0.4250455982504739	T	T	T
0.9312416519567654	0.6962968958482605	0.5145997319802172	T	T	T
1.0061237827606375	0.6482491044982603	0.5301227214046625	T	T	T

Figure S15(b) TS2

Si O Al Zn C H

1.0000000000000000

20.0219999999999985 0.0000000000000000 0.0000000000000000

0.0000000000000000 19.8990000000000009 0.0000000000000000

0.0000000000000000 0.0000000000000000 13.3829999999999991

94 193 2 2 2 8

Selective dynamics

Direct

0.4222891165236352	0.0575210536705035	0.6467232112817668	T	T	T
0.3020650808224375	0.0309077972471839	0.7874210576143856	T	T	T
0.2815918916275888	0.0540290223918696	0.0147592652332407	T	T	T
0.1216841779322319	0.0659060091543608	0.0116406967587348	T	T	T
0.0674222237506883	0.0325541216763991	0.7995305716148166	T	T	T
0.1788243800378822	0.0679916971012003	0.6619121625083777	T	T	T
0.4174324195445106	0.8269770932124820	0.6726278540083191	T	T	T
0.2954605041555143	0.8726310871280267	0.7943313630181180	T	T	T
0.2666239943969032	0.8285305169303507	0.0146443366791677	T	T	T
0.1087720704428785	0.8251143252002808	0.0127988240532690	T	T	T
0.0668570836265836	0.8757303627001445	0.7979285693931135	T	T	T
0.1744684290610492	0.8267883777829500	0.6553069190183929	T	T	T
0.0745940167316384	0.9428930725928086	0.1471782245147757	T	T	T
0.1955067389348475	0.9693257401843167	0.2865209442819688	T	T	T
0.2147233160483254	0.9450786282518570	0.5142182096018114	T	T	T
0.3750137003202875	0.9328738389945571	0.5137651637308566	T	T	T
0.4312347112946175	0.9657322076350389	0.3024402419944351	T	T	T
0.3194733171597760	0.9318982875194285	0.1622207194453027	T	T	T
0.0808013140797736	0.1732553830057964	0.1674342079309238	T	T	T
0.2011827875433611	0.1276095034567251	0.2937783783025206	T	T	T
0.2309358780346280	0.1698884705473096	0.5123810523785244	T	T	T
0.3880834411215563	0.1732062351628481	0.5088310695403913	T	T	T

Structure files (CONTCAR) involved in this work:

0.4337700309371464	0.1235584499653427	0.2956456032105754	T	T	T
0.3222772018790784	0.1714689553542900	0.1578839384790915	T	T	T
0.5765452386052372	0.5547394489942153	0.3550416544105510	T	T	T
0.6887201620182303	0.5246922031159974	0.2016551891671940	T	T	T
0.7145002235038147	0.5651989247495989	0.9857442634745425	T	T	T
0.8738129383874755	0.5711635397766128	0.9835615867423430	T	T	T
0.9242787299321982	0.5285978651913964	0.1891500635442962	T	T	T
0.8109431702187985	0.5509150534266175	0.3377571301915820	T	T	T
0.5718601957489852	0.3270499226641930	0.3298140630472007	T	T	T
0.6906983193739225	0.3706762900952413	0.1891264064938736	T	T	T
0.7285517657570301	0.3254501230076740	0.9760773117590651	T	T	T
0.8827519258297833	0.3236011355062344	0.9929620869344374	T	T	T
0.9382174407170133	0.3743220503259705	0.1900373741350501	T	T	T
0.9213688438023210	0.4428963744839534	0.8615219008624634	T	T	T
0.8035914568486865	0.4719355641711060	0.7157306592805627	T	T	T
0.7776219001926435	0.4353730884151794	0.4906401613241347	T	T	T
0.6187513598033482	0.4272175172519257	0.4876044159363912	T	T	T
0.5697580137703563	0.4689174948296702	0.6988366437731897	T	T	T
0.6782107818825173	0.4454661186457760	0.8516303677551059	T	T	T
0.9229080351346337	0.6765672278642278	0.8312592928338636	T	T	T
0.7682783120199791	0.6687556079794794	0.4631900788198735	T	T	T
0.6133751907934517	0.6731410254484352	0.4863709567347594	T	T	T
0.5613013492772765	0.6265539463012287	0.6955348155248896	T	T	T
0.6741271305000507	0.6714676257322012	0.8253183711493970	T	T	T
0.5767887396032086	0.9451771032155919	0.3588459697353932	T	T	T
0.6970862688338609	0.9717260866552523	0.2139782435456210	T	T	T
0.7184376636539631	0.9343933727615650	0.9937633036406013	T	T	T
0.8779374570667102	0.9325144480601588	0.9945112426524024	T	T	T
0.9295037426102009	0.9704710291471730	0.2037573079584628	T	T	T
0.8211220414125393	0.9465300440464087	0.3551644543317923	T	T	T
0.5759008003205929	0.1716919762619967	0.3313806104885627	T	T	T
0.6970809218137153	0.1290889664784498	0.1958072940897216	T	T	T
0.7309872320104424	0.1695387167314342	0.9749359502768217	T	T	T
0.8855605355079328	0.1717295056968587	0.9844457924583377	T	T	T
0.9350309325476271	0.1280218476770688	0.1972125899896306	T	T	T
0.8197315457006985	0.1710687840715416	0.3318269208860749	T	T	T
0.9223666542825437	0.0528489021646103	0.8563015400195402	T	T	T
0.8008178533922163	0.0245272037825811	0.7116481795285217	T	T	T
0.7803891201268099	0.0659603699976721	0.4930035952721357	T	T	T
0.6201269659417314	0.0703893234390571	0.4906942163231631	T	T	T
0.5681713493057906	0.0299937233108712	0.6990604872331924	T	T	T
0.6767928618583242	0.0504789265168908	0.8523622631062758	T	T	T
0.9238456989534345	0.8293864517496015	0.8383620879505564	T	T	T
0.8036132215197678	0.8671610404470222	0.6957404791490673	T	T	T
0.7697629851698488	0.8260748067961587	0.4776998194310630	T	T	T
0.6147097422313447	0.8261722920387402	0.4898306545372381	T	T	T
0.5640855257865991	0.8730575055643157	0.6977400099024488	T	T	T
0.6789650352122066	0.8302164743435998	0.8327655949864274	T	T	T
0.4232884191587638	0.4417728318014394	0.6474187096883318	T	T	T
0.3038641110010000	0.4683113945119527	0.7876682487416165	T	T	T
0.2835308184810247	0.4473678550361900	0.0162935670019977	T	T	T
0.1266006706840869	0.4345585086049442	0.0168843421399426	T	T	T
0.0692532772589842	0.4637831513746319	0.8071330722746256	T	T	T

Structure files (CONTCAR) involved in this work:

0.1786270107681049	0.4316365420521759	0.6633591366550321	T	T	T
0.4145763265621459	0.6719399315811884	0.6725115167554144	T	T	T
0.2960945144319007	0.6261226251140269	0.7953981738847562	T	T	T
0.2665011154756298	0.6702945915541397	0.0151910907636310	T	T	T
0.1095101337797873	0.6733829084907142	0.0112463200033268	T	T	T
0.0668122676684859	0.6231988093198716	0.7981003546716853	T	T	T
0.1756235866093532	0.6702070202161133	0.6538859321990390	T	T	T
0.0711747339928193	0.5555563075093588	0.1453566548283519	T	T	T
0.1923249750730398	0.5291892035557195	0.2848477018750730	T	T	T
0.2140373035192601	0.5523373470598543	0.5126668805004505	T	T	T
0.3728803914217567	0.5658854666389643	0.5167765209639491	T	T	T
0.4295837074233338	0.5333512843972008	0.3068201408867766	T	T	T
0.3198999141060381	0.5675877053884472	0.1630530682861736	T	T	T
0.0843612513111388	0.3272668603115925	0.1676908250950215	T	T	T
0.1996573526109713	0.3715934386186611	0.2964123975635756	T	T	T
0.2310292281079752	0.3302881911111862	0.5147502464286963	T	T	T
0.3873352816639339	0.3267080147862079	0.5090220229747455	T	T	T
0.4298652028708245	0.3759847576743067	0.2951877960544721	T	T	T
0.3191943010020613	0.3279126203770654	0.1567157950712736	T	T	T
0.3595410771029466	0.0677949142555758	0.7219334341353363	T	T	T
0.3148001871220142	0.0458451922110857	0.9047914993630037	T	T	T
0.2009291029463904	0.0500827755942219	0.0067094046555048	T	T	T
0.0913995614991208	0.0712514144453701	0.8999408620920670	T	T	T
0.1024075315148666	0.0667337226631131	0.7024759755625756	T	T	T
0.2290950073946508	0.0602575908610881	0.7570424680111706	T	T	T
0.3607641074707279	0.8305949114247261	0.7593806638142818	T	T	T
0.2884581155742796	0.8686650097670222	0.9144385519331547	T	T	T
0.1873824802289694	0.8395745422924713	0.0344445826731996	T	T	T
0.0938115166680052	0.8347640443565996	0.8946949073428392	T	T	T
0.0999045310910647	0.8425837823609696	0.6983116423525424	T	T	T
0.2288652189219499	0.8411858898318955	0.7432522358798525	T	T	T
0.3046934312679050	0.9508198949453757	0.7619322733758334	T	T	T
0.0896709121287495	0.9539028983981622	0.8071886325730366	T	T	T
0.4327762006450163	0.1247865322324772	0.5795856621201846	T	T	T
0.4110685482549093	0.9942765906624284	0.5721714744865670	T	T	T
0.3902077698959379	0.8626054988886159	0.5711520524068973	T	T	T
0.1916790684558569	0.1402065908704406	0.6086336524919812	T	T	T
0.1898734230100914	0.0063554583523379	0.5844824659264973	T	T	T
0.1894827527810671	0.8733267839454499	0.5582961437966032	T	T	T
0.9871540276136664	0.0394436317070132	0.7861761910965605	T	T	T
0.9859600772038492	0.8715031330701305	0.7902828382240819	T	T	T
0.1381882381959473	0.9326135183763146	0.2206412782262936	T	T	T
0.182485782202424	0.9548745729503674	0.4039105089815100	T	T	T
0.2954599559563915	0.9465317259430480	0.5076195550363695	T	T	T
0.4054193151368872	0.9270840762643805	0.4020540694842315	T	T	T
0.3954119491220311	0.9337349316644420	0.2044410176487304	T	T	T
0.2683779336705721	0.9395462942466903	0.2564547531500030	T	T	T
0.1390525956718881	0.1711293275479284	0.2515388982101359	T	T	T
0.2011743129254462	0.1328566248420789	0.4141924080851169	T	T	T
0.3099490007132688	0.1523966916985345	0.5215220603274719	T	T	T
0.4099594396476612	0.1663804129659327	0.3926887837817777	T	T	T
0.3975190551691907	0.1540874089705124	0.1965386202569042	T	T	T
0.2709322007022131	0.1573272361869913	0.2501743479905625	T	T	T

Structure files (CONTCAR) involved in this work:

0.1926722508268683	0.0494245661842184	0.2610104111527023	T	T	T
0.4126192526553646	0.0453162957293368	0.3109983513564432	T	T	T
0.0640086458032376	0.8757411118246125	0.0798223304031767	T	T	T
0.0843632136237899	0.0062618383464058	0.0723877656599891	T	T	T
0.1072205885631339	0.1373691934877056	0.0658602765489354	T	T	T
0.3080412976327173	0.8597953972464170	0.1078138246214827	T	T	T
0.3082426903821632	0.9933563473319152	0.0845928625412830	T	T	T
0.3038467085532514	0.1260978434504797	0.0610153159656726	T	T	T
0.5111223037784394	0.9552399677613840	0.2894203315544738	T	T	T
0.5143012496872174	0.1294994349279558	0.2818376794991645	T	T	T
0.6379336424019938	0.5618712977619064	0.2774654653706068	T	T	T
0.6959595929509261	0.5715947493050202	0.1033219814290490	T	T	T
0.7945772808922600	0.5578369778921179	0.9682141350498885	T	T	T
0.8918182665828406	0.5745920892270517	0.1017864167205197	T	T	T
0.8854947169716918	0.5427497713107045	0.2936468717238386	T	T	T
0.7610811079608529	0.5200781469482126	0.2562418002128475	T	T	T
0.6365468670940529	0.3317305840059485	0.2586532351737722	T	T	T
0.6874334790039671	0.3358318244894144	0.0789572575242783	T	T	T
0.8057527255312856	0.3493124035837410	0.9919626564652811	T	T	T
0.9103360282457226	0.3218006864909090	0.1071587619831918	T	T	T
0.9042354727296409	0.3557828581187755	0.2967101755182200	T	T	T
0.7639285958776785	0.3667437757969590	0.2372592931016401	T	T	T
0.6653369165977160	0.4487641445938687	0.1764316831341073	T	T	T
0.9176238715539415	0.4502494881357384	0.1565490327923675	T	T	T
0.5685311218437991	0.6252394839567726	0.4148633482542377	T	T	T
0.5894251620324602	0.4944607253375705	0.4349995924305580	T	T	T
0.5868212097647511	0.3600549080002998	0.4392351874410250	T	T	T
0.7970311050290526	0.6292488520138779	0.3651395116882548	T	T	T
0.7996804125800263	0.5106149554217093	0.4463851635551162	T	T	T
0.8239393379352370	0.3795701093626961	0.4371396233925101	T	T	T
0.0022443487663535	0.5474691576184658	0.2083355001360835	T	T	T
0.0188083436044457	0.3699850243337683	0.2004349946300806	T	T	T
0.8590884907128447	0.4345697758466460	0.7837423919979978	T	T	T
0.7977318505439331	0.4339998566770923	0.6080516756195425	T	T	T
0.6994241921302231	0.4242997181717141	0.4701830595174664	T	T	T
0.6026245872027983	0.4277541105811249	0.6058803127555001	T	T	T
0.6046819273072233	0.4444387128480217	0.8017259877775372	T	T	T
0.7313921634824453	0.4729808040011769	0.7685325977895150	T	T	T
0.8648736014436411	0.6786896145279074	0.7495035034286321	T	T	T
0.8135591201742316	0.6445878591769152	0.5594504846441267	T	T	T
0.6910159103529309	0.6474979636845920	0.4839543377664308	T	T	T
0.5851671312206743	0.6697998856193145	0.5992313984193480	T	T	T
0.5961051496555402	0.6576031420358042	0.7948470522676345	T	T	T
0.7222577394602598	0.6472933270996208	0.7356938704320913	T	T	T
0.8277659585140614	0.5487567523683310	0.6892645466926449	T	T	T
0.5825326721727798	0.5484340520916555	0.6793981145480564	T	T	T
0.9276288055527953	0.3755611019059906	0.9285975954928787	T	T	T
0.9131847466626346	0.5090182966141812	0.9310931752883211	T	T	T
0.8969203061342914	0.6417431689685901	0.9349485338125916	T	T	T
0.6965969820310718	0.3699212791356254	0.8863164570016715	T	T	T
0.6786912061769013	0.4969028447078457	0.9454493394363326	T	T	T
0.6882961780599383	0.6316634226639853	0.9294581710429799	T	T	T
0.4910223355546934	0.4525362743112904	0.7113636728495141	T	T	T

Structure files (CONTCAR) involved in this work:

0.4807516303482616	0.6311320959247038	0.7075180293813754	T	T	T
0.6417373028830784	0.9390711837364912	0.2875209560225275	T	T	T
0.6988870661715241	0.9286624126413564	0.1109984251343574	T	T	T
0.7984422451973971	0.9447345709652593	0.9788449655289350	T	T	T
0.8962354428538066	0.9281513956793661	0.1123449259441159	T	T	T
0.8961596388503458	0.9491936297902670	0.3096052873570302	T	T	T
0.7698392267694251	0.9676048894636260	0.2666544467977970	T	T	T
0.6398980848148390	0.1688904139013676	0.2577470262070915	T	T	T
0.6967678283474176	0.1595322441197749	0.0835332408940201	T	T	T
0.8086460152003505	0.1452035200011734	0.9807196379122471	T	T	T
0.9127094388789891	0.1694166942650228	0.0982285273307742	T	T	T
0.8965149567309821	0.1565890497834556	0.2948558783003373	T	T	T
0.7697997937759222	0.1383633963418295	0.2474674590908941	T	T	T
0.6784057309555873	0.0495873757669490	0.1911129094116452	T	T	T
0.9171127612178610	0.0494281849314238	0.1801559423701992	T	T	T
0.5692108029429060	0.8756866178824136	0.4219315018455944	T	T	T
0.5824092288943830	0.0076874260980412	0.4367169958887039	T	T	T
0.5955404108363231	0.1403788062326471	0.4399311387593527	T	T	T
0.8077129469189229	0.8704408767940452	0.3939844966013245	T	T	T
0.8145131202308785	0.9979740462275105	0.4486412485594554	T	T	T
0.8089125772576929	0.1324742841865292	0.4383544861925407	T	T	T
0.0085929990681776	0.9544404691759392	0.2147375546214108	T	T	T
0.0151846223032136	0.1364425286673888	0.2131414808054278	T	T	T
0.8566110373413063	0.0551208796953503	0.7862393129276765	T	T	T
0.7986431835227322	0.0701599365366265	0.6111623660960678	T	T	T
0.6999817894391061	0.0607903165397132	0.4764970369305551	T	T	T
0.6005347716886937	0.0736482017555279	0.6082744248819932	T	T	T
0.6022550113512317	0.0499450662746632	0.8049013380635541	T	T	T
0.7284249481010762	0.0264242112836971	0.7658404031089278	T	T	T
0.8615108134629030	0.8322110246837590	0.7616020155351828	T	T	T
0.8053592226567335	0.8321942286932775	0.5861642607933649	T	T	T
0.6923773555824059	0.8507804712830811	0.4859278512713247	T	T	T
0.5886491553505371	0.8268656604623491	0.6045674346342337	T	T	T
0.6034194098792084	0.8502899908569369	0.7984076611144182	T	T	T
0.7307408825719937	0.8554804502047481	0.7464114640935349	T	T	T
0.8184691916995875	0.9470122117257002	0.6841255777847878	T	T	T
0.5803772034979940	0.9511314579899856	0.6725329873061099	T	T	T
0.9310624462777800	0.1251129931219794	0.9118737410696492	T	T	T
0.9174939948296191	0.9944447149924165	0.9413363978129551	T	T	T
0.9011524121639013	0.8619202830716564	0.9445706368113022	T	T	T
0.6927799613439878	0.1261129498314788	0.8901253419073848	T	T	T
0.6799497186482806	0.9989761546032536	0.9464849455882163	T	T	T
0.6955233720409989	0.8655423479633205	0.9391244556956858	T	T	T
0.4891161376408348	0.0453781573393675	0.7122663562494481	T	T	T
0.4843284202985764	0.8635214829595762	0.7148307029703738	T	T	T
0.3614437829168067	0.4301068219187875	0.7239094305944919	T	T	T
0.3153006170095832	0.4533197541182058	0.9052401656497067	T	T	T
0.2034082933925342	0.4601844071236154	0.0133539312271842	T	T	T
0.0989772645491314	0.4257578130472835	0.9043356021385195	T	T	T
0.1033367818849472	0.4322128941848704	0.7076933711735980	T	T	T
0.2306628672747384	0.4405128940820299	0.7559088725343764	T	T	T
0.3608907470791682	0.6701789713193835	0.7637184967477137	T	T	T
0.2867504243438989	0.6291392405751836	0.9151221218462382	T	T	T

Structure files (CONTCAR) involved in this work:

0.1875362166933235	0.6590709533051174	0.0372334491733795	T	T	T
0.0971059052153228	0.6650446960735988	0.8920823299199192	T	T	T
0.1016583245346571	0.6506827467082735	0.6959041760869407	T	T	T
0.2297985002676696	0.6559919298221693	0.7419276010284248	T	T	T
0.3079131255776347	0.5483429332478048	0.7622290768637056	T	T	T
0.0843540889519850	0.5440340726480302	0.8141210212893488	T	T	T
0.4333752221693522	0.3763131553875557	0.5761669963368474	T	T	T
0.4113236859194938	0.5071538985743727	0.5775657988708991	T	T	T
0.3814573951589197	0.6374542612352747	0.5737252859219290	T	T	T
0.1906703002254842	0.3592170350456256	0.6104690952248658	T	T	T
0.1865318183453454	0.4930076117916555	0.5844720244907601	T	T	T
0.1920669810766164	0.6254536400955588	0.5554330118899764	T	T	T
0.9899845654463144	0.4494046273858377	0.7995057361169362	T	T	T
0.9867026256698888	0.6333861251160121	0.7888966455739262	T	T	T
0.1325155462279665	0.5655357288763807	0.2231885133598077	T	T	T
0.1810598362837950	0.5433659118481570	0.4027237231117634	T	T	T
0.2946322161419797	0.5467297697777928	0.5051923794882356	T	T	T
0.4066266689889046	0.5724793469749297	0.4073714372083134	T	T	T
0.3939173553880433	0.5686190463707521	0.2117036764691292	T	T	T
0.2643207822609742	0.5590445509143102	0.2512304461139450	T	T	T
0.1358737183961908	0.3272477949344664	0.2614402458683398	T	T	T
0.2030449809285342	0.3692945397576919	0.4168617818030383	T	T	T
0.3097866616485361	0.3478555154617817	0.5267937651735076	T	T	T
0.4057479066371421	0.3323341610655638	0.3912749226385348	T	T	T
0.3936887536758524	0.3480546000364736	0.1947952155215493	T	T	T
0.2677218601928939	0.3408046664468393	0.2492129737116451	T	T	T
0.1897718359039277	0.4489949459037993	0.2600214369156940	T	T	T
0.4092212325489367	0.4541566183836609	0.3141362110674256	T	T	T
0.0637342891885632	0.6212079706724059	0.0742108861620092	T	T	T
0.0815306527004424	0.4897467101142036	0.0754758030078792	T	T	T
0.1204917658725624	0.3619159116769007	0.0716012065490410	T	T	T
0.3088549409495934	0.6391405942073947	0.1073481702928898	T	T	T
0.3167008434184370	0.5047754082544975	0.0860088805108065	T	T	T
0.2993078286722702	0.3728409852511178	0.0599332585696788	T	T	T
0.5094983901636004	0.5401309636459023	0.2914718973450680	T	T	T
0.5098626690223497	0.3677789855620396	0.2790538379825017	T	T	T
0.4335588082811715	0.7490702929171417	0.6463622653056362	T	T	T
0.1783238496760698	0.7486289668664692	0.6208870130927999	T	T	T
0.2841683168796758	0.7493231831866928	0.0026567371645930	T	T	T
0.0893669307529369	0.7489576078205544	0.0449050434730956	T	T	T
0.0636492031947772	0.2509032930265186	0.1401687720821280	T	T	T
0.3172389691881040	0.2495764882868760	0.1237846951570721	T	T	T
0.2189447759726685	0.2502260070666966	0.5049756723711556	T	T	T
0.3999325741594059	0.2500534585017087	0.5450280745209366	T	T	T
0.5522965992041171	0.2489343470572019	0.3474369443867394	T	T	T
0.8071173831533076	0.2495661816003786	0.3459126602423912	T	T	T
0.7257872103821903	0.2476014745985854	0.9411929930597550	T	T	T
0.8895790130751698	0.2490197891440545	0.9451705801502209	T	T	T
0.9474685195600343	0.7525678374161350	0.8583953523488311	T	T	T
0.6849342465840842	0.7504026394940183	0.8496343621186336	T	T	T
0.7745270746120234	0.7482148670281799	0.4420333220228040	T	T	T
0.6086765504083174	0.7500440071491417	0.4465544775000611	T	T	T
0.9380194142926800	0.5206414073686479	0.4782703556654210	T	T	T

Structure files (CONTCAR) involved in this work:

0.8192215733441631	0.3329800540010127	0.3218946494040232	T	T	T
0.8016328661633680	0.6359835585072534	0.6924241938498731	T	T	T
0.9298897481468112	0.3869037114930537	0.4455497540312792	T	T	T
0.8708453565880550	0.5577326427621920	0.5541093031821421	T	T	T
0.9937615727693281	0.5650153862858865	0.4623374890284120	T	T	T
0.0036648649321862	0.3433346002247243	0.5148043522073910	T	T	T
0.0092279607536573	0.3603347324343327	0.5922575935251048	T	T	T
0.0504189473403131	0.3523840854447262	0.4739419722191292	T	T	T
0.9930732674756610	0.2890344611859687	0.5137993038782581	T	T	T
0.9906307876547302	0.4984142410500288	0.6559927193337849	T	T	T
0.9824117453731533	0.4855456558037076	0.6047676880703260	T	T	T
0.0105363588556413	0.5611230780462158	0.3845193839144175	T	T	T
0.9801826869414033	0.6180427527656240	0.4760284344129235	T	T	T
0.0356512426822028	0.5525724323241711	0.5126782539717856	T	T	T

Figure S15(b) Zn-CH₃+O_M-CH₃+H₂

Si O Al Zn C H

1.0000000000000000

20.0219999999999985 0.0000000000000000 0.0000000000000000

0.0000000000000000 19.8990000000000009 0.0000000000000000

0.0000000000000000 0.0000000000000000 13.3829999999999991

94 193 2 2 2 8

Selective dynamics

Direct

0.4223603188870387	0.0582287041406425	0.6472142839369737	T	T	T
0.3028041511444481	0.0316034894008291	0.7886625568688632	T	T	T
0.2813667171212555	0.0548189033077563	0.0155471266287245	T	T	T
0.1215006230722699	0.0657585574594103	0.0112488139945335	T	T	T
0.0671807568288442	0.0317853942764541	0.7985379519930935	T	T	T
0.1795631690474724	0.0677679035670253	0.6626783203754579	T	T	T
0.4178177766125133	0.8270155425745083	0.6722032764325280	T	T	T
0.2963971124191556	0.8733541580529475	0.7950763567563494	T	T	T
0.2665190612181439	0.8293082607810963	0.0149794852366448	T	T	T
0.1085375474693565	0.8256625419875518	0.0125873171861897	T	T	T
0.0659709990522032	0.8744532407936043	0.7968331518198731	T	T	T
0.1755134366197643	0.8273200873922121	0.6562889107486268	T	T	T
0.0743603168315152	0.9431830242961355	0.1476552592303657	T	T	T
0.1948696924157994	0.9700072824732182	0.2873116894572813	T	T	T
0.2151262043809749	0.9451394579596493	0.5144493805700673	T	T	T
0.3754236212395284	0.9332498747004697	0.5139199392970731	T	T	T
0.4313831607874279	0.9660993202443320	0.3019483859334698	T	T	T
0.3189262900465681	0.9326515275383630	0.1630628547789222	T	T	T
0.0807412790510698	0.1738495521028572	0.1660573225192666	T	T	T
0.2005217915577273	0.1283632460047110	0.2941324406851498	T	T	T
0.2312230740897130	0.1694665152771215	0.5124196149810331	T	T	T
0.3878310040845248	0.1727566159844017	0.5074001898987825	T	T	T
0.4343576554398965	0.1238250140334093	0.2942330670415885	T	T	T
0.3216687123431619	0.1721492812638622	0.1592358732644759	T	T	T
0.5764114483397098	0.5550967038697969	0.3524425642679683	T	T	T
0.6899384558648715	0.5238387674482529	0.1985653401415058	T	T	T
0.7147994778212156	0.5646787315139437	0.9840385384992529	T	T	T
0.8741092172103317	0.5679729090827867	0.9837002751630916	T	T	T
0.9256373283357303	0.5286880378178369	0.1926104667841163	T	T	T
0.8108861711139012	0.5520895532536780	0.3343751076837245	T	T	T

Structure files (CONTCAR) involved in this work:

0.5734921903419358	0.3261830162975397	0.3241515651482189	T	T	T
0.6932495055463277	0.3697342923068575	0.1851845883797959	T	T	T
0.7325661261795724	0.3263492772457083	0.9705770170758178	T	T	T
0.8873416387686388	0.3251152855890024	0.9853379173631349	T	T	T
0.9383420255541137	0.3729577697919053	0.1916721288746490	T	T	T
0.9212575207237698	0.4433554078794186	0.8524916053076923	T	T	T
0.8025017080750428	0.4716971846837018	0.7116486298767998	T	T	T
0.7757315340081976	0.4363400513089368	0.4862930824292769	T	T	T
0.6167283688715103	0.4278900816076684	0.4833542104372168	T	T	T
0.5688910182077158	0.4676313714416099	0.6955192393029047	T	T	T
0.6781916710840020	0.4462976655862609	0.8480979677515181	T	T	T
0.9219846671895178	0.6754694997852343	0.8316494362104364	T	T	T
0.7696229588479047	0.6678737326209788	0.4621326774426431	T	T	T
0.6149685570139852	0.6730670181407986	0.4860386645013000	T	T	T
0.5621291141278292	0.6254748657425272	0.6942831418725421	T	T	T
0.6778795008772369	0.6700550366296809	0.8202993932141268	T	T	T
0.5772632307355124	0.9453640398013740	0.3566012761433786	T	T	T
0.6975838240851644	0.9716202065503754	0.2097463433709873	T	T	T
0.7187319022693858	0.9330515278368817	0.9910901495464053	T	T	T
0.8781473540332695	0.9330091860836683	0.9934769355274903	T	T	T
0.9292543947673999	0.9717391786624777	0.2032783360802727	T	T	T
0.8204558734104639	0.9457917134544300	0.3531880157595784	T	T	T
0.5766766493995076	0.1707870811962483	0.3283854994544397	T	T	T
0.6986919511941913	0.1287571115274837	0.1923995132750762	T	T	T
0.7333271217174780	0.1706827265188053	0.9728176309168448	T	T	T
0.8880220192089341	0.1727216636459755	0.9828992069346006	T	T	T
0.9354920906984909	0.1293569082761462	0.1966351900077837	T	T	T
0.8196150922433014	0.1704052633187900	0.3310368738431830	T	T	T
0.9228699949563076	0.0534445359007142	0.8552025703782020	T	T	T
0.8017391793785624	0.0251883835835368	0.7113887196934831	T	T	T
0.7802601508551593	0.0648855721166317	0.4919278723415040	T	T	T
0.6198635073813643	0.0704225711697391	0.4894733833705434	T	T	T
0.5683218210392348	0.0305802672444252	0.6986940654635994	T	T	T
0.6775094790772794	0.0503284318179846	0.8514752013935666	T	T	T
0.9229462331301579	0.8283827583323925	0.8385997016781698	T	T	T
0.8044570355859316	0.8681412295623335	0.6948477931591794	T	T	T
0.7710506053520796	0.8261775832799968	0.4769281615613646	T	T	T
0.6158231989331161	0.8263775770078265	0.4883873752904158	T	T	T
0.5643294285693851	0.8732668373817559	0.6968237003052479	T	T	T
0.6800610192913230	0.8296541500328171	0.8288871656077158	T	T	T
0.4221426110267187	0.4410422337725637	0.6459264455300364	T	T	T
0.3039522439122468	0.4675776654558101	0.7890944435567986	T	T	T
0.2794421927971497	0.4466364292647748	0.0146871280773912	T	T	T
0.1218905883967969	0.4349556964076739	0.0112468953873818	T	T	T
0.0657032677733455	0.4664571954166910	0.7998818555819691	T	T	T
0.1794001488286180	0.4318630620195640	0.6641027933215100	T	T	T
0.4156492785542134	0.6717766181778629	0.6723377520808307	T	T	T
0.2967155233410326	0.6256912959792134	0.7964588611847351	T	T	T
0.2667357265217482	0.6706396103907165	0.0165047088995275	T	T	T
0.1099761495502830	0.6735432756280704	0.0134333017489822	T	T	T
0.0675069968962232	0.6250227956648176	0.7986471505003030	T	T	T
0.1762159603570565	0.6711818742633169	0.6554166441970815	T	T	T
0.0715002152287978	0.5561125552863937	0.1468947532191311	T	T	T

Structure files (CONTCAR) involved in this work:

0.1923116415286551	0.5297323676125254	0.2868872672182510	T	T	T
0.2139643110378892	0.5533041525300234	0.5135761643095919	T	T	T
0.3733273040580058	0.5661945635626719	0.5149096006326471	T	T	T
0.4302532059404681	0.5333343738239268	0.3045488061612866	T	T	T
0.3176783596107679	0.5673699028296231	0.1636664110835064	T	T	T
0.0834241888032052	0.3278335171133721	0.1644742943778446	T	T	T
0.1993904042987456	0.3717196386790547	0.2965297101147319	T	T	T
0.2307698404072826	0.3304922018519205	0.5136705409867736	T	T	T
0.3868587928197139	0.3267300643340563	0.5053858096042171	T	T	T
0.4315904496469013	0.3755526345106096	0.2927590604332419	T	T	T
0.3181460832890030	0.3289227668817095	0.1586235435489508	T	T	T
0.3598381988520086	0.0689298976121456	0.7228192516550757	T	T	T
0.3153247509856237	0.0468988657694159	0.9060164563179949	T	T	T
0.2008105106782198	0.0501196773091448	0.0064690809338279	T	T	T
0.0912080118768755	0.0697856449995824	0.8994697974393285	T	T	T
0.1029935144240695	0.0662113258672507	0.7023721074069309	T	T	T
0.2294015800636342	0.0598680166267988	0.7582951786155800	T	T	T
0.3607519088023633	0.8305274906743721	0.7583724406081580	T	T	T
0.2904851091778317	0.8686624144285958	0.9152184738373484	T	T	T
0.1871504029005976	0.8414090476347148	0.0317891751064356	T	T	T
0.0920075497483581	0.8340973942964793	0.8947626146812693	T	T	T
0.1003284570151747	0.8410487696740160	0.6983262330922246	T	T	T
0.2287497586085528	0.8433363582111276	0.7451695417823779	T	T	T
0.3065015871368947	0.9515213126392008	0.7634602030960639	T	T	T
0.0882592176049004	0.9527736845443568	0.8054739582736079	T	T	T
0.4326319754302373	0.1254766162403244	0.5798318037212888	T	T	T
0.4107173010729919	0.9947374032586445	0.5731990116454535	T	T	T
0.3910128836741554	0.8627746340734855	0.5705683628482677	T	T	T
0.1929787075406881	0.1399415412599294	0.6096537936156894	T	T	T
0.1909564464713536	0.0063237677655306	0.5851679253324841	T	T	T
0.1898326900772747	0.8735545280106884	0.5588894922447571	T	T	T
0.9870596037554109	0.0392859940659052	0.7840974946539810	T	T	T
0.9852381793322423	0.8687246153967474	0.7876474963017513	T	T	T
0.1378420891930380	0.9327677564237995	0.2214258803261243	T	T	T
0.1821934026216640	0.9551903582043726	0.4047062548307515	T	T	T
0.2957882176088430	0.9460922740767171	0.5070724097469330	T	T	T
0.4062223595075065	0.9281429840176276	0.4024598758467023	T	T	T
0.3949641472348785	0.9335361298735577	0.2048916666635871	T	T	T
0.2680508761755863	0.9408909857874125	0.2574527793425150	T	T	T
0.1396847863393108	0.1724200675366746	0.2491884927521899	T	T	T
0.1989604023871450	0.1343086732790873	0.4144850545460443	T	T	T
0.3100072556624662	0.1499777934985616	0.5174724332391135	T	T	T
0.4119791442818865	0.1664603356660255	0.3922449176853665	T	T	T
0.3973707001891486	0.1551345567807606	0.1962467246460121	T	T	T
0.2712955950957088	0.1570006239795437	0.2524435532271026	T	T	T
0.1914495205034666	0.0501057191056407	0.2620021630950380	T	T	T
0.4127506138292734	0.0457013150820156	0.3093781046279262	T	T	T
0.0638860321780973	0.8759987296714786	0.0802554113841550	T	T	T
0.0844766308888214	0.0064223191479999	0.0729374083909056	T	T	T
0.1068208799590316	0.1375047313900076	0.0644766961320860	T	T	T
0.3067844173557998	0.8605017967012439	0.1092230455874106	T	T	T
0.3081945835984060	0.9942310634504272	0.0854563174408550	T	T	T
0.3026733443853934	0.1270575364077541	0.0622618477440707	T	T	T

Structure files (CONTCAR) involved in this work:

0.5111334256183560	0.9552776450054205	0.2881713417821072	T	T	T
0.5147851880059521	0.1290987937310117	0.2786137706811503	T	T	T
0.6400414987277104	0.5583816581481158	0.2784033350391754	T	T	T
0.6938263584830094	0.5719103668583569	0.1008629452625778	T	T	T
0.7948603570833763	0.5531124062216090	0.9721996534820032	T	T	T
0.8942337440302317	0.5723537391616600	0.1013480818840362	T	T	T
0.8878744794288510	0.5466045974911067	0.2980029854168433	T	T	T
0.7639092231008822	0.5204633024645797	0.2498648747842618	T	T	T
0.6374342260308163	0.3304915161735840	0.2515686098479836	T	T	T
0.6923097497927452	0.3359245473712479	0.0743023091721362	T	T	T
0.8099832842799671	0.3504437352530213	0.9835053044520320	T	T	T
0.9150361717133070	0.3257076953458505	0.0988805172177639	T	T	T
0.9041951604698554	0.3484237053278605	0.2939244365379427	T	T	T
0.7652889165616740	0.3658479344666727	0.2364418312612536	T	T	T
0.6678610722328030	0.4478690229314305	0.1721339901594117	T	T	T
0.9170304342847098	0.4501344031929458	0.1647765428512045	T	T	T
0.5713965620142045	0.6258812541128744	0.4119663107220202	T	T	T
0.5834163219061291	0.4940878353801300	0.4329817151229753	T	T	T
0.5886146657045992	0.3596702232359615	0.4332254918235710	T	T	T
0.7941413634284751	0.6300189221018931	0.3602284753378966	T	T	T
0.8015113598249561	0.5112240082722879	0.4430264288420067	T	T	T
0.8206801342274385	0.3784193394353944	0.4359715570993992	T	T	T
0.0035457024176796	0.5475776887767185	0.2119774166038882	T	T	T
0.0193471376281996	0.3705713336474970	0.2025529064557630	T	T	T
0.8564388346010554	0.4326534231207214	0.7802313464375594	T	T	T
0.7943459473241928	0.4339031188941075	0.6043066209208491	T	T	T
0.6972932823403133	0.4303109116616364	0.4643501362534158	T	T	T
0.6006550003824566	0.4262063950307167	0.6017359044587963	T	T	T
0.6048243454737513	0.4429683007327739	0.7976260911919025	T	T	T
0.7306616489165982	0.4759692398284626	0.7652565105225388	T	T	T
0.8664682358725423	0.6774678227597565	0.7460664291672326	T	T	T
0.8181250112781562	0.6405166929477744	0.5531703808948272	T	T	T
0.6926941034978999	0.6475283704888232	0.4872631466090512	T	T	T
0.5847200165336971	0.6691600540923738	0.5976630949977892	T	T	T
0.5996258735362292	0.6546651877409799	0.7925808076446677	T	T	T
0.7255479287694475	0.6452039735819030	0.7303833057247687	T	T	T
0.8314587559780054	0.5466719155457580	0.6845589812386330	T	T	T
0.5816759893118494	0.5471445312996754	0.6757146230367572	T	T	T
0.9322415597233729	0.3748290952422851	0.9159349669026680	T	T	T
0.9132394531306408	0.5066090416353122	0.9283688419776301	T	T	T
0.8946495761952581	0.6389317415571469	0.9331654351376235	T	T	T
0.6991424864049772	0.3713548305499199	0.8823959764636705	T	T	T
0.6767590024697081	0.4981798874394737	0.9415119054270716	T	T	T
0.6936143438910380	0.6322416913725175	0.9257305418557507	T	T	T
0.4900696995370925	0.4518965025442048	0.7095523664373707	T	T	T
0.4818651209364213	0.6317074438496809	0.7094762693535519	T	T	T
0.6415474852080928	0.9409910693346307	0.2838922068857705	T	T	T
0.6990794573985618	0.9267772200846974	0.1083165587805137	T	T	T
0.7986580542952321	0.9446139520544903	0.9768174163140048	T	T	T
0.8960250460054994	0.9296401181913446	0.1115242988605059	T	T	T
0.8957695823091680	0.9503352051200642	0.3090219584064361	T	T	T
0.7698381634646392	0.9670489128304993	0.2639284956021661	T	T	T
0.6408770498209091	0.1666524747491468	0.2555449730047468	T	T	T

Structure files (CONTCAR) involved in this work:

0.6993418488920928	0.1624666710817263	0.0820833390500672	T	T	T
0.8109904154851435	0.1465115948171780	0.9786795947779595	T	T	T
0.9141849042439600	0.1708168455079318	0.0972003402293281	T	T	T
0.8967834831894940	0.1587064866646477	0.2934807414088215	T	T	T
0.7708376658563171	0.1364671824491624	0.2461286838434828	T	T	T
0.6804749246751843	0.0492590281712142	0.1827905760832533	T	T	T
0.9171616185656170	0.0507399701824094	0.1798330036067846	T	T	T
0.5710558038865421	0.8751665806981493	0.4183341466859969	T	T	T
0.5827402921312285	0.0071133086146746	0.4358860260546598	T	T	T
0.5949292208153398	0.1399655308156638	0.4377903781156795	T	T	T
0.8078516931185505	0.8690174551226431	0.3901509687357015	T	T	T
0.8120377876928978	0.9955204248756360	0.4483143940679587	T	T	T
0.8105615088782484	0.1300727473682107	0.4364501546133523	T	T	T
0.0081894809022908	0.9549450644316743	0.2147293916983319	T	T	T
0.0157044996895473	0.1367706062177244	0.2131945685317160	T	T	T
0.8567695154457992	0.0573976870112290	0.7858799112379947	T	T	T
0.7990194626165913	0.0695566176782286	0.6098196191307125	T	T	T
0.6997828851486064	0.0616949251320855	0.4759138041549139	T	T	T
0.5998593285541653	0.0738161065905983	0.6068582796623100	T	T	T
0.6030416774295908	0.0513701963288270	0.8036894360644371	T	T	T
0.7290208220568815	0.0264384916872635	0.7646322526424990	T	T	T
0.8600766931427328	0.8311390546807127	0.7627607321093386	T	T	T
0.8076903557067199	0.8347056043890633	0.5842741304061922	T	T	T
0.6936150549363282	0.8506713146005372	0.4858645852962864	T	T	T
0.5884076854868082	0.8279870866727584	0.6023442227246580	T	T	T
0.6039003442833502	0.8492221846151693	0.7967105526429125	T	T	T
0.7304336968044385	0.8574341744414099	0.7422365605375706	T	T	T
0.8212321524359476	0.9477205068387498	0.6863027444905280	T	T	T
0.5806316867848099	0.9515596540671175	0.6733495668523615	T	T	T
0.9334430553452938	0.1249878016267410	0.9118266903770966	T	T	T
0.9175776596922568	0.9945636438691919	0.9394151827087711	T	T	T
0.9019723899669527	0.8622627313223050	0.9445987238090052	T	T	T
0.6945488918916830	0.1253873840121193	0.8907152883070928	T	T	T
0.6795189268786246	-0.0028004511645487	0.9437327664912993	T	T	T
0.6970433709782186	0.8637746096063503	0.9361509533784351	T	T	T
0.4892848736489009	0.0458934496945614	0.7124822312580570	T	T	T
0.4846306918131553	0.8635981140679578	0.7146212595797602	T	T	T
0.3603814395091101	0.4293937175559987	0.7228734859292529	T	T	T
0.3159974152345587	0.4517117483746497	0.9064956065372803	T	T	T
0.1994869696715452	0.4573142422243783	0.0008991323421939	T	T	T
0.0881601329044046	0.4286129972218682	0.9016787090785380	T	T	T
0.1028590209885455	0.4325907632432466	0.7044298134707881	T	T	T
0.2298717966549329	0.4409951730531509	0.7584968003045532	T	T	T
0.3609167795781602	0.6697168043880686	0.7621886632867642	T	T	T
0.2881093109057581	0.6302766331578210	0.9162076900115314	T	T	T
0.1878927277528497	0.6582605199387542	0.0384156113625037	T	T	T
0.0976225903529735	0.6645654626112117	0.8944002539854348	T	T	T
0.1012232687426298	0.6555955587081755	0.6974445384929532	T	T	T
0.2295357695612756	0.6541581123382483	0.7434612856614210	T	T	T
0.3088556366801628	0.5477029275201777	0.7650005403935983	T	T	T
0.0856878057576307	0.5455644352932835	0.8074693325826863	T	T	T
0.4322819333819579	0.3755814540599962	0.5747557681266897	T	T	T
0.4098918387619110	0.5062981171397497	0.5758015044360476	T	T	T

Structure files (CONTCAR) involved in this work:

0.3840939578716322	0.6372375036353650	0.5724756126370161	T	T	T
0.1928800347126633	0.3596053268985771	0.6116530129277478	T	T	T
0.1884033608511545	0.4933046792434548	0.5856575080228492	T	T	T
0.1903291155520883	0.6256717367320354	0.5569841237146114	T	T	T
0.9858837400092308	0.4569922217963320	0.7816034272573646	T	T	T
0.9872329953192783	0.6337120644934079	0.7907373313228014	T	T	T
0.1332833273191064	0.5659988552837325	0.2238265025680420	T	T	T
0.1795484686654499	0.5435221429779834	0.4046783561626059	T	T	T
0.2944300197751893	0.5496736174218582	0.5039578778608327	T	T	T
0.4066818725124153	0.5723739463299772	0.4050765269047040	T	T	T
0.3927439961224262	0.5650856234345074	0.2083325400842254	T	T	T
0.2643241309255012	0.5606284750454422	0.2553353973216926	T	T	T
0.1378297389811053	0.3275685633705657	0.2543168197304741	T	T	T
0.1981496427213363	0.3674130709732449	0.4171112580004943	T	T	T
0.3094616860403588	0.3502202973155036	0.5183045841224195	T	T	T
0.4085484621067817	0.3311087247964205	0.3887447944633970	T	T	T
0.3933208216495169	0.3500461219420991	0.1925169766824577	T	T	T
0.2694283469701291	0.3418943899534922	0.2544933027337259	T	T	T
0.1905942950753587	0.4496001876562708	0.2616157469179124	T	T	T
0.4129599014725005	0.4537073733214745	0.3154231314149419	T	T	T
0.0635426544115146	0.6223807038235796	0.0770428001301098	T	T	T
0.0817038073941221	0.4911368028815023	0.0754601658638571	T	T	T
0.1160670266203189	0.3621903783913334	0.0653222182259770	T	T	T
0.3088319329148574	0.6396707832245508	0.1091303196893720	T	T	T
0.3080663157298835	0.5056146600965188	0.0860002581208949	T	T	T
0.2947797830297399	0.3733039649644285	0.0629692045874624	T	T	T
0.5095874290828696	0.5442835341631437	0.2864275932796065	T	T	T
0.5111153441651718	0.3663629092192344	0.2734248265701889	T	T	T
0.4339772135914676	0.7490795165382070	0.6462964062248379	T	T	T
0.1821813908557381	0.7492740069295084	0.6222558176970638	T	T	T
0.2833325262992586	0.7498749163530340	0.0045904212068521	T	T	T
0.0906991499927840	0.7494139841377916	0.0462699822969778	T	T	T
0.0628577816964723	0.2511755739162039	0.1382094551962032	T	T	T
0.3159109906198845	0.2504574588390094	0.1262357419442602	T	T	T
0.2207570010154347	0.2500533703041886	0.5077350630238180	T	T	T
0.3967358103501288	0.2500740586272512	0.5433903237859076	T	T	T
0.5540029289993338	0.2483129207514196	0.3434099433177903	T	T	T
0.8034702392594693	0.2479911026432691	0.3470591622661611	T	T	T
0.7287389569539608	0.2483059983096067	0.9360654261499980	T	T	T
0.8933985831944236	0.2493142080404071	0.9414269077872075	T	T	T
0.9452532851993597	0.7514317788375547	0.8610180392545304	T	T	T
0.6875765428481044	0.7495919072831736	0.8416886030432856	T	T	T
0.7763430053586048	0.7476489715327371	0.4447799220138031	T	T	T
0.6105227522564516	0.7499306845322806	0.4462484555704738	T	T	T
0.9363573253781463	0.4856902975704124	0.4961990113181960	T	T	T
0.8200414550432092	0.3307413731132465	0.3214493476322451	T	T	T
0.8049767187152125	0.6335022223074260	0.6866285923528218	T	T	T
0.9236468476073592	0.3828237541251865	0.4733070946535793	T	T	T
0.8766684777543735	0.5514295329162636	0.5478781317957502	T	T	T
0.0050258120754576	0.5023548816534668	0.4739268222064811	T	T	T
0.9892743215356660	0.3167510523650893	0.5170076652689980	T	T	T
1.0051991016892075	0.3267327099815467	0.5941502450561524	T	T	T
0.0331376548630755	0.3193854335936116	0.4676433407963849	T	T	T

Structure files (CONTCAR) involved in this work:

0.9679244084066075	0.2659948056889486	0.5121321991853667	T	T	T
-0.0324401678511664	0.6137648847338786	0.6081382644341651	T	T	T
-0.0430937583187714	0.6332894254322972	0.5619171785944898	T	T	T
0.0238668074202609	0.4681601411089722	0.4156488284736212	T	T	T
1.0092559549581386	0.5537414072999149	0.4444392815447016	T	T	T
0.0367536150932544	0.4968236096664222	0.5406544681962130	T	T	T

Figure S15(b) TS3

Si O Al Zn C H

1.0000000000000000

20.0219999999999985 0.0000000000000000 0.0000000000000000

0.0000000000000000 19.8990000000000009 0.0000000000000000

0.0000000000000000 0.0000000000000000 13.3829999999999991

94 193 2 2 2 6

Selective dynamics

Direct

0.4225355430732007	0.0581796653437728	0.6469034727249174	T	T	T
0.3028726188252389	0.0315206305370057	0.7881135724486681	T	T	T
0.2816754139062738	0.0544142440061262	0.0152115858785257	T	T	T
0.1218173509937294	0.0653544848608078	0.0111376240062004	T	T	T
0.0672825657903222	0.0319585544545968	0.7984060610805076	T	T	T
0.1795310850453631	0.0678273160193240	0.6623526826915375	T	T	T
0.4179713407717876	0.8272236729961555	0.6726605783362628	T	T	T
0.2965513729712885	0.8733190076269394	0.7950362222623791	T	T	T
0.2667143074233487	0.8292971490803794	0.0150171459960507	T	T	T
0.1089623892701213	0.8254806078580179	0.0124897222501349	T	T	T
0.0665326657271486	0.8745134365901804	0.7967421547368621	T	T	T
0.1757953271733900	0.8271786948864901	0.6557877367364363	T	T	T
0.0746103696857746	0.9428107045087758	0.1474752676748076	T	T	T
0.1952388203826295	0.9699719558283001	0.2869265256431861	T	T	T
0.2151783541878863	0.9452456980408114	0.5141741802029037	T	T	T
0.3753991249175715	0.9331411246368346	0.5141344298274340	T	T	T
0.4315810284024929	0.9656370228120128	0.3025762691904947	T	T	T
0.3194699217915449	0.9324839137992976	0.1628933467687558	T	T	T
0.0812843308685123	0.1734379291884021	0.1657927038751754	T	T	T
0.2010236703971984	0.1283781426627776	0.2938183353371928	T	T	T
0.2315538701753572	0.1696464221262740	0.5123581119230478	T	T	T
0.3882769426592046	0.1728726111709122	0.5071200536828752	T	T	T
0.4345325362719591	0.1232503885357414	0.2943276245799605	T	T	T
0.3222753393045700	0.1717218130035434	0.1585897046372063	T	T	T
0.5769818725613137	0.5541835874672303	0.3540506732940865	T	T	T
0.6901489538401229	0.5246367159012166	0.1984617883880762	T	T	T
0.7131836671460443	0.5647882121573242	0.9853964734843423	T	T	T
0.8728772572369602	0.5686130808181502	0.9843417598655604	T	T	T
0.9258279382460876	0.5296366269662784	0.1915629854517514	T	T	T
0.8107717238397443	0.5514459191183247	0.3344335303885871	T	T	T
0.5731842881223629	0.3264109136396705	0.3262702101312726	T	T	T
0.6947842971837435	0.3698793294582706	0.1892549559233431	T	T	T
0.7307456980168939	0.3255783384496705	0.9747687147248963	T	T	T
0.8852435160796150	0.3253877748669520	0.9902960877390330	T	T	T
0.9391596751473871	0.3754014090897267	0.1910209536700752	T	T	T
0.9198471591269287	0.4429038825207511	0.8546797566282962	T	T	T
0.8002130504059937	0.4721131139637297	0.7157299875032349	T	T	T
0.7742243957763891	0.4355587242458507	0.4882267544532520	T	T	T

Structure files (CONTCAR) involved in this work:

0.6159823248949109	0.4266608809023741	0.4852953791691384	T	T	T
0.5690346041739460	0.4675460835845374	0.6975837492827023	T	T	T
0.6760052576324157	0.4455553409603193	0.8529740111742821	T	T	T
0.9210594934800713	0.6759210651957652	0.8313821951289959	T	T	T
0.7699349952045637	0.6675015174207453	0.4627388737875003	T	T	T
0.6149579888098273	0.6725970020804906	0.4861945115052013	T	T	T
0.5619072363045339	0.6254496018666006	0.6950751019593785	T	T	T
0.6757604181486515	0.6715108610419527	0.8215316980705561	T	T	T
0.5774954035992775	0.9451931435732989	0.3576235922321256	T	T	T
0.6978921404391700	0.9715365239959862	0.2111452400649013	T	T	T
0.7190629165250015	0.9339997987526624	0.9919219151771864	T	T	T
0.8784240428464117	0.9332237452068231	0.9938153996463805	T	T	T
0.9295804519498314	0.9706929261682958	0.2035309263697285	T	T	T
0.8209213140726271	0.9455616951283740	0.3540486666414976	T	T	T
0.5766905233108029	0.1707720844005171	0.3285255435698917	T	T	T
0.6990159457285657	0.1290129283092707	0.1934903301944956	T	T	T
0.7331107574960898	0.1702366958167902	0.9733106180474116	T	T	T
0.8877554956219628	0.1726855655896737	0.9842169212727905	T	T	T
0.9361755577465257	0.1280073499296282	0.1969470828414384	T	T	T
0.8211603360980919	0.1707447282764796	0.3315076546577968	T	T	T
0.9229277238865625	0.0538106815650415	0.8558216000176757	T	T	T
0.8017923825632689	0.0251053198098873	0.7118462203915257	T	T	T
0.7804786261121672	0.0652053957937521	0.4922628128400307	T	T	T
0.6200809311949647	0.0705231462460491	0.4898220858170540	T	T	T
0.5684495651832311	0.0307690663648179	0.6986027564143850	T	T	T
0.6775478275245842	0.0505754876685632	0.8516619374838200	T	T	T
0.9233875116009994	0.8283674160210583	0.8391802610849695	T	T	T
0.8045409419519771	0.8678377971136703	0.6957353789606818	T	T	T
0.7714026517592554	0.8257101823675175	0.4778558928483491	T	T	T
0.6160052726034057	0.8259687354189336	0.4891807588319689	T	T	T
0.5644568875575497	0.8737493590730219	0.6968065704070675	T	T	T
0.6795899385914324	0.8303457513537246	0.8302976221444797	T	T	T
0.4228983055220865	0.4413054623801616	0.6447420085581137	T	T	T
0.3042473868993356	0.4676320245794767	0.7877314331298397	T	T	T
0.2804799176832808	0.4464197379094398	0.0136211520126818	T	T	T
0.1227496660671553	0.4352543398481281	0.0112040761912059	T	T	T
0.0650443373268472	0.4659522339508743	0.7995236103840004	T	T	T
0.1796029927570777	0.4319240271111391	0.6637371573019054	T	T	T
0.4159389533919925	0.6720437197543605	0.6714251233046874	T	T	T
0.2966491321649894	0.6257788073067003	0.7952239575194675	T	T	T
0.2670474983911303	0.6706672974427508	0.0151278245867401	T	T	T
0.1100063667444003	0.6732334827151346	0.0116378103398833	T	T	T
0.0659971108579487	0.6249080456828850	0.7965311542248200	T	T	T
0.1760152506005336	0.6710188963303402	0.6547398758973266	T	T	T
0.0720464517765818	0.5561528891891242	0.1470945603330113	T	T	T
0.1938204564636686	0.5294163521863576	0.2857761264874858	T	T	T
0.2157490200565201	0.5533473740134814	0.5136530233637157	T	T	T
0.3750552756448629	0.5664981269408639	0.5140534450824473	T	T	T
0.4312496553053022	0.5334104588789795	0.3032182140094817	T	T	T
0.3190870761570428	0.5672689992020561	0.1615780210421326	T	T	T
0.0843486713854582	0.3273808389463874	0.1632154857169551	T	T	T
0.2005761381777133	0.3713218036683249	0.2951041523536602	T	T	T
0.2316358732970918	0.3305391356217457	0.5131148077140162	T	T	T

Structure files (CONTCAR) involved in this work:

0.3877922459832427	0.3268274747031961	0.5044827149927571	T	T	T
0.4322636243018673	0.3756684186335996	0.2914342014303505	T	T	T
0.3192670461208620	0.3285436000729220	0.1568019061142017	T	T	T
0.3598658286950754	0.0688768816720742	0.7222431744342860	T	T	T
0.3153916539879288	0.0467761654753581	0.9054694601345255	T	T	T
0.2010875628179938	0.0494095569034375	0.0065760841322065	T	T	T
0.0916051342169615	0.0697239233552758	0.8993743196775381	T	T	T
0.1029821388266557	0.0665099045198040	0.7022267390129118	T	T	T
0.2294785413799235	0.0598251122284406	0.7577961393545050	T	T	T
0.3612253456581315	0.8305219209166105	0.7594063077733360	T	T	T
0.2898915497960142	0.8690303754470281	0.9151599274204240	T	T	T
0.1874414441467436	0.8410679012606840	0.0331636888341766	T	T	T
0.0933339356938055	0.8346526333911135	0.8945950979291092	T	T	T
0.1007284939848082	0.8411286794305162	0.6981262683657496	T	T	T
0.2293031820292063	0.8430238506871065	0.7443596560159494	T	T	T
0.3065681349991040	0.9514342762278741	0.7630257291934939	T	T	T
0.0883444596599392	0.9529847279748602	0.8048471238819226	T	T	T
0.4329456634203408	0.1253588290187236	0.5793921024315827	T	T	T
0.4110750902013552	0.9946082195234555	0.5729650174149259	T	T	T
0.3903540692935737	0.8627419147401414	0.5713259196712630	T	T	T
0.1929794217260374	0.1399612127941396	0.6092250978652607	T	T	T
0.1906264947697972	0.0063899312446922	0.5847452055071658	T	T	T
0.1900393744535574	0.8735392789117268	0.5584257209902257	T	T	T
0.9871418034839149	0.0397866433570639	0.7847006733589413	T	T	T
0.9858418090940397	0.8684781414564077	0.7883197718614118	T	T	T
0.1382166014397747	0.9327720009893506	0.2210579399994605	T	T	T
0.1824358763795513	0.9552219754854451	0.4042778289477877	T	T	T
0.2958614674469383	0.9466260387622797	0.5071321740071690	T	T	T
0.4062023542669264	0.9273658689417311	0.4027055557387471	T	T	T
0.3953936055032436	0.9333507285343198	0.2051043306932392	T	T	T
0.2683736559361902	0.9408537427669654	0.2569456385675968	T	T	T
0.1400472574279834	0.1724338420280380	0.2491577771064230	T	T	T
0.1996168961145450	0.1344502374617624	0.4141640158113608	T	T	T
0.3103796937862516	0.1504778910868475	0.5180788934558129	T	T	T
0.4117729637413493	0.1662887859348058	0.3916976297056103	T	T	T
0.3977420605483045	0.1539452909192363	0.1957660052541618	T	T	T
0.2716236470002112	0.1572038309859328	0.2516952081910499	T	T	T
0.1918364045643465	0.0501120950629337	0.2617687316032918	T	T	T
0.4128880204791732	0.0452249176979805	0.3104395053536550	T	T	T
0.0640706806187117	0.8755929381217742	0.0801516209294159	T	T	T
0.0844255111632825	0.0061700235556949	0.0727353487915831	T	T	T
0.1074165555601392	0.1371925185018536	0.0642946198664072	T	T	T
0.3074389404118677	0.8603313243381771	0.1089442282027067	T	T	T
0.3088994543604291	0.9939774371543956	0.0850801510605204	T	T	T
0.3027965356240831	0.1267468368136120	0.0617588478361785	T	T	T
0.5113617991455992	0.9549630675962766	0.2891382844680735	T	T	T
0.5149866123355745	0.1285625838493230	0.2791402416626811	T	T	T
0.6414430080156269	0.5571537227034115	0.2816484529027151	T	T	T
0.6905334338563505	0.5734903782153487	0.1014195100689704	T	T	T
0.7934859528693941	0.5532745216969218	0.9758620605671112	T	T	T
0.8938380698686369	0.5742389359412792	0.1021345275507035	T	T	T
0.8882590318423176	0.5417967009089077	0.2993737616427034	T	T	T
0.7656214686907694	0.5240483200723208	0.2445566268965169	T	T	T

Structure files (CONTCAR) involved in this work:

0.6395766732887159	0.3322896984800264	0.2589374513189845	T	T	T
0.6919213833514968	0.3335363717011570	0.0800969791586292	T	T	T
0.8080058686622748	0.3504921197832170	0.9868217698737661	T	T	T
0.9108635283078691	0.3248316069965132	0.1059406608049189	T	T	T
0.9062994589149660	0.3593607818175282	0.2998833907789403	T	T	T
0.7676495997742053	0.3664021522691208	0.2384617813918999	T	T	T
0.6699717928437944	0.4479344578890919	0.1729387681998417	T	T	T
0.9194223836710805	0.4516531261056033	0.1584880377830721	T	T	T
0.5711056004259640	0.6253171333892271	0.4125622799446544	T	T	T
0.5834912700592408	0.4935188901723628	0.4351055095675415	T	T	T
0.5843379497389745	0.3592965054806346	0.4368169659224524	T	T	T
0.7971397378942353	0.6298156922589803	0.3620595092529146	T	T	T
0.7968454135037671	0.5105819341695722	0.4410872422792794	T	T	T
0.8222006578079193	0.3798096620151089	0.4400801610262160	T	T	T
0.0037020943534404	0.5485243404034722	0.2121321007072344	T	T	T
0.0196968566209330	0.3696748004817413	0.2006839587418029	T	T	T
0.8554411859260246	0.4319330061944346	0.7814360869878094	T	T	T
0.7883736159639061	0.4370486894616765	0.6073560577534894	T	T	T
0.6961098614138118	0.4256527550906643	0.4632649349804679	T	T	T
0.6016680026308843	0.4263806956406015	0.6042679860041437	T	T	T
0.6031629392233101	0.4426505372773508	0.8008571211338464	T	T	T
0.7293323235508246	0.4747169060871755	0.7720875630582839	T	T	T
0.8645025893998840	0.6795845337756874	0.7474636056217399	T	T	T
0.8161746078629420	0.6404711161506796	0.5568276453824793	T	T	T
0.6927181369629584	0.6471466803569194	0.4852414385481074	T	T	T
0.5852055384630694	0.6684861800564507	0.5981389249345299	T	T	T
0.5975306461974400	0.6560446224849246	0.7940641666810175	T	T	T
0.7223498574153817	0.6493675966253321	0.7290728655252039	T	T	T
0.8269646070405887	0.5483114547860731	0.6936408659224801	T	T	T
0.5821612212640617	0.5471116311942784	0.6784902050187535	T	T	T
0.9302879895044793	0.3759911785621438	0.9227363660492975	T	T	T
0.9117939666462503	0.5072927387428696	0.9286608572264585	T	T	T
0.8934999446247610	0.6391142980368840	0.9327362293765468	T	T	T
0.6956244039623515	0.3705106012670430	0.8883423509757440	T	T	T
0.6746921812292009	0.4977709023271999	0.9458933340181868	T	T	T
0.6930939809635952	0.6314853597889860	0.9243926751456064	T	T	T
0.4900991326231237	0.4517566699317360	0.7099547659201718	T	T	T
0.4815084029825274	0.6312455963349376	0.7089455834963188	T	T	T
0.6417804226326430	0.9406035436867689	0.2848857015661264	T	T	T
0.6994584017435364	0.9274247582214293	0.1090931884085320	T	T	T
0.7989891610326088	0.9452251520974678	0.9772559504564331	T	T	T
0.8961667103765824	0.9287994152348578	0.1118508019608068	T	T	T
0.8961721668245104	0.9496427008616157	0.3094421474381888	T	T	T
0.7702098079785555	0.9665609076582802	0.2648656044569729	T	T	T
0.6409621244678801	0.1671660794003211	0.2557592593622697	T	T	T
0.6991641372899194	0.1612133249782828	0.0823257540479872	T	T	T
0.8108482382048642	0.1462903100401628	0.9791237643891394	T	T	T
0.9140511400872560	0.1699804376346004	0.0984244740748191	T	T	T
0.8979957444582901	0.1561157039564033	0.2949565230569395	T	T	T
0.7711335090184230	0.1384399619297784	0.2468252400646304	T	T	T
0.6811115093286566	0.0494251285341503	0.1856619870458913	T	T	T
0.9178047499398588	0.0496121226770313	0.1792577237352257	T	T	T
0.5713130931555747	0.8751124473037550	0.4195494299190017	T	T	T

Structure files (CONTCAR) involved in this work:

0.5828968997337760	0.0071792210691848	0.4364934255925669	T	T	T
0.5953904789932720	0.1400657514887852	0.4378415614455059	T	T	T
0.8081579672819912	0.8689702924038005	0.3915240081072728	T	T	T
0.8128575435330191	0.9961831474897066	0.4482673868782360	T	T	T
0.8098718130945517	0.1311031589581038	0.4371136219504687	T	T	T
0.0085711057940126	0.9542367996081744	0.2149254348479334	T	T	T
0.0163694513175137	0.1361863335396929	0.2128573080541772	T	T	T
0.8568307075535940	0.0572452228550042	0.7864250161149429	T	T	T
0.7993106588791026	0.0694920747979202	0.6102139586139533	T	T	T
0.6999840783117708	0.0613749654378688	0.4764188207733370	T	T	T
0.6000519138427624	0.0743851580559802	0.6071891174123248	T	T	T
0.6030368178678187	0.0509958149464235	0.8039799154007954	T	T	T
0.7290254936611165	0.0264102708354929	0.7649760459030288	T	T	T
0.8606158358912605	0.8313859319315515	0.7632764210825828	T	T	T
0.8078843630281278	0.8345090352523762	0.5851479107867011	T	T	T
0.6938840550198001	0.8498775183005297	0.4863939190637001	T	T	T
0.5887722888565520	0.8277192668787061	0.6032741139946516	T	T	T
0.6038446264756365	0.8506260210487315	0.7972303705670587	T	T	T
0.7306417778162974	0.8562350249286904	0.7432538676727601	T	T	T
0.8209007171217693	0.9475399612084558	0.6870232623099188	T	T	T
0.5807596464959309	0.9518996332491938	0.6721375686815130	T	T	T
0.9331990162615414	0.1256842387797884	0.9119813936018049	T	T	T
0.9179133007604289	0.9951167775013058	0.9404579607741421	T	T	T
0.9022665586204499	0.8626295444584606	0.9447667787203000	T	T	T
0.6945171869239264	0.1258314168542378	0.8900309710224641	T	T	T
0.6799883017699632	0.9983705940546301	0.9450184424289894	T	T	T
0.6969691037527499	0.8650925833851570	0.9367611695507589	T	T	T
0.4893774922540420	0.0460057136019993	0.7124755654331179	T	T	T
0.4847155657800395	0.8642839600114106	0.7143396547192145	T	T	T
0.3603973295697244	0.4298768408813211	0.7204946859316639	T	T	T
0.3164158598014980	0.4513468383737624	0.9049765560083379	T	T	T
0.2004176961006156	0.4577727484533219	0.0022425571375566	T	T	T
0.0898083461272923	0.4293906533136491	0.9013222799516452	T	T	T
0.1030324486727581	0.4326063001702482	0.7040841765317539	T	T	T
0.2300919084413926	0.4408387763297341	0.7580123193425113	T	T	T
0.3604882957234399	0.6699647190663021	0.7601929237185351	T	T	T
0.2887143401136608	0.6303865894846072	0.9150109979548695	T	T	T
0.1881145389803827	0.6581607873508221	0.0361874006324427	T	T	T
0.0965552348063036	0.6637201088881032	0.8930447956578378	T	T	T
0.1009608220598901	0.6552916718066177	0.6960731540909568	T	T	T
0.2291238650952986	0.6540010757133862	0.7431019941344499	T	T	T
0.3088823959425321	0.5477873045506463	0.7638695608240255	T	T	T
0.0836191433289662	0.5453790004127805	0.8055009857635158	T	T	T
0.4332005474488923	0.3759310748857718	0.5734454616923860	T	T	T
0.4122516711432484	0.5068444202496194	0.5745213020479455	T	T	T
0.3854288345436210	0.6378992125309177	0.5705987768234080	T	T	T
0.1931683222680462	0.3600288741992599	0.6103427448217591	T	T	T
0.1888458248237872	0.4934935559849841	0.5852273492775369	T	T	T
0.1911933372490449	0.6255952429191725	0.5563454640532082	T	T	T
0.9853891499632754	0.4541412377616282	0.7849065617905832	T	T	T
0.9858906351244855	0.6344237141894378	0.7890091133535881	T	T	T
0.1334281356218147	0.5654650034409410	0.2250816303460964	T	T	T
0.1826692993469488	0.5432635051689269	0.4038611760506594	T	T	T

Structure files (CONTCAR) involved in this work:

0.2961385447174265	0.5492877048763358	0.5056459935904122	T	T	T
0.4071538271629460	0.5725223633722327	0.4034181476694573	T	T	T
0.3940005894452099	0.5654634022564876	0.2068677613135758	T	T	T
0.2653445920505232	0.5603139075567791	0.2526150784820171	T	T	T
0.1385454515458666	0.3275647593037368	0.2532113717566785	T	T	T
0.2003669403076450	0.3670753848311353	0.4154810224027032	T	T	T
0.3103622065130983	0.3498145477839579	0.5187920303789111	T	T	T
0.4088341655357687	0.3314271609421023	0.3875146383852895	T	T	T
0.3941620877468070	0.3502414820215153	0.1909817566771327	T	T	T
0.2702584498381032	0.3413582782917775	0.2523137868009735	T	T	T
0.1914894333143196	0.4493235258392201	0.2606330751539303	T	T	T
0.4135721690512094	0.4538488871750570	0.3137458178750578	T	T	T
0.0643393699677706	0.6221218186800875	0.0768082437025410	T	T	T
0.0821017247159205	0.4906775744942614	0.0765497986983811	T	T	T
0.1166027043961322	0.3620308192241756	0.0641495241597782	T	T	T
0.3093460948727072	0.6395441721895351	0.1074330794741899	T	T	T
0.3102226967325332	0.5052760630349776	0.0841810979920935	T	T	T
0.2956294375738021	0.3728166761002790	0.0611447492219699	T	T	T
0.5107997066729679	0.5435987811301152	0.2863338577758752	T	T	T
0.5117911880507462	0.3661203707392000	0.2719024253371328	T	T	T
0.4346925473305863	0.7494185446173371	0.6466639556748510	T	T	T
0.1821698329304821	0.7491266986341090	0.6216053635673773	T	T	T
0.2836105102397468	0.7499301361903965	0.0037034052386595	T	T	T
0.0907530704451620	0.7490724517338739	0.0447932587641349	T	T	T
0.0632988571996971	0.2507749597962757	0.1377461255370777	T	T	T
0.3174346941700385	0.2499897102590258	0.1250371089434455	T	T	T
0.2209049512304289	0.2501868823308731	0.5077059202130235	T	T	T
0.3980127337830004	0.2502117509531392	0.5425111719699262	T	T	T
0.5536131032518337	0.2482284934738885	0.3427573441422889	T	T	T
0.8098778564889958	0.2493386686902614	0.3459474389867386	T	T	T
0.7281254764883759	0.2480310047142809	0.9380348820080159	T	T	T
0.8928768146641165	0.2499878278790065	0.9456393290386133	T	T	T
0.9453056703875790	0.7514139535591760	0.8621344032982990	T	T	T
0.6853660004240727	0.7504871149269828	0.8465897000693174	T	T	T
0.7770643837668004	0.7472209882316186	0.4456828752282351	T	T	T
0.6102241317756106	0.7495929569343751	0.4469109803950390	T	T	T
0.9400864850300716	0.4951944848919209	0.5170595546002409	T	T	T
0.8217945290175335	0.3334781093810338	0.3266486843169605	T	T	T
0.8023906211626640	0.6349224332847315	0.6907871391146526	T	T	T
0.9371376229801068	0.4190939822675722	0.4264066213985264	T	T	T
0.8721055712838913	0.5549799925296212	0.5534456571962409	T	T	T
0.0254201502420942	0.5263358819182717	0.4729049677282362	T	T	T
0.0373082067012090	0.4029865513704232	0.4498631788204832	T	T	T
0.0545796182107051	0.4068344913009254	0.5274342892135195	T	T	T
0.0759436663534395	0.4196861231512465	0.3975496144098479	T	T	T
0.0248520870434328	0.3509051263656642	0.4332573962768034	T	T	T
0.0378752767538731	0.5247724710880558	0.3926960615571547	T	T	T
0.0034154265128747	0.5725600906204350	0.4962091328189514	T	T	T
0.0679662883707734	0.5099059648532973	0.5186842862634329	T	T	T

Figure S15(b) C₂H₆

Si O Al Zn C H

1.0000000000000000

20.0219999999999985 0.0000000000000000 0.0000000000000000

Structure files (CONTCAR) involved in this work:

0.0000000000000000 19.8990000000000009 0.0000000000000000
0.0000000000000000 0.0000000000000000 13.3829999999999991
94 193 2 2 2 6

Selective dynamics

Direct

0.4229482152690781	0.0599786305784233	0.6486819759598966	T	T	T
0.3047179664755420	0.0309972583327772	0.7910928380130958	T	T	T
0.2824776243888498	0.0571093001150775	0.0168251072696511	T	T	T
0.1223677908810176	0.0645153818083080	0.0127446535515275	T	T	T
0.0672706003081856	0.0316784034706491	0.8004474190099925	T	T	T
0.1799265952321179	0.0643133017235490	0.6638997577050834	T	T	T
0.4194341538748848	0.8278261750824787	0.6680670898675916	T	T	T
0.3014623915879526	0.8721386645945297	0.8001965406444088	T	T	T
0.2672365878508642	0.8316848883074703	0.0194508071592544	T	T	T
0.1119620728464495	0.8271496102779982	0.0105044367794200	T	T	T
0.0654500605823256	0.8740373006669213	0.7965316308754368	T	T	T
0.1797316349874462	0.8276299187141244	0.6645941654908237	T	T	T
0.0768003539686149	0.9410258617606302	0.1484728270514912	T	T	T
0.1949926137176134	0.9698390862003614	0.2908713492444312	T	T	T
0.2167011112536841	0.9429592574168112	0.5161443370573503	T	T	T
0.3768494374239024	0.9363249459359497	0.5131528374162087	T	T	T
0.4335726670253309	0.9680899625489916	0.3010118160375876	T	T	T
0.3201005213942409	0.9362471537888537	0.1646344219706711	T	T	T
0.0814358145061145	0.1734355599391527	0.1668866079404885	T	T	T
0.1986650644005985	0.1287091583418013	0.3002307679875595	T	T	T
0.2323725823965376	0.1696654755604273	0.5185763348533596	T	T	T
0.3879975425487280	0.1736457679528513	0.5093478564346994	T	T	T
0.4361024538475189	0.1266333339648588	0.2955330748713472	T	T	T
0.3199952299412865	0.1722528744214696	0.1656510820082742	T	T	T
0.5746079456948711	0.5553923267641132	0.3561805761902156	T	T	T
0.6894773044774121	0.5253999661100404	0.2011425591826672	T	T	T
0.7116151961496466	0.5689201443118215	0.9883504214333426	T	T	T
0.8718822267064932	0.5710528513525237	0.9852805577019222	T	T	T
0.9270581729563246	0.5319233863409891	0.1920500842554150	T	T	T
0.8112637924262075	0.5524876194946039	0.3361267969164216	T	T	T
0.5741244326903767	0.3277681983386551	0.3313312467813204	T	T	T
0.6938995517402308	0.3709916189211749	0.1902448619838438	T	T	T
0.7293863159698841	0.3263975228388001	0.9785095397470935	T	T	T
0.8839899027358753	0.3265762206386994	0.9969189755333996	T	T	T
0.9403356784043105	0.3770732916460380	0.1956029233291368	T	T	T
0.9185651865965870	0.4430614847062810	0.8581912417276397	T	T	T
0.8009982221263307	0.4711568787780917	0.7166961169887157	T	T	T
0.7713624827940732	0.4381063228509586	0.4905079484752315	T	T	T
0.6134599597080747	0.4305249213961932	0.4891924271762974	T	T	T
0.5678202025781237	0.4690087032617595	0.7023748954376976	T	T	T
0.6764593366723887	0.4479783068694258	0.8557352824530899	T	T	T
0.9202998749137338	0.6767433639047250	0.8303354191107780	T	T	T
0.7710587252652360	0.6669692138851770	0.4653764308306342	T	T	T
0.6156611344390241	0.6728899759466016	0.4868409065447865	T	T	T
0.5613129868544491	0.6276380413201400	0.6972893603277496	T	T	T
0.6760197318945829	0.6728047989701919	0.8227214296717975	T	T	T
0.5782031038780363	0.9446515072541287	0.3584212091848772	T	T	T
0.6986922683125201	0.9722692031330048	0.2139132663321793	T	T	T

Structure files (CONTCAR) involved in this work:

0.7200921361018181	0.9353033843604875	0.9928122455393767	T	T	T
0.8801893722901905	0.9336241555947596	0.9947174431215642	T	T	T
0.9322564933894253	0.9692399665903626	0.2044896969033887	T	T	T
0.8226471365430121	0.9453244455792340	0.3544298843319371	T	T	T
0.5790524299162483	0.1725071081867000	0.3300468963400519	T	T	T
0.6987386646490922	0.1302346248178927	0.1929805789111864	T	T	T
0.7326610745259668	0.1707644574399117	0.9728685043025719	T	T	T
0.8874682686412890	0.1734906129404081	0.9878777843916134	T	T	T
0.9372362366954164	0.1266498326899671	0.1993508319177031	T	T	T
0.8211462044081458	0.1702676705594938	0.3299918140511172	T	T	T
0.9229237722612796	0.0556287481021855	0.8576311549501867	T	T	T
0.8031922340262562	0.0267378375159031	0.7111864001934124	T	T	T
0.7809086954601466	0.0645931209799147	0.4923178229710943	T	T	T
0.6208086260723468	0.0689929826024215	0.4907780507047534	T	T	T
0.5684069142690120	0.0313310540027152	0.6996110529188595	T	T	T
0.6791195610970667	0.0518364830863307	0.8497450273366600	T	T	T
0.9233648491267933	0.8292096759974433	0.8372008454371298	T	T	T
0.8042330657211643	0.8701452697180430	0.6963852260975629	T	T	T
0.7717591617579020	0.8259568076943364	0.4790128724313189	T	T	T
0.6166670064628430	0.8264219291249029	0.4904138753796259	T	T	T
0.5649183589166042	0.8742287449073449	0.6980148605618015	T	T	T
0.6802508000649024	0.8323397955841755	0.8305522253082183	T	T	T
0.4235729568837784	0.4425684792680072	0.6415395811297626	T	T	T
0.3039655795306307	0.4699890613494597	0.7823663052513784	T	T	T
0.2812179072821847	0.4428201950467678	0.0070966809300552	T	T	T
0.1225268989964207	0.4361932647674629	0.0110190872238352	T	T	T
0.0647029741826336	0.4680325650075282	0.8001111531132956	T	T	T
0.1760818325801960	0.4388281875370597	0.6557563227546912	T	T	T
0.4171697339073584	0.6743168668565760	0.6622246523606502	T	T	T
0.3010813300909581	0.6283044862161430	0.7964291140489284	T	T	T
0.2679514374134691	0.6705948816608840	0.0161210626395878	T	T	T
0.1131066451424513	0.6730937242720036	0.0063396149939400	T	T	T
0.0640482115577604	0.6269091061300986	0.7948862549539224	T	T	T
0.1785551357926028	0.6697050627518663	0.6612369920581046	T	T	T
0.0730655572064874	0.5588297833243721	0.1438969396607665	T	T	T
0.1936586867435432	0.5290112150716558	0.2823760084638317	T	T	T
0.2166894496126048	0.5569398390469037	0.5110179530832959	T	T	T
0.3757229433333140	0.5656300107282879	0.5111314048008140	T	T	T
0.4291763894876092	0.5311132570304097	0.2990241100149122	T	T	T
0.3209584803881901	0.5609854776246201	0.1505666901077598	T	T	T
0.0839894764976864	0.3263378612915205	0.1630690844440067	T	T	T
0.1969414853580875	0.3714342385655222	0.2995978395952402	T	T	T
0.2314587556996010	0.3308811612639749	0.5182739124543074	T	T	T
0.3866016781262734	0.3276697003233313	0.5046275658671550	T	T	T
0.4326468455371830	0.3730179532452179	0.2915112883104161	T	T	T
0.3171623499586962	0.3301024438963927	0.1614752075502353	T	T	T
0.3592090199315515	0.0697148296821976	0.7223333033146191	T	T	T
0.3157266158031430	0.0525594750077783	0.9065462092939278	T	T	T
0.2019720025554589	0.0504538433038013	0.0096463986271343	T	T	T
0.0928053763791573	0.0694040991835087	0.9007155262159883	T	T	T
0.1033399329346253	0.0648786116308278	0.7035925562172992	T	T	T
0.2293395430962213	0.0518542710887724	0.7587249230772032	T	T	T
0.3611964771127481	0.8277180488288979	0.7524587952004301	T	T	T

Structure files (CONTCAR) involved in this work:

0.3021225777252836	0.8620213790929857	0.9199511971012563	T	T	T
0.1888526791976372	0.8529338097719193	0.0197235519812250	T	T	T
0.0878070311417893	0.8326692765632487	0.8954888217096624	T	T	T
0.1030946902039441	0.8416952974920124	0.6998987389846176	T	T	T
0.2295256806538296	0.8481019616253790	0.7561931831854567	T	T	T
0.3147552148091101	0.9506628021052111	0.7737020863731249	T	T	T
0.0867748367889171	0.9524073875360566	0.8082852133010335	T	T	T
0.4333152012000067	0.1282192012558057	0.5836536993325524	T	T	T
0.4125472772848650	0.9975423822398058	0.5723548119069797	T	T	T
0.3928341478685816	0.8656770173688936	0.5683465230059430	T	T	T
0.1961068921958729	0.1371409258419306	0.6152153197239306	T	T	T
0.1884105013248289	0.0046875571219665	0.5824914726581176	T	T	T
0.1964438814156212	0.8710970674552586	0.5650835926330406	T	T	T
0.9873248045799107	0.0416039097473258	0.7869831278971248	T	T	T
0.9850806431354878	0.8680652976531265	0.7819741310257688	T	T	T
0.1414004540581334	0.9312528169653235	0.2204070781084107	T	T	T
0.1832189452102206	0.9477485434637893	0.4059793606759312	T	T	T
0.2971319884366416	0.9495455877398652	0.5085786419229515	T	T	T
0.4068779328800663	0.9313188757212977	0.4014176334234857	T	T	T
0.3966392903449630	0.9359050379754035	0.2041813429607559	T	T	T
0.2706123301380863	0.9493103326899971	0.2592858598715104	T	T	T
0.1412218195689991	0.1742275035363986	0.2486592858520343	T	T	T
0.1957934537622340	0.1404579899596414	0.4196097640181528	T	T	T
0.3107393688246468	0.1481731413063655	0.5157841336061216	T	T	T
0.4144168823594411	0.1674331779703340	0.3954288747637911	T	T	T
0.3970198175865252	0.1590124950655805	0.1999809099114681	T	T	T
0.2718367734542277	0.1507772120592750	0.2587738337012899	T	T	T
0.1842681664631574	0.0502414002250999	0.2747914166729813	T	T	T
0.4163583822443393	0.0479334182740217	0.3077875417445535	T	T	T
0.0657085716265857	0.8731122665208387	0.0828162681115784	T	T	T
0.0857643879829215	0.0041527267559855	0.0728531485446319	T	T	T
0.1065499649210199	0.1358742775969639	0.0661823723863445	T	T	T
0.3043657327049493	0.8632623956956309	0.1160749035260693	T	T	T
0.3111400958888650	0.9953619340605737	0.0826097761872771	T	T	T
0.3026930769604353	0.1287184855647747	0.0664652410915667	T	T	T
0.5130634354406427	0.9549354925324032	0.2878867274594822	T	T	T
0.5163160923238521	0.1332048913579622	0.2785640727677214	T	T	T
0.6396854807384714	0.5554818501248679	0.2847982225051638	T	T	T
0.6900277915739983	0.5753258425012023	0.1053035762028491	T	T	T
0.7920004013112618	0.5597765413588657	0.9764658004593145	T	T	T
0.8923940461387734	0.5748958265019651	0.1034160546544525	T	T	T
0.8887155916014741	0.5425117525944420	0.2997311609748836	T	T	T
0.7647088181467740	0.5243960163421414	0.2482096188542587	T	T	T
0.6411756787340808	0.3350066352790703	0.2655633860895691	T	T	T
0.6887579492770951	0.3326925690995765	0.0828219423151971	T	T	T
0.8065591432833318	0.3508668771766950	0.9941585134039603	T	T	T
0.9095918377581891	0.3260412913340769	0.1133153331689923	T	T	T
0.9053830620539111	0.3632108464378219	0.3061601912915877	T	T	T
0.7681631360409903	0.3671625141669185	0.2351484927470311	T	T	T
0.6700110149220950	0.4489417698107128	0.1721967532017760	T	T	T
0.9228610912337282	0.4530773042180530	0.1612448573951457	T	T	T
0.5705881944507697	0.6274648955558171	0.4121319932687609	T	T	T
0.5784010402072114	0.4963221530940946	0.4402038701235994	T	T	T

Structure files (CONTCAR) involved in this work:

0.5833977276966380	0.3624188850999507	0.4408711252199351	T	T	T
0.7980064571173028	0.6308294748269809	0.3630328728673703	T	T	T
0.7991122167189229	0.5106482526029830	0.4421678905826765	T	T	T
0.8142619986676838	0.3785249573241803	0.4394655717937166	T	T	T
0.0046393324600699	0.5525531876286410	0.2091981927925627	T	T	T
0.0201604926553802	0.3674337277635955	0.2082958065487520	T	T	T
0.8552938282789778	0.4299804575536317	0.7832484007185546	T	T	T
0.7861758700688835	0.4357563531458611	0.6091544725101670	T	T	T
0.6931201074658653	0.4332636118391396	0.4647103815285472	T	T	T
0.6011191512197411	0.4290390925406361	0.6084040185114744	T	T	T
0.6031980981629228	0.4437116897801351	0.8045228317450976	T	T	T
0.7304380709808229	0.4758647580874539	0.7746019198344526	T	T	T
0.8615901352662910	0.6792895761741101	0.7500576882461364	T	T	T
0.8170180646293831	0.6379505044584967	0.5577532566789823	T	T	T
0.6932104053471170	0.6467759773384831	0.4854539419836173	T	T	T
0.5859570582414595	0.6679162500599320	0.5985855674977303	T	T	T
0.5972608156622256	0.6603871103425039	0.7944606233656980	T	T	T
0.7226316445365125	0.6442226572000394	0.7340788797300964	T	T	T
0.8305830593059373	0.5462148198279884	0.6929346782385939	T	T	T
0.5804744514541995	0.5487276087268584	0.6857000684349592	T	T	T
0.9287614097185483	0.3775782113792927	0.9297822555838854	T	T	T
0.9079694027870845	0.5080569804088089	0.9299416158313965	T	T	T
0.8964646323237986	0.6403785885348158	0.9342692994661381	T	T	T
0.6958861288841203	0.3731663214743293	0.8930414182372497	T	T	T
0.6746802203180211	0.5014646118312061	0.9470734869886940	T	T	T
0.6890262866872930	0.6360256517535131	0.9300261538986118	T	T	T
0.4887815987788265	0.4518246145023214	0.7121090859865854	T	T	T
0.4807655986180528	0.6345917656346374	0.7092113134627213	T	T	T
0.6437078585306043	0.9396184530134513	0.2880360075576761	T	T	T
0.6990822574293492	0.9305747051619500	0.1096626138807453	T	T	T
0.8004096308771903	0.9442647596417120	0.9803973658768608	T	T	T
0.8993776888330361	0.9276398697608145	0.1121225963285385	T	T	T
0.8979047126733619	0.9481141867357130	0.3095900014362620	T	T	T
0.7717892809881437	0.9665111474075156	0.2653115158111034	T	T	T
0.6424012593416719	0.1710707271750742	0.2550890602656768	T	T	T
0.6963573052576102	0.1582846601862476	0.0794415018666655	T	T	T
0.8104694109088689	0.1475279368964787	0.9822562545064174	T	T	T
0.9142578476652952	0.1691977252276700	0.1017833651476431	T	T	T
0.8981667697356530	0.1528077740422920	0.2979141284362711	T	T	T
0.7721936469257120	0.1415903774460511	0.2414158667021495	T	T	T
0.6806137630372543	0.0505961358587345	0.1936562062500715	T	T	T
0.9205770370801835	0.0481529035990815	0.1799655002884985	T	T	T
0.5710842559419647	0.8748740459544603	0.4208283145469475	T	T	T
0.5821750779594586	0.0067019699819608	0.4373572404059830	T	T	T
0.5993832864273722	0.1386865250328571	0.4364350377300898	T	T	T
0.8091319422155956	0.8690801659484417	0.3929185966549826	T	T	T
0.8160289661652750	0.9972171859167637	0.4474945712108030	T	T	T
0.8051727331082172	0.1316994129951277	0.4348092494807946	T	T	T
0.0112572759493705	0.9529543943665654	0.2170452469505879	T	T	T
0.0171008342348459	0.1365578788029753	0.2164796510475600	T	T	T
0.8569169785746578	0.0590044484024293	0.7878691025700508	T	T	T
0.8019975864561867	0.0710541714018936	0.6092607874615251	T	T	T
0.7004583643993119	0.0562089466915035	0.4805619978613871	T	T	T

Structure files (CONTCAR) involved in this work:

0.5991892102697316	0.0748284552265031	0.6073558362728901	T	T	T
0.6039726447753901	0.0514829847613285	0.8043473841185379	T	T	T
0.7295403181417801	0.0277644606206877	0.7616368358587855	T	T	T
0.8586751489538902	0.8324308443152432	0.7651992758466207	T	T	T
0.8073767205324170	0.8358361642845132	0.5866660710295917	T	T	T
0.6943579782902443	0.8507463834376711	0.4859033466154184	T	T	T
0.5903137526287263	0.8283513628850215	0.6049609272606767	T	T	T
0.6037933312482856	0.8512580886579557	0.7990414462873250	T	T	T
0.7299746130535627	0.8617245612180627	0.7441444477428890	T	T	T
0.8229433378161745	0.9493162501555287	0.6865808619443102	T	T	T
0.5806579016310670	0.9524861246849489	0.6732394362295979	T	T	T
0.9326738031683359	0.1276184079115893	0.9137473147813198	T	T	T
0.9178379425580453	0.9970706084846959	0.9424127117214115	T	T	T
0.9051362004538843	0.8642981032137884	0.9433164295402424	T	T	T
0.6964446187030418	0.1275779548331967	0.8858741597825832	T	T	T
0.6833854046965427	0.0005447133324061	0.9440905778988665	T	T	T
0.6968856042225395	0.8664496682563386	0.9380468465283298	T	T	T
0.4894203496398080	0.0468596693940895	0.7148541635827615	T	T	T
0.4850989740484690	0.8643842652226593	0.7143954822117871	T	T	T
0.3576342544782706	0.4323944022608812	0.7107622712323985	T	T	T
0.3098659027221863	0.4390055033489882	0.8940014891351517	T	T	T
0.2010532934660741	0.4565587587773279	0.0089677623789735	T	T	T
0.0937299430499615	0.4302775775621123	0.8986422801760499	T	T	T
0.1008557294370233	0.4375943169094051	0.7011298144802511	T	T	T
0.2279117880344994	0.4581341543537898	0.7446343343500961	T	T	T
0.3568139716381304	0.6747988382394947	0.7430502941556348	T	T	T
0.3023821557842181	0.6438229664045489	0.9145235681575554	T	T	T
0.1899521895076317	0.6476408750865587	0.0179084640452701	T	T	T
0.0910727809325381	0.6695580439066738	0.8901281793617369	T	T	T
0.1016223686019855	0.6551297461493554	0.6950741757013663	T	T	T
0.2273807273960201	0.6452424576261345	0.7517928901286896	T	T	T
0.3202058482947432	0.5499623424590694	0.7786821511541664	T	T	T
0.0812850767285247	0.5477715675575632	0.8101609548619669	T	T	T
0.4336212040072897	0.3762272970682919	0.5720734985945319	T	T	T
0.4178550627828751	0.5078782738450995	0.5690201142928668	T	T	T
0.3915618961896308	0.6385453165936843	0.5598598687490671	T	T	T
0.1940022529421326	0.3644133819060897	0.6134266979447720	T	T	T
0.1800262619856168	0.4946353474320959	0.5671097996884019	T	T	T
0.1951170746410358	0.6285115840278652	0.5594805064355582	T	T	T
0.9850092165583378	0.4543649483175712	0.7908126456082364	T	T	T
0.9840936861081760	0.6359786915983703	0.7826663013730286	T	T	T
0.1362100723232962	0.5678912932171541	0.2189813037265565	T	T	T
0.1933736377610430	0.5571235130690686	0.3954342976243111	T	T	T
0.2969598157503557	0.5470872941709723	0.5202320290542387	T	T	T
0.3981883927742776	0.5697527997919926	0.3951799945878584	T	T	T
0.3952833446025299	0.5602670987538073	0.1980736063828059	T	T	T
0.2672625018209946	0.5420221588499692	0.2368353714076026	T	T	T
0.14109088271110745	0.3237351132435795	0.2485827066788754	T	T	T
0.1950673458593082	0.3588247295199501	0.4184710018619734	T	T	T
0.3095733471453880	0.3532039556050818	0.5152207539579446	T	T	T
0.4092991305348059	0.3295602229165115	0.3882904626798594	T	T	T
0.3942070778105658	0.3457694758158310	0.1923583296183014	T	T	T
0.2703478948986658	0.3531968431411933	0.2554322185896020	T	T	T

Structure files (CONTCAR) involved in this work:

0.1772637250482706	0.4490874048060345	0.2765889993633449	T	T	T
0.4140842227244324	0.4512995232576893	0.3113502397671581	T	T	T
0.0656730972689450	0.6250169760763028	0.0738528333707736	T	T	T
0.0812516300397992	0.4927695708275691	0.0734450308984848	T	T	T
0.1123763490121930	0.3632243839142289	0.0635763034565494	T	T	T
0.3064195133735576	0.6362746537265908	0.1096024894360398	T	T	T
0.3178725036832375	0.5056079641529592	0.0616031502868473	T	T	T
0.2972379113068038	0.3717497428074145	0.0616343388289380	T	T	T
0.5086429441264592	0.5447025528626941	0.2883797306360263	T	T	T
0.5123531445442985	0.3640461263795796	0.2729660530663091	T	T	T
0.4375414604668557	0.7512106432714856	0.6369019977092928	T	T	T
0.1891361573360184	0.7488164776800663	0.6370738977482945	T	T	T
0.2749754122196213	0.7510578120369694	0.0239845875465680	T	T	T
0.1057742486556772	0.7495661605150878	0.0463875658466771	T	T	T
0.0622412225008748	0.2501487132417963	0.1360320679938780	T	T	T
0.3079432403292001	0.2507525493810228	0.1379435129961439	T	T	T
0.2244926688104140	0.2502852567048892	0.5250818958514156	T	T	T
0.3935235548339029	0.2512805029295312	0.5452383511629206	T	T	T
0.5571053594482726	0.2494850989055997	0.3511961794458563	T	T	T
0.8126830150624164	0.2492479554562867	0.3447540398437412	T	T	T
0.7273464026722454	0.2491362105164084	0.9402901526083188	T	T	T
0.8923838320082405	0.2513992844461099	0.9520774284537237	T	T	T
0.9447717330528905	0.7522533650852017	0.8600280808710130	T	T	T
0.6890942052157025	0.7522786377966403	0.8416743849398596	T	T	T
0.7776215896979664	0.7470796526600547	0.4493328276789154	T	T	T
0.6113643130756223	0.7500569175424147	0.4486787193810761	T	T	T
0.9355792770187953	0.4779629867988744	0.5244335777730093	T	T	T
0.8188277283474048	0.3333125845246403	0.3256621355671163	T	T	T
0.8024190931847459	0.6320146818222376	0.6907011239857680	T	T	T
0.9150109323280415	0.4200332780186668	0.4264498062962871	T	T	T
0.8814782509867285	0.5499497111950780	0.5565015451064605	T	T	T
0.0379762723900072	0.5825389010012917	0.4479946987252142	T	T	T
-0.0079412627323439	0.6345279879482600	0.4951092412742133	T	T	T
0.0719925743378169	0.5610105299662722	0.5036882545774881	T	T	T
0.0677975503498058	0.6049858636062928	0.3879377401979958	T	T	T
0.0093600145662904	0.5404811236822713	0.4171216652590755	T	T	T
0.9515898150003337	0.6499671603434887	0.4443497070023105	T	T	T
-0.0296895426206927	0.6158281322925584	0.5665339777339846	T	T	T
0.0189069270570982	0.6802929447858022	0.5177381061651061	T	T	T

Figure S15(b)TS4

Si O Al Zn C H

1.0000000000000000

20.0219999999999985 0.0000000000000000 0.0000000000000000

0.0000000000000000 19.8990000000000009 0.0000000000000000

0.0000000000000000 0.0000000000000000 13.3829999999999991

94 193 2 2 2 6

Selective dynamics

Direct

0.4231186789575326	0.0600280371513692	0.6489163348239140	T	T	T
0.3048464791764791	0.0306580747822721	0.7911272431788534	T	T	T
0.2826612623120333	0.0570396479985675	0.0167886628674486	T	T	T
0.1224451143466746	0.0643786675719463	0.0126684177873713	T	T	T
0.0674801788955570	0.0313996901850847	0.8003705575662486	T	T	T

Structure files (CONTCAR) involved in this work:

0.1801081824455195	0.0641187067423501	0.6638206870260364	T	T	T
0.4190823132593871	0.8275590342450654	0.6678200568973901	T	T	T
0.3014023442507296	0.8718195469933694	0.8004403162408109	T	T	T
0.2668957587997328	0.8316813410537568	0.0195569871260919	T	T	T
0.1116628644418040	0.8271554989995028	0.0106157266170786	T	T	T
0.0652355343160163	0.8739180928116418	0.7966040081591537	T	T	T
0.1797082481197908	0.8275942774956767	0.6651686351602194	T	T	T
0.0767523774233652	0.9410066413698762	0.1486645859105511	T	T	T
0.1949094187714198	0.9696226147710945	0.2912851994129175	T	T	T
0.2170115742229123	0.9427853203088359	0.5163184526441510	T	T	T
0.3771424625635507	0.9365990303477129	0.5130481248032472	T	T	T
0.4335243600219774	0.9684895007863017	0.3006753079474480	T	T	T
0.3199703283513129	0.9361812526962880	0.1647109740615139	T	T	T
0.0810271468631763	0.1731634775045780	0.1669407306668945	T	T	T
0.1984347672062984	0.1286609224168960	0.3004713807273492	T	T	T
0.2325344647006729	0.1697200576081472	0.5189148143460329	T	T	T
0.3879992285547606	0.1736288477692949	0.5098560952990817	T	T	T
0.4360234807744546	0.1269304191104643	0.2958536762862519	T	T	T
0.3199771425930920	0.1721764928029559	0.1656421826431479	T	T	T
0.5731688024014940	0.5563337467854114	0.3547765949019961	T	T	T
0.6896884494217429	0.5255620274337616	0.2043104559040202	T	T	T
0.7116532111391118	0.5684826513136215	0.9879847529438669	T	T	T
0.8713715181572298	0.5708652034974344	0.9839066000824158	T	T	T
0.9246530261503491	0.5292116248388042	0.1900109516989277	T	T	T
0.8127589746751659	0.5528287905038257	0.3407283531255910	T	T	T
0.5752086624090677	0.3277941859265562	0.3305422917038996	T	T	T
0.6933298520653993	0.3712743513852816	0.1879093704360132	T	T	T
0.7293678073252270	0.3268479990827617	0.9756348479437926	T	T	T
0.8841429137359156	0.3253840906043161	0.9926607063932096	T	T	T
0.9397502358696713	0.3744862877554054	0.1918824016864674	T	T	T
0.9186464996759699	0.4434036739413263	0.8568188138765079	T	T	T
0.8006246360659842	0.4712567882952394	0.7142787914809360	T	T	T
0.7742313313113801	0.4390530792461567	0.4901584970184352	T	T	T
0.6159810300975639	0.4320260173760867	0.4873573431258504	T	T	T
0.5685716090589660	0.4697074636918599	0.7000612374839184	T	T	T
0.6767592078352320	0.4483661581392633	0.8534354641084866	T	T	T
0.9202080897608431	0.6760516791768467	0.8311233362791349	T	T	T
0.7685995534356677	0.6693737458838684	0.4636891642466878	T	T	T
0.6134957694547855	0.6734755893346877	0.4839013152233522	T	T	T
0.5612046855249286	0.6281847398466944	0.6955833548351663	T	T	T
0.6739500678918636	0.6721028000344059	0.8254953229518800	T	T	T
0.5778886988608120	0.9452260707918877	0.3581238679004317	T	T	T
0.6983814311878607	0.9723308181811137	0.2137683813530489	T	T	T
0.7202474860481135	0.9348738422571595	0.9931566840352176	T	T	T
0.8803005943548053	0.9328401927643323	0.9944856239612377	T	T	T
0.9320827483172694	0.9695655153449049	0.2041842800421878	T	T	T
0.8224476833243651	0.9466521204858002	0.3543105431096781	T	T	T
0.5791384219820925	0.1726474128152436	0.3310762448681202	T	T	T
0.6981041897780734	0.1296365188095024	0.1928533915325888	T	T	T
0.7320822416461904	0.1708066680175235	0.9728944805127383	T	T	T
0.8870426504721460	0.1728569889188559	0.9861260888482496	T	T	T
0.9364251739027341	0.1272208254263200	0.1985261791017767	T	T	T
0.8198869993580731	0.1703006993857266	0.3296038130785522	T	T	T

Structure files (CONTCAR) involved in this work:

0.9229910650884116	0.0542287846070613	0.8569888978688296	T	T	T
0.8025602213306519	0.0256670170462563	0.7105284797098717	T	T	T
0.7810281025362301	0.0653331043538636	0.4926685837644275	T	T	T
0.6209607118610512	0.0691568736971339	0.4912444530340848	T	T	T
0.5683901289588393	0.0309508808002960	0.7001303698652502	T	T	T
0.6789618536915712	0.0513940679105563	0.8503385573475410	T	T	T
0.9230070186336170	0.8289258853283681	0.8360650232342436	T	T	T
0.8031792178659780	0.8689053972313046	0.6948450770906442	T	T	T
0.7694983678557525	0.8267389091390883	0.4772087671684763	T	T	T
0.6148359815428062	0.8269703048751484	0.4898678677340987	T	T	T
0.5642976020323358	0.8737577780094133	0.6984296918549326	T	T	T
0.6797306469984624	0.8315796390984970	0.8311968066419505	T	T	T
0.4234524131669167	0.4428621906208530	0.6397480712132516	T	T	T
0.3043076230038503	0.4699888495036167	0.7813942271588143	T	T	T
0.2810636431661425	0.4420887752387981	0.0057531850502696	T	T	T
0.1223237346498787	0.4349389875457088	0.0080973520578005	T	T	T
0.0645800893287506	0.4679726003912746	0.7987629696800749	T	T	T
0.1759826595404717	0.4392536196978113	0.6545133164454797	T	T	T
0.4164998187572403	0.6740979502010060	0.6604327922578217	T	T	T
0.3009110212496502	0.6281149471431312	0.7952864095418631	T	T	T
0.2672135084965624	0.6705867010456061	0.0155016108611192	T	T	T
0.1125195888290090	0.6731409842341308	0.0062325287145887	T	T	T
0.0637780463817876	0.6267682283688493	0.7952277699345491	T	T	T
0.1777910088906412	0.6696132284007379	0.6604939997678120	T	T	T
0.0716574107592010	0.5576882532741565	0.1402353850186809	T	T	T
0.1915153579046819	0.5292996880794498	0.2813081103825535	T	T	T
0.2141995602931819	0.5575149259901440	0.5090549133397364	T	T	T
0.3736720856731482	0.5658444627006288	0.5093328312981663	T	T	T
0.4278393834067037	0.5301829409804376	0.2984443986177294	T	T	T
0.3194533651555611	0.5608416974301837	0.1501824878122730	T	T	T
0.0838538543530383	0.3261256841902156	0.1617544508102035	T	T	T
0.1969429868948363	0.3713517618464667	0.2985483543790617	T	T	T
0.2316667472000187	0.3308933615606209	0.5175325620035438	T	T	T
0.3866375441387893	0.3274327534466067	0.5040532314585094	T	T	T
0.4327822772005204	0.3723349553179186	0.2915060467307386	T	T	T
0.3175167943310954	0.3298753908427113	0.1608069834945501	T	T	T
0.3592492974289782	0.0694702922920918	0.7223691463050090	T	T	T
0.3158303697886851	0.0523785495527608	0.9064940955426177	T	T	T
0.2021257504354780	0.0507890286372230	0.0097169825391145	T	T	T
0.0929066967462880	0.0692539234304011	0.9006102964778261	T	T	T
0.1035459991249876	0.0646092352156156	0.7035435471333104	T	T	T
0.2294790827500179	0.0514273399928665	0.7586066701821241	T	T	T
0.3606036688563827	0.8270906915852362	0.7518750984988086	T	T	T
0.3023454536374302	0.8617092073701698	0.9202378150818858	T	T	T
0.1885454916365799	0.8531569080203802	0.0192266359283701	T	T	T
0.0872161600311976	0.8324885455132890	0.8957176068338528	T	T	T
0.1029787159691103	0.8416361414878450	0.6999901089282707	T	T	T
0.2291897403982707	0.8479839288605265	0.7571873758720498	T	T	T
0.3149557654623092	0.9503090965468726	0.7739204330965076	T	T	T
0.0869705328132484	0.9521554704443809	0.8085544696555179	T	T	T
0.4334558591911798	0.1284345750231190	0.5842594837658326	T	T	T
0.4129079344890744	0.9977725560214210	0.5722410026495621	T	T	T
0.3929267139305302	0.8659572945239374	0.5683097269013416	T	T	T

Structure files (CONTCAR) involved in this work:

0.1961872502184177	0.1370472151678834	0.6153792117684247	T	T	T
0.1885192939110216	0.0046751642794245	0.5821291506846725	T	T	T
0.1970998242230937	0.8710492475575042	0.5659326690111123	T	T	T
0.9875717134433843	0.0410586064270723	0.7864037428163890	T	T	T
0.9848599775533634	0.8682104322701287	0.7817863711021448	T	T	T
0.1412694808812683	0.9311495362882840	0.2207494094273675	T	T	T
0.1833880434125839	0.9469360889394584	0.4062010395104266	T	T	T
0.2974040283314737	0.9498317076271159	0.5084890797753158	T	T	T
0.4072475369752957	0.9317182436646322	0.4013285945983334	T	T	T
0.3965247288946552	0.9358361917824097	0.2042065948692116	T	T	T
0.2705624255472120	0.9495055639549258	0.2593509325681907	T	T	T
0.1406811025111077	0.1738335113959782	0.2489237103590981	T	T	T
0.1958432217309745	0.1410814535016631	0.4197041876326695	T	T	T
0.3108110109335297	0.1479312107667996	0.5161085405391208	T	T	T
0.4143731689836580	0.1674704831084622	0.3959679051667048	T	T	T
0.3970008837321145	0.1595719716252307	0.2004457277228731	T	T	T
0.2715118266875073	0.1505226593993179	0.2583299125667423	T	T	T
0.1839636248035513	0.0500749504097678	0.2760387357288375	T	T	T
0.4159209500116290	0.0482665595384251	0.3072946586879174	T	T	T
0.0655300353323468	0.8729704511593969	0.0833224119749150	T	T	T
0.0861449164553750	0.0037911715992013	0.0725736608298029	T	T	T
0.1061944657936150	0.1355316169399074	0.0663648846871491	T	T	T
0.3038833112077100	0.8631919863846356	0.1163767656505126	T	T	T
0.3111070872625318	0.9951802304812793	0.0824889294581922	T	T	T
0.3032741533423427	0.1285487380034081	0.0663535429428981	T	T	T
0.5130966780919867	0.9561185038975020	0.2870160014987636	T	T	T
0.5162613533079226	0.1336067173974055	0.2794537703877648	T	T	T
0.6372634905967403	0.5586454953130618	0.2815680191335806	T	T	T
0.6950751855630374	0.5735351418259704	0.1067039855688155	T	T	T
0.7916790876278176	0.5616473266287701	0.9685827078540165	T	T	T
0.8881966018743795	0.5724368575087421	0.1033344217781380	T	T	T
0.8884508963313473	0.5407272692183552	0.2986959200187260	T	T	T
0.7623682924224113	0.5225136163538373	0.2591783892343200	T	T	T
0.6411114324532698	0.3332678869626707	0.2618094785038420	T	T	T
0.6877892139336202	0.3356762486226975	0.0786017090332461	T	T	T
0.8068529328343982	0.3501481502693994	0.9920211656248905	T	T	T
0.9109956445943318	0.3236014191901020	0.1082078945177443	T	T	T
0.9052181315643982	0.3573702645621979	0.3014425670346472	T	T	T
0.7679879118335741	0.3665832894422876	0.2311274897622539	T	T	T
0.6689569755737288	0.4494398373486965	0.1754876307307276	T	T	T
0.9193878701217617	0.4502680459843356	0.1600810970273239	T	T	T
0.5665035004531462	0.6280095540874890	0.4115841073520752	T	T	T
0.5798017403731111	0.4971186779621480	0.4382939795073523	T	T	T
0.5873912280248059	0.3633199268266038	0.4388229032852021	T	T	T
0.8003648296142962	0.6314275524905949	0.3653665883725857	T	T	T
0.8050915209676498	0.5125176255536718	0.4495704556434167	T	T	T
0.8158460381593674	0.3801591274323753	0.4348191286501262	T	T	T
0.0026621921092833	0.5491071273779362	0.2030300542551400	T	T	T
0.0198579085070887	0.3677389588150690	0.2056263024793252	T	T	T
0.8550355123602109	0.4317729950531196	0.7824369808986371	T	T	T
0.7886773852805882	0.4323660549851492	0.6086776074639356	T	T	T
0.6958524598177722	0.4368930415340688	0.4635782970243406	T	T	T
0.6029592475813117	0.4300759826219283	0.6065347643501349	T	T	T

Structure files (CONTCAR) involved in this work:

0.6032436003967304	0.4443136964907070	0.8028907843755709	T	T	T
0.7299428106397542	0.4770938689624190	0.7713784248669722	T	T	T
0.8603099598394294	0.6770366538589362	0.7530946952106184	T	T	T
0.8111379058433934	0.6460987251475712	0.5606595597017240	T	T	T
0.6905103499098395	0.6468474803287558	0.4766988214391631	T	T	T
0.5867972346643010	0.6685519435813908	0.5975114925594746	T	T	T
0.5954607802575677	0.6611519887859379	0.7940210020870221	T	T	T
0.7213342892505152	0.6416000208667453	0.7394875265285408	T	T	T
0.8293070573799664	0.5462571850132468	0.6857962424915054	T	T	T
0.5811818170037679	0.5494540057619767	0.6841662705619285	T	T	T
0.9287581530839759	0.3767501524783957	0.9258573957017497	T	T	T
0.9082886734315228	0.5076601259713220	0.9300347989759407	T	T	T
0.8987328127903648	0.6403456720008130	0.9367364410138380	T	T	T
0.6973327538961110	0.3732305485222745	0.8882963867952158	T	T	T
0.6753961782829899	0.5005063287492180	0.9466728173332245	T	T	T
0.6844647078984663	0.6355362235905629	0.9337627225646142	T	T	T
0.4894486054017800	0.4526431926975651	0.7084631390494645	T	T	T
0.4804116574859709	0.6340407489834509	0.7056419111601253	T	T	T
0.6436823309289843	0.9394573503320636	0.2882997269302586	T	T	T
0.6995917732092235	0.9298791204067709	0.1101695729754832	T	T	T
0.8005592801955476	0.9439036042849093	0.9804164229661435	T	T	T
0.8998027583180892	0.9274329692031142	0.1118311175027840	T	T	T
0.8976458485635824	0.9482211355929747	0.3091142900678605	T	T	T
0.7715389493965640	0.9684657234580151	0.2654722284346748	T	T	T
0.6423474195338450	0.1705696222043896	0.2559358386383680	T	T	T
0.6961273189641016	0.1588929499640131	0.0799152014791931	T	T	T
0.8098633471071160	0.1473664593201947	0.9818862700456180	T	T	T
0.9141233701389730	0.1692654239135821	0.0999973630532069	T	T	T
0.8971374857173676	0.1545659930739018	0.2963569474817051	T	T	T
0.7716283760276126	0.1394461310307180	0.2418311243553318	T	T	T
0.6790867429928871	0.0502163201595704	0.1918455077553482	T	T	T
0.9197727586566145	0.0485374929209350	0.1801704379244771	T	T	T
0.5692224913599345	0.8758072562404879	0.4208764497042149	T	T	T
0.5823009182320126	0.0072647238555902	0.4369949583438859	T	T	T
0.5992065800090079	0.1390725921094622	0.4377609986326063	T	T	T
0.8077736702187598	0.8709958473972674	0.3934793423292410	T	T	T
0.8169695944190601	0.9986833824418638	0.4473015385328802	T	T	T
0.8053723014788127	0.1325486708283849	0.4355181768037060	T	T	T
0.0111726071337972	0.9536519398942643	0.2168781540544746	T	T	T
0.0163157262497853	0.1368048392209639	0.2162899246218064	T	T	T
0.8569959412747005	0.0564618939685185	0.7873339271435523	T	T	T
0.8016239206376183	0.0713103370528675	0.6098599586100363	T	T	T
0.7006323740693303	0.0566146541708479	0.4804290857679144	T	T	T
0.5996204351706168	0.0742818391771156	0.6080300243249858	T	T	T
0.6037679841158584	0.0507627329624955	0.8051414743378934	T	T	T
0.7292850113775634	0.0272626286261042	0.7621250882690193	T	T	T
0.8587006565082205	0.8323562672349740	0.7632657437367469	T	T	T
0.8051169090116295	0.8335018271444101	0.5856938222981397	T	T	T
0.6922952361426864	0.8521045207678093	0.4856494896157360	T	T	T
0.5889161310980980	0.8281288156205798	0.6046996981422829	T	T	T
0.6033823459741631	0.8505801266525936	0.7991721501563818	T	T	T
0.7295344977284440	0.8603936379163576	0.7445383668333494	T	T	T
0.8209920025357046	0.9482685359845054	0.6833607475960519	T	T	T

Structure files (CONTCAR) involved in this work:

0.5800916556074136	0.9520349437275035	0.6738271539561752	T	T	T
0.9320467644352707	0.1263864252887634	0.9127341343249935	T	T	T
0.9185585505374273	0.9958818918575348	0.9420765216189282	T	T	T
0.9044732856069796	0.8633555262577934	0.9426491882883141	T	T	T
0.6957972094177226	0.1273116909115781	0.8862960525864532	T	T	T
0.6836526207501306	0.0003395265791689	0.9449048152278287	T	T	T
0.6966043254334642	0.8662353288559733	0.9382368861389103	T	T	T
0.4895009872560783	0.0469837983529123	0.7152201995380763	T	T	T
0.4845127367214234	0.8638511865508963	0.7153664786075873	T	T	T
0.3581967914460819	0.4322367098178943	0.7103124460461762	T	T	T
0.3102143505754482	0.4387926165397842	0.8929209754741054	T	T	T
0.2008215582392715	0.4546836444948924	0.0056240561376379	T	T	T
0.0930669768241145	0.4285040361206324	0.8960473302252613	T	T	T
0.1006893390146195	0.4379670870288420	0.6996288219557076	T	T	T
0.2282606166845385	0.4587662773375015	0.7428176794547996	T	T	T
0.3567482057677315	0.6746756252184966	0.7423279264429042	T	T	T
0.3010991062026379	0.6444553425397190	0.9131438293193059	T	T	T
0.1892605463041787	0.6473774055558037	0.0182783910399664	T	T	T
0.0909053429989771	0.6698581286745360	0.8898412707045844	T	T	T
0.1010751893297733	0.6552433015313688	0.6954097546142458	T	T	T
0.2273277113438948	0.6437928783237278	0.7492471097271235	T	T	T
0.3208901435499564	0.5498852341290758	0.7785795060207111	T	T	T
0.0814947919341262	0.5476062267693870	0.8105473718878508	T	T	T
0.4337869561104653	0.3764111401272563	0.5705860738884121	T	T	T
0.4155168299809388	0.5079218757488474	0.5673271439659564	T	T	T
0.3896482447627488	0.6386095626202253	0.5584935352009863	T	T	T
0.1941769980505389	0.3649523295119259	0.6122288926877728	T	T	T
0.1785939520333522	0.4949553783856451	0.5657544990856509	T	T	T
0.1923665298137340	0.6289436508309192	0.5575999630688213	T	T	T
0.9847026117056056	0.4552971570812553	0.7887374083165246	T	T	T
0.9838046957109667	0.6352378517841919	0.7828090712559074	T	T	T
0.1336472062851836	0.5667925554006943	0.2172281678795290	T	T	T
0.1887796068784350	0.5576466800980927	0.3943378998984308	T	T	T
0.2946197839101981	0.5480509894856752	0.5167720699603088	T	T	T
0.3966675308902893	0.5696342117064456	0.3936639916544578	T	T	T
0.3938045558792034	0.5587694835702428	0.1973176611595915	T	T	T
0.2651996848033245	0.5436502220602389	0.2367153954946015	T	T	T
0.1408824408786083	0.3239149534358571	0.2473765910741895	T	T	T
0.1952218235777693	0.3580836207720349	0.4172883580034387	T	T	T
0.3097166885958290	0.3534045593080872	0.5141756035626077	T	T	T
0.4094685629435953	0.3283516737189576	0.3877702148350282	T	T	T
0.3946496209692739	0.3449344986354930	0.1920834874529642	T	T	T
0.2703650145984764	0.3534973436623102	0.2541180061902181	T	T	T
0.1769968431022700	0.4489871559336027	0.2760889331651458	T	T	T
0.4130150565512146	0.4503335642030520	0.3116694590671206	T	T	T
0.0643946014679285	0.6248922546326933	0.0724249222258858	T	T	T
0.0814255860944769	0.4925054476394813	0.0686991785568098	T	T	T
0.1121389068860472	0.3624120105657475	0.0617795867991443	T	T	T
0.3062992261914383	0.6361281046680846	0.1082685466312995	T	T	T
0.3158192816882186	0.5053681429412548	0.0614891617763085	T	T	T
0.2980738555415795	0.3713619652225794	0.0605643244937033	T	T	T
0.5072296006950351	0.5435755477379409	0.2877979018000966	T	T	T
0.5126952659673782	0.3642286653768944	0.2740189764509182	T	T	T

Structure files (CONTCAR) involved in this work:

0.4369582167961041	0.7510610843625072	0.6355389997996022	T	T	T
0.1890710837069327	0.7487650743974736	0.6376329210490194	T	T	T
0.2741021865774668	0.7510099340524622	0.0242310640866260	T	T	T
0.1055687869586860	0.7495462403210634	0.0466178292636911	T	T	T
0.0620571656041538	0.2498603544379958	0.1357511968025083	T	T	T
0.3076096317960059	0.2505790485120167	0.1376891882260400	T	T	T
0.2249498904524773	0.2503644620892279	0.5259553562500832	T	T	T
0.3932283238685066	0.2512909292491119	0.5457996258606752	T	T	T
0.5578137440932356	0.2498180208108010	0.3523128402286413	T	T	T
0.8086978533671639	0.2490320821317860	0.3438042410259033	T	T	T
0.7265445615541515	0.2490923951666739	0.9398098583347660	T	T	T
0.8919267744824312	0.2502456809670434	0.9475287462799441	T	T	T
0.9446371703548883	0.7519809919861490	0.8583075955857766	T	T	T
0.6882210951242405	0.7515338275599610	0.8434928554833742	T	T	T
0.7733769828269319	0.7491082880370507	0.4414076303383644	T	T	T
0.6088232280885871	0.7509450770444203	0.4469884545687155	T	T	T
0.9428548378246466	0.4710834305266416	0.5159326714533176	T	T	T
0.8175057004268584	0.3326188269351741	0.3225737773335593	T	T	T
0.8000952256550437	0.6329824497919143	0.6902538737046103	T	T	T
0.9195566538465511	0.4110262192772181	0.4223698012717671	T	T	T
0.8872324603116513	0.5507311354774923	0.5623092033569662	T	T	T
1.0084193269582951	0.6153713161008416	0.4179899740502506	T	T	T
0.9823171802509126	0.5984192753845049	0.5226691958421564	T	T	T
0.0248640733990442	0.5698981211112580	0.3788085152312945	T	T	T
0.0512766690368440	0.6498621297563308	0.4215497625495011	T	T	T
0.9697975399632193	0.6388319228955983	0.3712856072718235	T	T	T
0.9549428145602866	0.6423879772847998	0.5532126718583625	T	T	T
0.9683202203410881	0.5322997130157242	0.5101887222506621	T	T	T
0.0228898277368170	0.5903460506594709	0.5765558432615777	T	T	T

Figure S15(b) Zn-C₂H₅+O_M-H

Si O Al Zn C H

1.0000000000000000

20.0219999999999985 0.0000000000000000 0.0000000000000000

0.0000000000000000 19.8990000000000009 0.0000000000000000

0.0000000000000000 0.0000000000000000 13.3829999999999991

94 193 2 2 2 6

Selective dynamics

Direct

0.4231408149805674	0.0603933603982790	0.6487367953972639	T	T	T
0.3050717134725821	0.0310710083795759	0.7913688041600396	T	T	T
0.2827371717450503	0.0575743371432121	0.0165794200854368	T	T	T
0.1225751190868731	0.0647847765534900	0.0124064562069606	T	T	T
0.0676932696891459	0.0306272976584290	0.8008396227974269	T	T	T
0.1802216768562542	0.0639954625032094	0.6642175558871842	T	T	T
0.4193139664719366	0.8278301604115706	0.6683200937361025	T	T	T
0.3015054048933147	0.8722178071393210	0.8010498380835134	T	T	T
0.2670102218452679	0.8318941653227452	0.0198198820523240	T	T	T
0.1119004797980161	0.8273710416692459	0.0114573414689045	T	T	T
0.0655981966615142	0.8734683981086782	0.7976144085478167	T	T	T
0.1800955017711271	0.8279117291304822	0.6662422111653487	T	T	T
0.0763651121580136	0.9415996749637494	0.1486960245745032	T	T	T
0.1944671337225725	0.9697104415002213	0.2919976906356582	T	T	T
0.2174477551571035	0.9427454023524443	0.5166407023981310	T	T	T

Structure files (CONTCAR) involved in this work:

0.3777187433479685	0.9367605043687461	0.5127257486384548	T	T	T
0.4330170906792760	0.9694849656323099	0.3002232051120312	T	T	T
0.3194952575645156	0.9366146487504258	0.1646351535508844	T	T	T
0.0807115591821710	0.1729374829528810	0.1670269970423960	T	T	T
0.1980235342865305	0.1289641785393319	0.3014662966709264	T	T	T
0.2324489596654487	0.1700634134472502	0.5202211486480771	T	T	T
0.3877410325191527	0.1741635325527631	0.5106660181006304	T	T	T
0.4352479404013840	0.1275251040273613	0.2965413497303305	T	T	T
0.3194951665862624	0.1726641284612944	0.1660073193057928	T	T	T
0.5736713179252396	0.5568883952707173	0.3562157360342792	T	T	T
0.6912283389133295	0.5269324060605755	0.2084553847431198	T	T	T
0.7142875469274718	0.5687401542739657	0.9904861346839647	T	T	T
0.8741846454382557	0.5727955374000500	0.9898284711772011	T	T	T
0.9267714380763311	0.5299220370375833	0.1963097069376230	T	T	T
0.8145089465884527	0.5527694948493092	0.3472096983426006	T	T	T
0.5754116666328808	0.3277286705616796	0.3282810949979699	T	T	T
0.6922547981277923	0.3724621549364013	0.1852462978767501	T	T	T
0.7299920552486338	0.3285413205727427	0.9718287871862998	T	T	T
0.8852942360947083	0.3261553485974292	0.9908504153677197	T	T	T
0.9404444438920576	0.3746367223969294	0.1921953761041733	T	T	T
0.9197417752876471	0.4460509299713437	0.8587829945375473	T	T	T
0.8035526555259060	0.4728504340073085	0.7109340952946429	T	T	T
0.7753922428365343	0.4383183781099994	0.4921071591471786	T	T	T
0.6170654818523019	0.4315448325362414	0.4871363008948606	T	T	T
0.5698093317980520	0.4703129931370290	0.6986895617576064	T	T	T
0.6804477791047671	0.4502420118775531	0.8503561454687013	T	T	T
0.9220741113573658	0.6754483337701660	0.8366754221406519	T	T	T
0.7671111932345835	0.6724382067850926	0.4652881505198038	T	T	T
0.6125485372109899	0.6745766060742391	0.4834245878372058	T	T	T
0.5622227966581160	0.6282833237413240	0.6943262968370628	T	T	T
0.6747995187633536	0.6696310404041955	0.8274284679399022	T	T	T
0.5770365242014299	0.9463651646317499	0.3568329878722667	T	T	T
0.6972305171220159	0.9727986660401059	0.2114747064466790	T	T	T
0.7190533111058767	0.9339818086119424	0.9925458619540785	T	T	T
0.8788405387609568	0.9328181147017367	0.9929093509078148	T	T	T
0.9311249631052857	0.9695955927457293	0.2018935973006299	T	T	T
0.8210950012000618	0.9480788370060510	0.3516286662695693	T	T	T
0.5785479695219011	0.1725909118281833	0.3314052890513204	T	T	T
0.6973609862950073	0.1292750304291018	0.1921095498937087	T	T	T
0.7318836755929728	0.1720078530270531	0.9728223560102572	T	T	T
0.8873435352618985	0.1734482011670447	0.9843614089869435	T	T	T
0.9357299370267756	0.1270213763926230	0.1967073571352041	T	T	T
0.8191284542496565	0.1692931526493740	0.3288610367260704	T	T	T
0.9227323595984348	0.0537313751420539	0.8559615460689646	T	T	T
0.8017942179371147	0.0247228357540293	0.7101360808619647	T	T	T
0.7804707067282998	0.0657095344793250	0.4921508615306062	T	T	T
0.6204417505695415	0.0694978407702575	0.4911781452051071	T	T	T
0.5683006825913840	0.0310052594373835	0.7006206100791517	T	T	T
0.6784124730236183	0.0511530789898534	0.8513249044156066	T	T	T
0.9226262852460978	0.8288639666337285	0.8334038071854235	T	T	T
0.8031063632678684	0.8674043329912581	0.6912098386642638	T	T	T
0.7669082936772513	0.8277062925439627	0.4727648758424483	T	T	T
0.6126254259343096	0.8278772572541435	0.4878248813009528	T	T	T

Structure files (CONTCAR) involved in this work:

0.5641349597416242	0.8734692985308258	0.6987332509399455	T	T	T
0.6804340400178273	0.8294094805522867	0.8303041134111280	T	T	T
0.4242185629981400	0.4430152569493114	0.6419828359801256	T	T	T
0.3051837124935625	0.4700139225455649	0.7839648192649603	T	T	T
0.2803167693024851	0.4431173650853517	0.0085329759514362	T	T	T
0.1217537390994074	0.4363205374579628	0.0120111454938571	T	T	T
0.0660200409794425	0.4697464134909879	0.8020025307491502	T	T	T
0.1765118799494813	0.4397443306376539	0.6566828008776258	T	T	T
0.4171295859387373	0.6743310894720371	0.6622670848714058	T	T	T
0.3021526458374525	0.6280423923065627	0.7976630026572967	T	T	T
0.2675484761857878	0.6707099975154334	0.0185180909759348	T	T	T
0.1133340191065796	0.6735684993096264	0.0117811043568806	T	T	T
0.0662661315086680	0.6277938886667531	0.7998273731704005	T	T	T
0.1789270201279365	0.6704077049586822	0.6623702807558770	T	T	T
0.0721461424848025	0.5586012603593015	0.1452682993117960	T	T	T
0.1930444395007288	0.5293481444472744	0.2834532543600680	T	T	T
0.2142048236003360	0.5579439021015319	0.5113524058861544	T	T	T
0.3737139030707458	0.5660578877990290	0.5117059767427026	T	T	T
0.4282574637808482	0.5302098441035535	0.3005501739440765	T	T	T
0.3205264776165618	0.5614576635233112	0.1523366328932562	T	T	T
0.0841978069821758	0.3259018010115101	0.1639280050830558	T	T	T
0.1973278724641132	0.3712285179237501	0.3008277260942613	T	T	T
0.2315274543893371	0.3312179157785859	0.5195790366280519	T	T	T
0.3863566000054016	0.3280231271087688	0.5052782349819983	T	T	T
0.4324120152969054	0.3725750139678103	0.2926051650605515	T	T	T
0.3170590432569463	0.3300951641691064	0.1627336165601996	T	T	T
0.3591458728545105	0.0697745076840528	0.7219700319128254	T	T	T
0.3162741362649533	0.0532686686901103	0.9065164951583136	T	T	T
0.2022458521126819	0.0514842735740965	0.0087406546336605	T	T	T
0.0926078234468516	0.0695003166439088	0.9005703276392772	T	T	T
0.1036058579111220	0.0636270017333511	0.7036572344460035	T	T	T
0.2295535942785659	0.0515184332086293	0.7590671376465855	T	T	T
0.3599256013373889	0.8273210140786765	0.7508972149582347	T	T	T
0.3031218494375069	0.8614673622205188	0.9207160021522193	T	T	T
0.1887488512817622	0.8537710523700947	0.0186968824475179	T	T	T
0.0870996448613474	0.8314774705895680	0.8965534406427476	T	T	T
0.1031375848999179	0.8411087215667408	0.7007828371132340	T	T	T
0.2288412690426941	0.8491336178288921	0.7586803354284166	T	T	T
0.3154110769106662	0.9507037753049958	0.7750020542071178	T	T	T
0.0879842380822246	0.9515915889393638	0.8102168312893591	T	T	T
0.4335724650765333	0.1290551263530632	0.5846388475406400	T	T	T
0.4129097637374675	0.9984542721733858	0.5715206659773026	T	T	T
0.3943422676359087	0.8664440335891365	0.5682938814760827	T	T	T
0.1957147899263293	0.1372117215234172	0.6161899126176087	T	T	T
0.1894234210141781	0.0051012189996809	0.5819211221449463	T	T	T
0.1972287682595985	0.8714030359520736	0.5670130423269674	T	T	T
0.9877488850184289	0.0397173632822118	0.7865733080294129	T	T	T
0.9852343902575043	0.8689763324126498	0.7824992671061082	T	T	T
0.1403514494583537	0.9316626500525110	0.2218039557892724	T	T	T
0.1834743143089708	0.9465134137202929	0.4067595022691932	T	T	T
0.2978405913794346	0.9492355558031960	0.5083076851437874	T	T	T
0.4076989365410113	0.9320444121575291	0.4009030946130299	T	T	T
0.3960322140222544	0.9366814176258481	0.2039789007282838	T	T	T

Structure files (CONTCAR) involved in this work:

0.2699563155418139	0.9497714943125266	0.2591086144026544	T	T	T
0.1397521722915014	0.1734808694048836	0.2499514198956503	T	T	T
0.1957436826334938	0.1423541063896357	0.4204857009739602	T	T	T
0.3106434156240865	0.1481117750291175	0.5173039203196860	T	T	T
0.4138544701964953	0.1682592927101518	0.3966242965911667	T	T	T
0.3964837811999108	0.1605674738212186	0.2012134863491533	T	T	T
0.2708126821226058	0.1508463224012354	0.2583385353434991	T	T	T
0.1837038952445876	0.0502722554630239	0.2779576728451966	T	T	T
0.4143815905511202	0.0490368007982059	0.3078047100963696	T	T	T
0.0655461935343809	0.8736871615026344	0.0830667153939503	T	T	T
0.0865340498559225	0.0043541102840683	0.0728527268607341	T	T	T
0.1064765850170049	0.1359714017147459	0.0662799165057573	T	T	T
0.3037572321419638	0.8634596620626628	0.1167674740348616	T	T	T
0.3105968011910760	0.9954167197357535	0.0821304380085381	T	T	T
0.3032961885759758	0.1289327779228564	0.0666743643823393	T	T	T
0.5126627458699962	0.9584301548338703	0.2852596894821780	T	T	T
0.5155069359597104	0.1336090872188583	0.2800827829196337	T	T	T
0.6377938978693808	0.5614351424176878	0.2830707184914351	T	T	T
0.6977752225203557	0.5729123224536776	0.1091321016590293	T	T	T
0.7946130975969984	0.5661789707188444	0.9721420831977029	T	T	T
0.8903862190924143	0.5729807180325903	0.1095356978311712	T	T	T
0.8903593838528222	0.5394109148842645	0.3050359615314159	T	T	T
0.7635170623203222	0.5236970442091460	0.2645359322986029	T	T	T
0.6397362870306686	0.3319194219641760	0.2558379231058759	T	T	T
0.6872305211197174	0.3412070488160803	0.0729603214495656	T	T	T
0.8078338045663283	0.3501306626776445	0.9902003309155232	T	T	T
0.9121286586767293	0.3252722087232727	0.1065017402850731	T	T	T
0.9037469064436990	0.3564443963451223	0.3000318306924885	T	T	T
0.7668818598873233	0.3659279077294297	0.2285297215859215	T	T	T
0.6685911876922519	0.4510248113512157	0.1810632769945768	T	T	T
0.9223580671618264	0.4513462096709497	0.1634943785960712	T	T	T
0.5644962241479192	0.6278130867792612	0.4142785460602337	T	T	T
0.5816433064523996	0.4969902327861659	0.4383936751047074	T	T	T
0.5897741677947403	0.3632311813910280	0.4359036754936664	T	T	T
0.8023122356592405	0.6309183138492342	0.3727105403961751	T	T	T
0.8087070214246426	0.5094332343280548	0.4523825470548337	T	T	T
0.8158124920376254	0.3784356916808024	0.4341551772680476	T	T	T
0.0046198566046714	0.5505298379568880	0.2122045760980996	T	T	T
0.0200624869561894	0.3664367431450341	0.2096944235394012	T	T	T
0.8570677333311062	0.4350918676564035	0.7830020053892066	T	T	T
0.7917326982954794	0.4287492651732392	0.6096079728779943	T	T	T
0.6972148791023487	0.4363736523232083	0.4657095753170223	T	T	T
0.6029807158674853	0.4285328743316601	0.6061085657349157	T	T	T
0.6060245671263863	0.4483872407577394	0.8021842443362071	T	T	T
0.7325606478707837	0.4800051019723116	0.7674941364602399	T	T	T
0.8608392084252215	0.6721826572375466	0.7618586792318748	T	T	T
0.8058601527306666	0.6583914760141685	0.5673354496677252	T	T	T
0.6890850946899485	0.6478056663995180	0.4730522886450961	T	T	T
0.5877577479900020	0.6708907738195646	0.5983774272362693	T	T	T
0.5965310930930895	0.6584427379786538	0.7945173983258398	T	T	T
0.7230415758113599	0.6373034956385858	0.7445725066720258	T	T	T
0.8327526722598482	0.5464153831337533	0.6769130534743814	T	T	T
0.5812349644590028	0.5496570755397108	0.6775289373068477	T	T	T

Structure files (CONTCAR) involved in this work:

0.9299162841946697	0.3778367274045395	0.9244239099142726	T	T	T
0.9093950045161988	0.5087076280914059	0.9348991906530056	T	T	T
0.9043344529408066	0.6419779283793634	0.9455150909369194	T	T	T
0.7005867913737995	0.3739237267135925	0.8811190325722948	T	T	T
0.6817391999635217	0.4992491231421358	0.9473727675055478	T	T	T
0.6835375484667608	0.6345512809912719	0.9372408888624071	T	T	T
0.4908242976440251	0.4525095894415807	0.7095570867642336	T	T	T
0.4814830346584995	0.6342348407336688	0.7054396797077161	T	T	T
0.6431614956423150	0.9407583819727581	0.2877605891639634	T	T	T
0.6983273733044723	0.9284091982847781	0.1095977869858585	T	T	T
0.7991868974442278	0.9451773645965834	0.9807025185532179	T	T	T
0.8994715835596797	0.9266586769545474	0.1098259835877133	T	T	T
0.8964243237039711	0.9487747516917527	0.3067932596528857	T	T	T
0.7706119878032768	0.9711769907131933	0.2628204345482087	T	T	T
0.6418671543422829	0.1695172296220582	0.2565615811529843	T	T	T
0.6968717589979592	0.1615011829346231	0.0809043566433306	T	T	T
0.8098683399449912	0.1490484025490154	0.9803706713037040	T	T	T
0.9141286976394369	0.1696989680447346	0.0984308605724641	T	T	T
0.8963492920667271	0.1541754246080983	0.2947044754431941	T	T	T
0.7706556007179794	0.1367959323042552	0.2428913084540687	T	T	T
0.6773754563383985	0.0501869153941199	0.1862243201512846	T	T	T
0.9187138549259033	0.0485577032030979	0.1772420218223577	T	T	T
0.5670698846678776	0.8767205052823623	0.4185411195574968	T	T	T
0.5816425448706352	0.0078205988206330	0.4367325974971698	T	T	T
0.5982079085261033	0.1396467969029133	0.4386961117037603	T	T	T
0.8048877104417326	0.8727175692646750	0.3895943481783994	T	T	T
0.8166422382512296	0.9997410969710042	0.4452644496633125	T	T	T
0.8055872673312767	0.1333589093636247	0.4364393187182504	T	T	T
0.0102468612246046	0.9543415296010359	0.2155887756201806	T	T	T
0.0156023793132331	0.1365068758292620	0.2150659859713991	T	T	T
0.8572042686377621	0.0555261092458744	0.7854315924469112	T	T	T
0.8002642185699724	0.0706034305440024	0.6096876137906295	T	T	T
0.7000993730787554	0.0574127401628421	0.4788559747593752	T	T	T
0.5997295133542442	0.0739257561298509	0.6082246238413855	T	T	T
0.6034687541128984	0.0517189523391056	0.8052970253233600	T	T	T
0.7291734292028312	0.0268592956268276	0.7637257071206175	T	T	T
0.8605718454145890	0.8307148457485173	0.7561609141440101	T	T	T
0.8034570061433056	0.8340060503950938	0.5807637937769791	T	T	T
0.6898865085720953	0.8535383240248536	0.4836860482189002	T	T	T
0.5868308467528073	0.8291905947208796	0.6027070386323203	T	T	T
0.6042486445908422	0.8487427010128443	0.7976582850169791	T	T	T
0.7305082978212442	0.8571707756290057	0.7433980639533605	T	T	T
0.8195704567833766	0.9473252594415275	0.6823638428940573	T	T	T
0.5800875849199956	0.9519586145774023	0.6759135775968852	T	T	T
0.9316186013557062	0.1263093559206037	0.9108645373887813	T	T	T
0.9176765996436733	0.9959205073932912	0.9416650145746847	T	T	T
0.9010180659185857	0.8635645456307980	0.9385719462807873	T	T	T
0.6954569917287677	0.1268619699644192	0.8883125698687288	T	T	T
0.6814305062650525	-0.0009478248595151	0.9447516502009699	T	T	T
0.6971828795346127	0.8650223497095431	0.9368919799917388	T	T	T
0.4893679054381709	0.0470790924805277	0.7151684999200467	T	T	T
0.4844062396635701	0.8637731051391808	0.7175161984911247	T	T	T
0.3594828089185331	0.4320453835390599	0.7138139764003150	T	T	T

Structure files (CONTCAR) involved in this work:

0.3091798842352941	0.4386878348976394	0.8956120188988795	T	T	T
0.2001317944178894	0.4566457255898632	0.0094462876019619	T	T	T
0.0929174260228730	0.4296776072997557	0.8995248826564313	T	T	T
0.1009587318727553	0.4386459965204761	0.7021178480715817	T	T	T
0.2292244210733567	0.4593266693961587	0.7439611899530656	T	T	T
0.3588153239398418	0.6745232899565687	0.7466189623307117	T	T	T
0.3001236381833019	0.6439792862660378	0.9155789143988683	T	T	T
0.1897720302689765	0.6471402265549808	0.0251159940530651	T	T	T
0.0932038224497594	0.6701605098103948	0.8949855633828347	T	T	T
0.1028073255679263	0.6578334988582873	0.7007076511993977	T	T	T
0.2293925867523733	0.6435806459772470	0.7490684453842111	T	T	T
0.3222800239772649	0.5497300195705531	0.7816222737333326	T	T	T
0.0854560317901362	0.5486849393636076	0.8129034734759262	T	T	T
0.4336799151346046	0.3768622758626203	0.5717878622841734	T	T	T
0.4154596238279616	0.5082465060376443	0.5700973535200666	T	T	T
0.3890079640771342	0.6389329041483349	0.5609074244868180	T	T	T
0.1938542276620462	0.3652731934343989	0.6143206712496015	T	T	T
0.1779778577132753	0.4952327684342623	0.5675183627317413	T	T	T
0.1913380058919157	0.6291425661864616	0.5592758573795070	T	T	T
0.9858182281480127	0.4594164104588811	0.7905704061038523	T	T	T
0.9861531367773234	0.6346719185756742	0.7894381827257856	T	T	T
0.1358099047455154	0.5671889211591241	0.2189395628629365	T	T	T
0.1892314312755628	0.5573508495662152	0.3965080761395213	T	T	T
0.2945248304510358	0.5483417738616545	0.5197189141573713	T	T	T
0.3967624728506153	0.5694208234465673	0.3959423913645395	T	T	T
0.3949499856490236	0.5590067285911475	0.1989368301894669	T	T	T
0.2668612710292220	0.5439959595279928	0.2397351186278640	T	T	T
0.1415063367918068	0.3237779404939704	0.2490928310221546	T	T	T
0.1942968312305624	0.3582478286730494	0.4197237468085533	T	T	T
0.3094038410815482	0.3542419812523970	0.5156161278929191	T	T	T
0.4091613247965440	0.3286398432126643	0.3889856238434401	T	T	T
0.3943236040422560	0.3451999209460240	0.1930377095772866	T	T	T
0.2708795162108996	0.3527029303145706	0.2577946666829304	T	T	T
0.1782515010673060	0.4490190645197483	0.2776689914424381	T	T	T
0.4125651942019183	0.4504601465238430	0.3132975289365261	T	T	T
0.0643566451453535	0.6257558245995331	0.0774293733992577	T	T	T
0.0800375526458570	0.4932146551584031	0.0730562028983027	T	T	T
0.1117688814476997	0.3634249740100466	0.0645648548331648	T	T	T
0.3078276374492962	0.6369175480033755	0.1107711641332363	T	T	T
0.3159628176648450	0.5062689861773947	0.0632667317221452	T	T	T
0.2964040452203282	0.3724217527939561	0.0638984682970360	T	T	T
0.5077113488688780	0.5427800964304144	0.2897289709250884	T	T	T
0.5122042205257286	0.3646250876148892	0.2744400730219370	T	T	T
0.4370119383147191	0.7512598831512077	0.6364519412252754	T	T	T
0.1911128665719236	0.7492867082356031	0.6387276840460506	T	T	T
0.2739963636815234	0.7512233098734870	0.0252257239597710	T	T	T
0.1064948136276839	0.7503262223258516	0.0504987967005615	T	T	T
0.0624063614857319	0.2499426313897571	0.1364597890190166	T	T	T
0.3069546397962811	0.2510572270170467	0.1380288404641854	T	T	T
0.2251000724064350	0.2507425363842791	0.5283702833063422	T	T	T
0.3925607464801623	0.2518093912420654	0.5468855905364997	T	T	T
0.5576452144417300	0.2500097092737709	0.3513949075764913	T	T	T
0.8071201780020193	0.2481350408454893	0.3409721475504509	T	T	T

Structure files (CONTCAR) involved in this work:

0.7257179220365237	0.2501597128362453	0.9390088054256099	T	T	T
0.8936386661528131	0.2509227531514922	0.9461578785474153	T	T	T
0.9453606977236663	0.7525897234148280	0.8578770948102822	T	T	T
0.6885309456857774	0.7494551377451615	0.8438711378027820	T	T	T
0.7694184535777054	0.7510489644849462	0.4328620525935422	T	T	T
0.6062451966805305	0.7517744536256517	0.4453412661129192	T	T	T
0.9458388114691744	0.4584862420181603	0.5267146265416430	T	T	T
0.8157299685940843	0.3315355455817273	0.3197830211669719	T	T	T
0.8012076726315197	0.6327713117125769	0.6908881298111628	T	T	T
0.9139310330397183	0.4071734506599220	0.4235555261471850	T	T	T
0.9112288109360773	0.5589797356288105	0.5793252275358870	T	T	T
0.9789256816345635	0.6607194657442774	0.4465274310733595	T	T	T
0.9846809431111770	0.6200073915229687	0.5428714784013359	T	T	T
0.9754527458213978	0.6289592742315760	0.3796644719032790	T	T	T
0.0234548203151198	0.6929191829967786	0.4375535233308454	T	T	T
0.9351086252151067	0.6940274099895321	0.4476159406249038	T	T	T
0.9890901282307997	0.6538496931174841	0.6072406356826037	T	T	T
0.9944065945142923	0.4620470903683978	0.5294825251482499	T	T	T
0.0303320797497366	0.5889041361159563	0.5423443653636648	T	T	T

Figure S15(b)TS5

Si O Al Zn C H

1.0000000000000000					
20.0219999999999985	0.0000000000000000	0.0000000000000000			
0.0000000000000000	19.8990000000000009	0.0000000000000000			
0.0000000000000000	0.0000000000000000	13.3829999999999991			
94	193	2	2	2	6

Selective dynamics

Direct

0.4231770363453946	0.0604309633075302	0.6487026271874569	T	T	T
0.3052671932981027	0.0308254357357830	0.7918298825526684	T	T	T
0.2824949060425946	0.0578083093030998	0.0166311300987037	T	T	T
0.1223767077410148	0.0652339395910904	0.0125014227098768	T	T	T
0.0679351244493169	0.0310633141372054	0.8003931939438648	T	T	T
0.1807092590495113	0.0642486631648793	0.6643528679365885	T	T	T
0.4190042881328384	0.8276737850025133	0.6675676097357645	T	T	T
0.3018956607764654	0.8718714319065005	0.8019299866765386	T	T	T
0.2673975830900039	0.8317822784044956	0.0201790789228299	T	T	T
0.1122230806130994	0.8275637137663566	0.0106099390957009	T	T	T
0.0659522957798265	0.8740819921547394	0.7969259231860001	T	T	T
0.1807746276146623	0.8278204608289854	0.6673655341468187	T	T	T
0.0764767148525815	0.9416126194249774	0.1487864628172814	T	T	T
0.1941269500532594	0.9693607883428057	0.2930850180004711	T	T	T
0.2179007512893849	0.9427155621667379	0.5172334198297118	T	T	T
0.3780340971787708	0.9370588695224282	0.5122277963112036	T	T	T
0.4324795607526751	0.9708101586517619	0.2999801735057268	T	T	T
0.3190188329445431	0.9368535879240890	0.1651101754004264	T	T	T
0.0802739690881633	0.1727032031014379	0.1672956255621653	T	T	T
0.1975105312474947	0.1286587864305781	0.3021526974220370	T	T	T
0.2326334602448207	0.1704627835365535	0.5203137977138230	T	T	T
0.3878009255674380	0.1746148946843833	0.5112802292492501	T	T	T
0.4344734453086960	0.1283002429512819	0.2969501359983951	T	T	T
0.3187567708005347	0.1727822834846186	0.1663691654195182	T	T	T
0.5733683228971845	0.5570644216297889	0.3539959308068958	T	T	T

Structure files (CONTCAR) involved in this work:

0.6914467709574993	0.5277139850562784	0.2089829173783502	T	T	T
0.7154717298470873	0.5698729139812154	0.9901403079491543	T	T	T
0.8745882608716806	0.5743098945200424	0.9879712423411893	T	T	T
0.9251934263427141	0.5314939850887350	0.1949254347914754	T	T	T
0.8142308443767309	0.5538432497280273	0.3496520811748569	T	T	T
0.5760296638810096	0.3279097295642739	0.3264242133632008	T	T	T
0.6930429187799082	0.3731119826006510	0.1847961610488106	T	T	T
0.7316729377268217	0.3301276989572129	0.9698262693733676	T	T	T
0.8871957350965618	0.3266060688948616	0.9919256567283566	T	T	T
0.9406584230411176	0.3761077857938316	0.1937440766492944	T	T	T
0.9212136322508885	0.4463595881990248	0.8606327927196025	T	T	T
0.8063062844547791	0.4737776135453004	0.7119856437074019	T	T	T
0.7772872265402355	0.4385838452413222	0.4938238787185421	T	T	T
0.6185705434254866	0.4319222672687087	0.4858282546666192	T	T	T
0.5708030797524870	0.4711640318414440	0.6972157872588410	T	T	T
0.6828056199411776	0.4521921532514688	0.8494363691418484	T	T	T
0.9238274092487871	0.6758638748322615	0.8343519595134161	T	T	T
0.7645500232141477	0.6736619489645806	0.4655921621362291	T	T	T
0.6108193491645565	0.6750023171255763	0.4804551253526277	T	T	T
0.5625785071498748	0.6287357986636269	0.6917084135171963	T	T	T
0.6746155058342400	0.6686171429925047	0.8285430486749956	T	T	T
0.5768158365555639	0.9478829311472684	0.3543798606769434	T	T	T
0.6969824365304836	0.9742807320590331	0.2070534390026242	T	T	T
0.7186688868664476	0.9339910535884983	0.9900615500502082	T	T	T
0.8784720408039186	0.9324290877257260	0.9902833747850833	T	T	T
0.9308126605061291	0.9685868466819474	0.1994374132192023	T	T	T
0.8197614959891417	0.9485647315867858	0.3476659746329776	T	T	T
0.5780173178966455	0.1725571660972482	0.3310444306037283	T	T	T
0.6978286856396173	0.1305561656676772	0.1909627016385484	T	T	T
0.7321220156735992	0.1741926114597221	0.9723598929415350	T	T	T
0.8879669174054097	0.1738956794229888	0.9839426114138189	T	T	T
0.9354704847965167	0.1258410046697495	0.1958936227142804	T	T	T
0.8198056638634538	0.1695728602287173	0.3290172595836813	T	T	T
0.9230136792377538	0.0540106608250195	0.8548966513931664	T	T	T
0.8018176054983963	0.0253185835104488	0.7099534622167922	T	T	T
0.7804773563790511	0.0657994480487380	0.4905780716524448	T	T	T
0.6203182129390634	0.0696925086020014	0.4908148488328481	T	T	T
0.5683560824329067	0.0312211644608354	0.7005688980298427	T	T	T
0.6781393118240330	0.0525994654306316	0.8512282741354010	T	T	T
0.9229713239334667	0.8289735321405719	0.8297617730173643	T	T	T
0.8036238763204001	0.8671125699237560	0.6884064936079780	T	T	T
0.7653910649686642	0.8290358740600702	0.4697648110801244	T	T	T
0.6110176810533386	0.8283940962833086	0.4841743173437137	T	T	T
0.5635482426567129	0.8732959517323573	0.6968007538673521	T	T	T
0.6807891195346609	0.8281419819986140	0.8274969252720685	T	T	T
0.4249355282065906	0.4427187682433829	0.6458143730646507	T	T	T
0.3058654677449618	0.4701277029420388	0.7865214734551027	T	T	T
0.2799944612541497	0.4438106701152709	0.0116876171211559	T	T	T
0.1216377295047139	0.4362186424212492	0.0149744361028641	T	T	T
0.0670744864724447	0.4696877666941237	0.8039075483444847	T	T	T
0.1771825778056182	0.4392929417027240	0.6588569962983923	T	T	T
0.4164077303805237	0.6742428866284726	0.6625826775625944	T	T	T
0.3031964728684380	0.6281378128661165	0.7998375559657394	T	T	T

Structure files (CONTCAR) involved in this work:

0.2674123706448488	0.6706278775944475	0.0194423795713271	T	T	T
0.1133107094612518	0.6737611350257633	0.0090677047826715	T	T	T
0.0671515344759417	0.6275124263097065	0.7974381798819588	T	T	T
0.1808934763447562	0.6700224146663909	0.6626373619709427	T	T	T
0.0711222382788277	0.5593587155372498	0.1449231222359320	T	T	T
0.1907262495951746	0.5294381385527493	0.2851142528672245	T	T	T
0.2144770297366907	0.5567062464233719	0.5118311617598453	T	T	T
0.3735089350167001	0.5647975266632650	0.5134857793969134	T	T	T
0.4281999205805057	0.5299460489568247	0.3018224923016249	T	T	T
0.3189491233846644	0.5622444234800595	0.1561181570024004	T	T	T
0.0840123077949971	0.3258041134290586	0.1659464379397793	T	T	T
0.1965503458768257	0.3715513620835445	0.3022034642988447	T	T	T
0.2319541475423289	0.3317554623507236	0.5204974658150370	T	T	T
0.3867997845934464	0.3284246330942386	0.5076888309017531	T	T	T
0.4322061952458832	0.3724628484024739	0.2939742355814062	T	T	T
0.3164190836923455	0.3299588379602753	0.1643296579192390	T	T	T
0.3592449101735418	0.0693790897907219	0.7221212029157411	T	T	T
0.3164693787541989	0.0532437605066312	0.9068774853163405	T	T	T
0.2020374135754977	0.0520728016924643	0.0080785907077652	T	T	T
0.0920714251022185	0.0694946144999184	0.9008777041407682	T	T	T
0.1040707409339126	0.0643047742512428	0.7036527420829095	T	T	T
0.2297977742894874	0.0512678514512112	0.7593601567855209	T	T	T
0.3596175328584996	0.8269994941772768	0.7501322413278432	T	T	T
0.3045247681957867	0.8607546262510345	0.9215121644139399	T	T	T
0.1891571341037819	0.8537306562572075	0.0174741730811468	T	T	T
0.0869448286699050	0.8320917856884940	0.8960433008737303	T	T	T
0.1035686287868801	0.8409708599313760	0.7006599366174805	T	T	T
0.2288575976162912	0.8487430212531512	0.7607412679254624	T	T	T
0.3155725495101812	0.9503920274100272	0.7760012155077989	T	T	T
0.0886837244882170	0.9520791121952098	0.8091580043960127	T	T	T
0.4335533846049021	0.1291778514441834	0.5849101953328343	T	T	T
0.4131554232427422	0.9986523476353920	0.5712075468832876	T	T	T
0.3944370952237523	0.8666722434701120	0.5676755685036207	T	T	T
0.1964502227722544	0.1375093213231762	0.6167153804978283	T	T	T
0.1898211253169624	0.0052643305244413	0.5820651788660164	T	T	T
0.1984819077950671	0.8714218915496731	0.5685241042663486	T	T	T
0.9880452008912961	0.0400327532277263	0.7855177097060866	T	T	T
0.9856101614517953	0.8702686613250616	0.7811282401198878	T	T	T
0.1400341416626532	0.9314219000308996	0.2226660273674944	T	T	T
0.1833159512455274	0.9455651841708459	0.4076570987525905	T	T	T
0.2981787891432008	0.9495586827514463	0.5076869894286085	T	T	T
0.4083009675085098	0.9324365344943164	0.4005371090078166	T	T	T
0.3956575900150438	0.9374802239697623	0.2039711350563423	T	T	T
0.2696633166116619	0.9497645018426062	0.2598682859370826	T	T	T
0.1391234329645376	0.1728673605944367	0.2504792649559879	T	T	T
0.1955392414007115	0.1425214020110661	0.4210407720560904	T	T	T
0.3107840571554989	0.1483536774944128	0.5171997061320569	T	T	T
0.4139459847036642	0.1692995010326079	0.3971808680793891	T	T	T
0.3958137431438014	0.1614598092568466	0.2017031966982593	T	T	T
0.2702436452983167	0.1502118390112960	0.2584509374376519	T	T	T
0.1831325174748010	0.0498596315991666	0.2796279157418118	T	T	T
0.4126098240695711	0.0500422099727411	0.3084597859276877	T	T	T
0.0661803400113555	0.8737795984286364	0.0827195311729293	T	T	T

Structure files (CONTCAR) involved in this work:

0.0868328253233252	0.0048074800272031	0.0738029570743590	T	T	T
0.1064331406583644	0.1365973410640163	0.0659716351900484	T	T	T
0.3034582905700143	0.8635273151559647	0.1175499140822192	T	T	T
0.3096437334944562	0.9954444016058004	0.0824488865804408	T	T	T
0.3032227243750168	0.1290633411606000	0.0667858277713058	T	T	T
0.5122474297070151	0.9615650326111441	0.2838683315524496	T	T	T
0.5147248389950539	0.1337596599595694	0.2800844056648805	T	T	T
0.6362872406305174	0.5640132712922858	0.2788367358758111	T	T	T
0.7024368712572301	0.5727523790057381	0.1096755464416107	T	T	T
0.7952567366252867	0.5708314040744027	0.9661207237458680	T	T	T
0.8875979218676587	0.5740129417922085	0.1085384442581545	T	T	T
0.8892297016516048	0.5419221419183354	0.3037523326145222	T	T	T
0.7617378317939668	0.5243029890690943	0.2701200465295594	T	T	T
0.6389270319622318	0.3313529222181716	0.2511356727120151	T	T	T
0.6896508477130985	0.3436594809834871	0.0712892519938765	T	T	T
0.8097788583399501	0.3504918202453238	0.9881249820802421	T	T	T
0.9120667742201148	0.3262877439184207	0.1085099868081857	T	T	T
0.9045100653518447	0.3589722076207912	0.3019498655881293	T	T	T
0.7668028594064684	0.3663697529059935	0.2311181366394017	T	T	T
0.6688689058493303	0.4517122049815073	0.1823687919606996	T	T	T
0.9226067340760760	0.4527633143380596	0.1634961068609962	T	T	T
0.5622888587035509	0.6274749813683107	0.4132501489473662	T	T	T
0.5837097343330087	0.4971278544735110	0.4354398888915888	T	T	T
0.5929546247836823	0.3634171697946332	0.4332473075141003	T	T	T
0.8038762479486783	0.6321308456367658	0.3765676274414649	T	T	T
0.8098810182712686	0.5107019440535793	0.4551217751255209	T	T	T
0.8169397435910442	0.3787394471270110	0.4360749775595202	T	T	T
0.0024878963296574	0.5543640060374493	0.2099746682715389	T	T	T
0.0203071845421105	0.3675804769422060	0.2101008561669220	T	T	T
0.8587805600254702	0.4351621796538561	0.7844674983850196	T	T	T
0.7939007395387518	0.4294168086419680	0.6113945176286247	T	T	T
0.6989266655424305	0.4377422649593775	0.4686794388452993	T	T	T
0.6020644603878300	0.4284468283139399	0.6041629670390108	T	T	T
0.6087596621441583	0.4512256545773650	0.8001502219489666	T	T	T
0.7355227020675190	0.4829819764512798	0.7682002945577379	T	T	T
0.8617880358672019	0.6728452463666904	0.7610342176744939	T	T	T
0.7999344997192502	0.6613700242032468	0.5705727962447631	T	T	T
0.6870166435571561	0.6477463588331009	0.4671412688405541	T	T	T
0.5884161052107818	0.6721439621649083	0.5965980295397679	T	T	T
0.5969183203608435	0.6579775543812288	0.7923830543723742	T	T	T
0.7245663725155176	0.6345464370747970	0.7496292694884011	T	T	T
0.8371111633104574	0.5469470259236695	0.6764072256036023	T	T	T
0.5813956393234698	0.5502626400327406	0.6730666858811529	T	T	T
0.9323557352159438	0.3785571137763253	0.9266896692072514	T	T	T
0.9093249978074841	0.5089349720317906	0.9363080207188270	T	T	T
0.9079908472107759	0.6421119068748933	0.9437238407683148	T	T	T
0.7028618662142359	0.3756583725718798	0.8787731062991792	T	T	T
0.6838677439969384	0.4996565768435463	0.9481441606381572	T	T	T
0.6806740502635092	0.6346636032912061	0.9396437555386270	T	T	T
0.4921803398488598	0.4528386311716517	0.7118693895330817	T	T	T
0.4818672723044054	0.6345232005599587	0.7025091342175658	T	T	T
0.6427686051510689	0.9440965615199282	0.2847581595213798	T	T	T
0.6972721211669259	0.9279701588646028	0.1069040190635760	T	T	T

Structure files (CONTCAR) involved in this work:

0.7988357347555507	0.9455112078251316	0.9798260853027574	T	T	T
0.9001555519665744	0.9253655376924346	0.1067472181724091	T	T	T
0.8953414101252738	0.9477659407788669	0.3038057145621223	T	T	T
0.7704245332651263	0.9728994653052762	0.2582431687169861	T	T	T
0.6412359557028073	0.1684045792289389	0.2563301408634414	T	T	T
0.6986757894830895	0.1661678213844790	0.0820318484986095	T	T	T
0.8101066545634577	0.1510012611485003	0.9776190643064766	T	T	T
0.9133656000376462	0.1692552314279998	0.0986148725154819	T	T	T
0.8965019215620065	0.1523138502866595	0.2945124415971041	T	T	T
0.7703003730143597	0.1370996179044698	0.2443290983469917	T	T	T
0.6785275759294933	0.0515381456122020	0.1785844356561804	T	T	T
0.9185197922248411	0.0475153994320586	0.1744992666427189	T	T	T
0.5668465007444782	0.8768537372384438	0.4124209549543664	T	T	T
0.5818431265727207	0.0073667913571988	0.4374185586431514	T	T	T
0.5971447872576237	0.1396147104439696	0.4385719738353701	T	T	T
0.8015543978279730	0.8732286336107272	0.3839274739133017	T	T	T
0.8156258523352247	-0.0002101671895336	0.4418278745300238	T	T	T
0.8061558506393077	0.1339251132164453	0.4368551117834482	T	T	T
0.0098488430671703	0.9534917944108350	0.2149091270132797	T	T	T
0.0154082223251823	0.1350835325203994	0.2139400359714714	T	T	T
0.8576512582257811	0.0565554289089557	0.7841132341587610	T	T	T
0.8007585326482519	0.0693502379299021	0.6078891613697237	T	T	T
0.7000063107035973	0.0584786675260823	0.4775182476054030	T	T	T
0.5999552800258027	0.0737790918794258	0.6079787439033765	T	T	T
0.6033166071751666	0.0529514740236560	0.8048823985261520	T	T	T
0.7292441709297058	0.0297846667512519	0.7632465195115782	T	T	T
0.8621786443862300	0.8294650068023217	0.7500985232855788	T	T	T
0.8040723768857773	0.8373491344330704	0.5756944514766817	T	T	T
0.6883249625602347	0.8539669593058717	0.4828699202718014	T	T	T
0.5838175833054357	0.8305323465823052	0.5981590321268017	T	T	T
0.6047114436328899	0.8465231538533534	0.7934720792554332	T	T	T
0.7312962000701049	0.8540176993975336	0.7399501750423382	T	T	T
0.8189525912337419	0.9473447838217874	0.6854139724515278	T	T	T
0.5802330021303941	0.9519920253695726	0.6771046882355856	T	T	T
0.9320267210365423	0.1261280807424170	0.9110190106825020	T	T	T
0.9175826296224582	0.9954810181425832	0.9394825814131758	T	T	T
0.8990695426327296	0.8632862802461908	0.9341037675675059	T	T	T
0.6942410781910719	0.1278778078126421	0.8907501112574306	T	T	T
0.6811822033571227	0.9992328945681921	0.9429256886905192	T	T	T
0.6972318266405495	0.8654968848040233	0.9328424886500104	T	T	T
0.4894023421532263	0.0470470405508708	0.7149904239052614	T	T	T
0.4840122818733184	0.8634600632281004	0.7174509803990534	T	T	T
0.3610096849158028	0.4312738780083571	0.7189579669533408	T	T	T
0.3091272394397053	0.4403323877059828	0.8990050157350481	T	T	T
0.1998092707756975	0.4574689142848864	0.0129648902266517	T	T	T
0.0929250903886612	0.4301681320905061	0.9025375739480722	T	T	T
0.1025083095227179	0.4373924523581634	0.7060567677696683	T	T	T
0.2304368182059759	0.4589045480137136	0.7455710172140878	T	T	T
0.3601643505515613	0.6749215246841603	0.7500694439976887	T	T	T
0.3014712561392952	0.6431873122171256	0.9179987249426804	T	T	T
0.1895630704171295	0.6471559036518868	0.0224126461451505	T	T	T
0.0928981062629772	0.6712796362067822	0.8920845808817920	T	T	T
0.1039220144089866	0.6557202257012187	0.6969733856795448	T	T	T

Structure files (CONTCAR) involved in this work:

0.2302742688607333	0.6444010189918725	0.7515424566674553	T	T	T
0.3229162659601503	0.5499154987301541	0.7819970923977611	T	T	T
0.0864462244260974	0.5488606804042506	0.8140763834634629	T	T	T
0.4340777350224782	0.3767130063470273	0.5751962140448380	T	T	T
0.4149027088712114	0.5080796280611291	0.5745656597304007	T	T	T
0.3851288429819290	0.6380477562149369	0.5638877134794856	T	T	T
0.1948658715287389	0.3650714939238314	0.6160975219667488	T	T	T
0.1782793691215012	0.4955869648379917	0.5709301280124512	T	T	T
0.1954532066504784	0.6292038496237864	0.5598185027707920	T	T	T
0.9867791004279249	0.4607333853965663	0.7922677265888249	T	T	T
0.9871342572929749	0.6351569288409887	0.7838088702132895	T	T	T
0.1336516668717120	0.5680520892921593	0.2208747884425735	T	T	T
0.1859289456842291	0.5567319096109542	0.3986423202039893	T	T	T
0.2946643694196309	0.5450393751024347	0.5149140072716631	T	T	T
0.4001220545698203	0.5688558965510822	0.3996439382168538	T	T	T
0.3932273568072641	0.5609820725558543	0.2030919634182205	T	T	T
0.2648007358761602	0.5451096859961616	0.2429876554644846	T	T	T
0.1408485079018802	0.3232036094067349	0.2518953649827078	T	T	T
0.1947231030938334	0.3598515327049251	0.4213460541844772	T	T	T
0.3098980129762545	0.3547723478592643	0.5170047820127145	T	T	T
0.4102064492950320	0.3293290511285084	0.3917083468071201	T	T	T
0.3937784719019626	0.3436879015082849	0.1955746178446968	T	T	T
0.2700548735565079	0.3529405864336886	0.2588942044130566	T	T	T
0.1767702397255182	0.4490446919911392	0.2773483064720605	T	T	T
0.4112285226929281	0.4503435426717102	0.3126656015036073	T	T	T
0.0647070276284437	0.6254130257329575	0.0743599393342719	T	T	T
0.0790159047299522	0.4924448389678418	0.0761973218040911	T	T	T
0.1126089115755554	0.3629523634851861	0.0667692310269037	T	T	T
0.3058535392381132	0.6373905395445297	0.1136676610927127	T	T	T
0.3154642110704575	0.5064973514408019	0.0677922804837103	T	T	T
0.2964760695770843	0.3727039666452964	0.0655759713555031	T	T	T
0.5076091728166017	0.5411133142751305	0.2880168750102729	T	T	T
0.5120182897703172	0.3652790253478800	0.2753535033504272	T	T	T
0.4359383108945447	0.7510152827852488	0.6348718766719634	T	T	T
0.1917061437794996	0.7491650813646328	0.6395934776779041	T	T	T
0.2739144271624374	0.7511095477998713	0.0260249322567954	T	T	T
0.1065219543968814	0.7503175226089740	0.0488924438740376	T	T	T
0.0616158371159633	0.2499473168524328	0.1384978626983365	T	T	T
0.3055679548041567	0.2511174960637080	0.1388024166335569	T	T	T
0.2254977390748953	0.2511581198416112	0.5277295385593112	T	T	T
0.3925716548226469	0.2519958386161274	0.5486583601511343	T	T	T
0.5579558970104623	0.2502936707105807	0.3502585756125383	T	T	T
0.8094981608611599	0.2486689959944481	0.3401574867944156	T	T	T
0.7258433351927567	0.2519220802337432	0.9364540182866037	T	T	T
0.8965836162019852	0.2514834328633238	0.9472492715009543	T	T	T
0.9471366067474700	0.7531066228142204	0.8547708976395684	T	T	T
0.6888029202502353	0.7484460612023776	0.8439037194217189	T	T	T
0.7676440237678099	0.7519290178052648	0.4317713183544655	T	T	T
0.6045387389466275	0.7521380621966225	0.4421465607565330	T	T	T
0.9537913467796804	0.4645641262993864	0.5200656168139870	T	T	T
0.8171876807052952	0.3326283994394085	0.3216106164999887	T	T	T
0.8017574171419714	0.6323287388426320	0.6922624668114660	T	T	T
0.9169877690686752	0.4110945135486064	0.4256410091942430	T	T	T

Structure files (CONTCAR) involved in this work:

0.9131143166432897	0.5426612364083074	0.5726589511626508	T	T	T
0.9965201204879230	0.6252643669403033	0.4490052652036683	T	T	T
0.9568187799707485	0.6350936782889579	0.5337736695466140	T	T	T
0.0223100691841552	0.5428266763928680	0.4261496040027181	T	T	T
0.0504597976812116	0.6333531312853747	0.4503874547337449	T	T	T
0.9736268408003450	0.6245593641337408	0.3749649885505956	T	T	T
0.9075013588877194	0.6576925954853440	0.5208553040769627	T	T	T
0.0034093707743867	0.5087327035215313	0.4562165099882365	T	T	T
0.9820507160390869	0.6519110328886276	0.6017899525427451	T	T	T

Figure S15(b) C₂H₄+H₂

Si O Al Zn C H

1.0000000000000000

20.0219999999999985 0.0000000000000000 0.0000000000000000

0.0000000000000000 19.8990000000000009 0.0000000000000000

0.0000000000000000 0.0000000000000000 13.3829999999999991

94 193 2 2 2 6

Selective dynamics

Direct

0.4236599999999981	0.0600900000000024	0.6490799999999979	T	T	T
0.3055700000000030	0.0306700000000006	0.7918700000000030	T	T	T
0.2830900000000014	0.0578599999999980	0.0171199999999985	T	T	T
0.1229399999999998	0.0649099999999976	0.0131799999999984	T	T	T
0.0677499999999966	0.0310199999999980	0.8010000000000019	T	T	T
0.1806600000000032	0.0636999999999972	0.6643100000000004	T	T	T
0.4198499999999967	0.8276299999999992	0.6681700000000035	T	T	T
0.3026199999999974	0.8716900000000010	0.8020199999999988	T	T	T
0.2677100000000010	0.8322500000000019	0.0207300000000004	T	T	T
0.1127600000000015	0.8277100000000033	0.0108499999999978	T	T	T
0.0656099999999995	0.8731700000000018	0.7969500000000025	T	T	T
0.1811700000000016	0.8276499999999984	0.6670000000000016	T	T	T
0.0776699999999977	0.9415199999999970	0.1494300000000024	T	T	T
0.1955200000000019	0.9700899999999990	0.2926000000000002	T	T	T
0.2179599999999979	0.9425200000000018	0.5170400000000015	T	T	T
0.3780199999999994	0.9365799999999993	0.5132400000000032	T	T	T
0.4341000000000008	0.9688200000000009	0.3011100000000013	T	T	T
0.3204599999999971	0.9374200000000030	0.1654800000000023	T	T	T
0.0818500000000029	0.1738500000000016	0.1667599999999965	T	T	T
0.1987000000000023	0.1292499999999990	0.3017299999999992	T	T	T
0.2330100000000002	0.1700999999999979	0.5203100000000020	T	T	T
0.3882199999999969	0.1736700000000013	0.5100600000000028	T	T	T
0.4361999999999995	0.1269700000000000	0.2961600000000004	T	T	T
0.3200599999999980	0.1724999999999994	0.1665800000000033	T	T	T
0.5738199999999978	0.5562899999999971	0.3565499999999986	T	T	T
0.6888599999999983	0.5256200000000035	0.2032600000000002	T	T	T
0.7120999999999995	0.5676100000000019	0.9892499999999984	T	T	T
0.8718900000000005	0.5705099999999987	0.9856399999999965	T	T	T
0.9278100000000009	0.5326200000000014	0.1925600000000003	T	T	T
0.8113600000000005	0.5542500000000032	0.3365399999999994	T	T	T
0.5756700000000023	0.3269400000000005	0.3284200000000013	T	T	T
0.6935000000000002	0.3710799999999992	0.1863900000000029	T	T	T
0.7305599999999970	0.3278400000000019	0.9736699999999985	T	T	T
0.8852300000000000	0.3270899999999983	0.9937699999999978	T	T	T
0.9412999999999982	0.3772499999999965	0.1939899999999994	T	T	T

Structure files (CONTCAR) involved in this work:

0.9196099999999987	0.4442799999999991	0.8558599999999998	T	T	T
0.8033300000000025	0.4732199999999978	0.7117700000000013	T	T	T
0.7729700000000008	0.4403900000000007	0.4881999999999991	T	T	T
0.6150099999999981	0.4313199999999995	0.4863399999999984	T	T	T
0.5692499999999967	0.4693699999999978	0.6986500000000007	T	T	T
0.6793499999999995	0.4494600000000020	0.8509600000000006	T	T	T
0.9199500000000000	0.6766399999999990	0.8316500000000033	T	T	T
0.7691299999999970	0.6695399999999978	0.4624900000000025	T	T	T
0.6144800000000004	0.6739400000000018	0.4856300000000005	T	T	T
0.5627700000000004	0.6278099999999966	0.6961200000000005	T	T	T
0.6783300000000025	0.6712599999999966	0.8228700000000018	T	T	T
0.5786700000000025	0.9456399999999974	0.3577299999999966	T	T	T
0.6993599999999986	0.9724300000000028	0.2122799999999998	T	T	T
0.7206400000000031	0.9341799999999978	0.9926600000000008	T	T	T
0.8807699999999983	0.9338699999999989	0.9948800000000020	T	T	T
0.9329999999999998	0.9695899999999966	0.2046700000000001	T	T	T
0.8228900000000010	0.9470000000000027	0.3539900000000031	T	T	T
0.5793000000000035	0.1718699999999984	0.3312000000000026	T	T	T
0.6994400000000027	0.1299599999999970	0.1927900000000022	T	T	T
0.7329700000000017	0.1718699999999984	0.9733500000000035	T	T	T
0.8878800000000027	0.1738500000000016	0.9872399999999999	T	T	T
0.9375199999999992	0.1272499999999965	0.1991999999999976	T	T	T
0.8212600000000023	0.1708500000000015	0.3299599999999998	T	T	T
0.9233300000000000	0.0555599999999998	0.8575400000000002	T	T	T
0.8031900000000007	0.0266299999999973	0.7109200000000016	T	T	T
0.7813900000000018	0.0661699999999996	0.4924699999999973	T	T	T
0.6212599999999995	0.0691199999999981	0.4919200000000004	T	T	T
0.5690000000000026	0.0310699999999997	0.7011099999999999	T	T	T
0.6794999999999973	0.0516700000000014	0.8511099999999985	T	T	T
0.9231899999999982	0.8292300000000026	0.8367000000000004	T	T	T
0.8038999999999987	0.8697999999999979	0.6950900000000004	T	T	T
0.7702900000000028	0.8272800000000018	0.4777100000000019	T	T	T
0.6155100000000004	0.8272699999999986	0.4894000000000034	T	T	T
0.5648199999999974	0.8736699999999971	0.6987499999999969	T	T	T
0.6808800000000019	0.8309899999999999	0.8300500000000000	T	T	T
0.4240899999999996	0.4425600000000003	0.6414600000000021	T	T	T
0.3051800000000000	0.4699299999999980	0.7840800000000030	T	T	T
0.2804900000000004	0.4426199999999980	0.0078200000000024	T	T	T
0.1221099999999993	0.4369900000000015	0.0119800000000012	T	T	T
0.0659100000000024	0.4690200000000004	0.8008000000000024	T	T	T
0.1771999999999991	0.4399999999999977	0.6558899999999994	T	T	T
0.4184199999999976	0.6741000000000028	0.6616799999999969	T	T	T
0.3020500000000013	0.6280700000000010	0.7968600000000023	T	T	T
0.2686399999999978	0.6713700000000031	0.0177600000000027	T	T	T
0.1146099999999990	0.6737699999999975	0.0103000000000009	T	T	T
0.0656200000000027	0.6277400000000029	0.7995499999999964	T	T	T
0.1785500000000013	0.6697699999999998	0.6625999999999976	T	T	T
0.0731200000000030	0.5593700000000013	0.1454200000000014	T	T	T
0.1943300000000008	0.5295300000000012	0.2829400000000035	T	T	T
0.2154200000000017	0.5582800000000034	0.5112600000000000	T	T	T
0.3751499999999979	0.5659800000000033	0.5108699999999970	T	T	T
0.4290499999999966	0.5304199999999994	0.2990300000000019	T	T	T
0.3214699999999979	0.5608300000000028	0.1500199999999978	T	T	T

Structure files (CONTCAR) involved in this work:

0.0846799999999988	0.3267600000000002	0.1636000000000024	T	T	T
0.1976500000000030	0.3714200000000005	0.3013499999999993	T	T	T
0.2322899999999990	0.3311800000000034	0.5194699999999983	T	T	T
0.3871299999999991	0.3276600000000016	0.5042699999999982	T	T	T
0.4336800000000025	0.3723099999999988	0.2913500000000013	T	T	T
0.3171099999999996	0.3301999999999978	0.1632600000000011	T	T	T
0.3597099999999998	0.0692700000000031	0.7224300000000028	T	T	T
0.3162999999999982	0.0534200000000027	0.9068600000000018	T	T	T
0.2025900000000007	0.0511499999999998	0.0101799999999983	T	T	T
0.0934499999999971	0.0688299999999984	0.9010699999999972	T	T	T
0.1040899999999993	0.0638399999999990	0.7040799999999976	T	T	T
0.2300600000000017	0.0506000000000029	0.7589100000000002	T	T	T
0.3609799999999979	0.8268800000000027	0.7515300000000025	T	T	T
0.3048199999999994	0.8604100000000017	0.9215799999999987	T	T	T
0.1895400000000009	0.8543599999999998	0.0169100000000029	T	T	T
0.0869900000000001	0.8317499999999995	0.8964300000000023	T	T	T
0.1041499999999971	0.8412399999999991	0.7008000000000010	T	T	T
0.2298699999999982	0.8487300000000033	0.7595900000000029	T	T	T
0.3163300000000007	0.9502600000000001	0.7764799999999994	T	T	T
0.0865200000000002	0.9515900000000030	0.8093999999999966	T	T	T
0.4337299999999971	0.1286199999999980	0.5846299999999971	T	T	T
0.4136700000000033	0.9978699999999989	0.5722799999999992	T	T	T
0.3938800000000029	0.8659600000000012	0.5685100000000034	T	T	T
0.1967399999999984	0.1367499999999993	0.6163600000000002	T	T	T
0.1891299999999987	0.0046200000000027	0.5820399999999992	T	T	T
0.1985299999999981	0.8709399999999974	0.5676199999999980	T	T	T
0.9879000000000033	0.0414000000000030	0.7873099999999980	T	T	T
0.9854300000000009	0.8666300000000007	0.7805200000000028	T	T	T
0.1424000000000021	0.9316000000000031	0.2211199999999991	T	T	T
0.1841999999999970	0.9459000000000017	0.4069100000000034	T	T	T
0.2982900000000015	0.9498600000000010	0.5089499999999987	T	T	T
0.4081499999999991	0.9315500000000014	0.4015600000000035	T	T	T
0.3971200000000010	0.9363900000000029	0.2044700000000006	T	T	T
0.2714399999999983	0.9513200000000026	0.2603700000000018	T	T	T
0.1416600000000017	0.1743400000000008	0.2484499999999983	T	T	T
0.1957400000000007	0.1430199999999999	0.4206000000000003	T	T	T
0.3111000000000033	0.1476800000000011	0.5162499999999994	T	T	T
0.4148199999999989	0.1676300000000026	0.3962799999999973	T	T	T
0.3971700000000027	0.1597099999999969	0.2008300000000034	T	T	T
0.2720199999999977	0.1500699999999995	0.2593699999999970	T	T	T
0.1836100000000016	0.0505100000000027	0.2792200000000022	T	T	T
0.4158800000000014	0.0484099999999970	0.3082399999999978	T	T	T
0.0667600000000022	0.8738299999999981	0.0832400000000035	T	T	T
0.0865999999999971	0.0048800000000000	0.0743399999999994	T	T	T
0.1067600000000013	0.1364900000000020	0.0657300000000021	T	T	T
0.3035700000000006	0.8644999999999996	0.1178200000000018	T	T	T
0.3118600000000029	0.9961399999999969	0.0828100000000020	T	T	T
0.3032600000000016	0.1294400000000024	0.0667699999999982	T	T	T
0.5137300000000025	0.9569600000000023	0.2871000000000024	T	T	T
0.5164299999999997	0.1330400000000012	0.2792000000000030	T	T	T
0.6392000000000024	0.5574299999999965	0.2857500000000002	T	T	T
0.6894800000000032	0.5740699999999990	0.1056999999999988	T	T	T
0.7924099999999967	0.5568799999999996	0.9804999999999993	T	T	T

Structure files (CONTCAR) involved in this work:

0.8947000000000003	0.5754599999999996	0.1026000000000025	T	T	T
0.8884600000000020	0.5444900000000032	0.2985699999999980	T	T	T
0.7640000000000029	0.5241299999999995	0.2507400000000004	T	T	T
0.6414499999999990	0.3317800000000020	0.2592399999999984	T	T	T
0.6881199999999978	0.3371599999999972	0.0758099999999970	T	T	T
0.8078100000000035	0.3511400000000009	0.9920499999999990	T	T	T
0.9117999999999995	0.3273200000000003	0.1094900000000010	T	T	T
0.9052300000000031	0.3616400000000013	0.3028300000000002	T	T	T
0.7680900000000008	0.3663600000000002	0.2299099999999967	T	T	T
0.6682699999999997	0.4491799999999984	0.1762500000000031	T	T	T
0.9241000000000028	0.4538000000000011	0.1620199999999983	T	T	T
0.5680100000000010	0.6278700000000015	0.4136700000000033	T	T	T
0.5775999999999968	0.4963400000000036	0.4391299999999987	T	T	T
0.5874900000000025	0.3626599999999982	0.4365400000000008	T	T	T
0.7973399999999984	0.6327100000000030	0.3609799999999979	T	T	T
0.8023799999999994	0.5132100000000008	0.4438000000000031	T	T	T
0.8143299999999982	0.3807600000000022	0.4344299999999990	T	T	T
0.0052099999999982	0.5536499999999975	0.2123500000000007	T	T	T
0.0209499999999991	0.3678000000000026	0.2089599999999976	T	T	T
0.8568899999999999	0.4322400000000002	0.7799499999999995	T	T	T
0.7877900000000011	0.4350400000000008	0.6067200000000028	T	T	T
0.6945300000000003	0.4376200000000026	0.4623800000000031	T	T	T
0.6020699999999977	0.4282899999999970	0.6054000000000030	T	T	T
0.6059199999999976	0.4450700000000012	0.8002499999999984	T	T	T
0.7332800000000006	0.4801700000000011	0.7714399999999983	T	T	T
0.8648099999999985	0.6787300000000016	0.7458999999999989	T	T	T
0.8144899999999993	0.6449100000000030	0.5557500000000033	T	T	T
0.6915400000000034	0.6474800000000016	0.4806099999999986	T	T	T
0.5870600000000010	0.6699100000000016	0.5989100000000036	T	T	T
0.5996600000000001	0.6582099999999969	0.7941900000000004	T	T	T
0.7257099999999994	0.6423399999999972	0.7357299999999967	T	T	T
0.8344900000000024	0.5471199999999996	0.6830700000000007	T	T	T
0.5811800000000034	0.5490399999999980	0.6800100000000029	T	T	T
0.9295100000000005	0.3777800000000013	0.9253700000000009	T	T	T
0.9090100000000021	0.5086000000000013	0.9290900000000022	T	T	T
0.8926900000000018	0.6407099999999986	0.9336199999999977	T	T	T
0.7000099999999989	0.3740499999999969	0.8848699999999994	T	T	T
0.6758000000000024	0.5005299999999977	0.9453499999999977	T	T	T
0.6910200000000017	0.6352600000000024	0.9309500000000028	T	T	T
0.4902200000000008	0.4524199999999965	0.7099600000000024	T	T	T
0.4822699999999998	0.6351599999999991	0.7094999999999985	T	T	T
0.6443500000000029	0.9410600000000002	0.2876300000000001	T	T	T
0.6998600000000010	0.9288499999999971	0.1096500000000020	T	T	T
0.8009300000000010	0.9437599999999975	0.9805599999999970	T	T	T
0.9004100000000008	0.9278800000000018	0.1121300000000005	T	T	T
0.8982999999999990	0.9484500000000011	0.3095199999999991	T	T	T
0.7723799999999983	0.9679700000000011	0.2642700000000033	T	T	T
0.6430599999999984	0.1689099999999968	0.2572699999999983	T	T	T
0.6974099999999979	0.1613699999999980	0.0810699999999969	T	T	T
0.8107400000000027	0.1483199999999982	0.9820800000000034	T	T	T
0.9145600000000016	0.1694900000000032	0.1012399999999971	T	T	T
0.8983899999999991	0.1537700000000015	0.2975800000000035	T	T	T
0.7726899999999972	0.1398599999999988	0.2426000000000030	T	T	T

Structure files (CONTCAR) involved in this work:

0.6815199999999990	0.0503199999999993	0.1880700000000033	T	T	T
0.9214199999999977	0.0485499999999988	0.1803700000000035	T	T	T
0.5704100000000025	0.8755099999999985	0.4188199999999966	T	T	T
0.5830699999999993	0.0066300000000012	0.4383800000000022	T	T	T
0.5983599999999996	0.1386899999999969	0.4385499999999993	T	T	T
0.8083499999999972	0.8713899999999981	0.3935800000000000	T	T	T
0.8169400000000024	0.9995199999999969	0.4462800000000016	T	T	T
0.8058800000000019	0.1336900000000014	0.4361699999999971	T	T	T
0.0119600000000020	0.9530699999999968	0.2178299999999993	T	T	T
0.0173899999999989	0.1372199999999992	0.2162900000000008	T	T	T
0.8575400000000002	0.0579200000000029	0.7874300000000005	T	T	T
0.8021400000000014	0.0715999999999966	0.6096500000000020	T	T	T
0.7010000000000005	0.0575800000000015	0.4802400000000020	T	T	T
0.6003699999999981	0.0741000000000014	0.6088600000000000	T	T	T
0.6042800000000028	0.0513899999999978	0.8059799999999981	T	T	T
0.7298899999999975	0.0283799999999985	0.7624300000000019	T	T	T
0.8587199999999982	0.8327400000000011	0.7642400000000009	T	T	T
0.8065100000000029	0.8347399999999965	0.5856700000000004	T	T	T
0.6930400000000034	0.8523700000000005	0.4864499999999978	T	T	T
0.5885899999999964	0.8289699999999982	0.6036100000000033	T	T	T
0.6041999999999987	0.8489900000000006	0.7984799999999979	T	T	T
0.7298800000000014	0.8612899999999968	0.7434599999999989	T	T	T
0.8220099999999988	0.9491299999999967	0.6846800000000002	T	T	T
0.5810400000000016	0.9520600000000030	0.6759300000000010	T	T	T
0.9327899999999971	0.1277600000000021	0.9130099999999999	T	T	T
0.9181900000000027	0.9976300000000009	0.9431799999999981	T	T	T
0.9058800000000033	0.8649899999999988	0.9425200000000018	T	T	T
0.6962499999999991	0.1272799999999989	0.8884499999999989	T	T	T
0.6839399999999998	0.9995400000000032	0.9444000000000017	T	T	T
0.6975100000000012	0.8654300000000035	0.9374200000000030	T	T	T
0.4900400000000005	0.0470499999999987	0.7154400000000010	T	T	T
0.4850100000000026	0.8641700000000014	0.7162000000000006	T	T	T
0.3591399999999965	0.4324099999999973	0.7128399999999999	T	T	T
0.3088600000000028	0.4368800000000022	0.8947199999999995	T	T	T
0.2005300000000005	0.4575999999999993	0.0097499999999968	T	T	T
0.0932699999999969	0.4306500000000000	0.8996899999999997	T	T	T
0.1023199999999989	0.4384799999999984	0.7023099999999971	T	T	T
0.2294399999999968	0.4606500000000011	0.7434900000000013	T	T	T
0.3575700000000026	0.6738100000000031	0.7416800000000023	T	T	T
0.3016000000000005	0.6475099999999969	0.9136499999999970	T	T	T
0.1909899999999993	0.6471700000000027	0.0226800000000011	T	T	T
0.0936299999999974	0.6703100000000006	0.8937700000000035	T	T	T
0.1017300000000034	0.6572499999999977	0.6992400000000032	T	T	T
0.2284399999999991	0.6422000000000025	0.7496300000000033	T	T	T
0.3227699999999984	0.5496399999999966	0.7849799999999973	T	T	T
0.0835099999999969	0.5485600000000019	0.8119599999999991	T	T	T
0.4339700000000022	0.3760699999999986	0.5722299999999976	T	T	T
0.4161700000000010	0.5074100000000001	0.5685900000000004	T	T	T
0.3935999999999993	0.6385000000000005	0.5587599999999995	T	T	T
0.1958100000000016	0.3655100000000004	0.6148200000000017	T	T	T
0.1797299999999993	0.4950400000000030	0.5661800000000028	T	T	T
0.1910499999999971	0.6291500000000028	0.5591000000000008	T	T	T
0.9861999999999966	0.4565800000000024	0.7891699999999986	T	T	T

Structure files (CONTCAR) involved in this work:

0.985509999999979	0.635759999999977	0.789979999999999	T	T	T
0.136609999999975	0.567660000000036	0.219499999999965	T	T	T
0.192659999999965	0.558639999999969	0.395440000000007	T	T	T
0.295830000000023	0.550480000000003	0.522089999999986	T	T	T
0.396450000000015	0.568710000000029	0.394359999999989	T	T	T
0.395699999999979	0.558549999999968	0.197209999999983	T	T	T
0.267620000000009	0.543109999999986	0.236750000000007	T	T	T
0.142130000000016	0.324289999999977	0.248480000000007	T	T	T
0.194490000000018	0.357649999999996	0.419910000000016	T	T	T
0.310240000000003	0.353980000000000	0.513370000000019	T	T	T
0.410919999999973	0.328789999999979	0.388399999999972	T	T	T
0.394500000000007	0.345520000000005	0.192500000000026	T	T	T
0.271389999999967	0.353000000000015	0.258560000000028	T	T	T
0.179020000000013	0.449370000000018	0.278649999999990	T	T	T
0.415210000000019	0.450470000000028	0.311979999999984	T	T	T
0.065869999999968	0.626229999999996	0.076610000000023	T	T	T
0.080379999999981	0.493549999999990	0.074100000000014	T	T	T
0.112499999999972	0.363889999999978	0.064030000000025	T	T	T
0.308909999999974	0.636360000000034	0.108820000000015	T	T	T
0.317480000000033	0.505809999999968	0.060679999999978	T	T	T
0.295940000000016	0.372149999999978	0.064300000000029	T	T	T
0.508169999999998	0.545409999999968	0.288269999999971	T	T	T
0.513240000000032	0.363250000000007	0.271650000000011	T	T	T
0.438150000000003	0.751190000000011	0.636490000000020	T	T	T
0.191360000000031	0.748779999999964	0.640300000000034	T	T	T
0.274290000000006	0.751699999999996	0.028799999999968	T	T	T
0.107900000000008	0.750509999999985	0.049320000000016	T	T	T
0.062919999999983	0.250660000000034	0.136249999999969	T	T	T
0.307389999999981	0.250970000000024	0.139449999999965	T	T	T
0.226149999999970	0.250689999999987	0.529449999999971	T	T	T
0.393009999999968	0.251390000000007	0.545760000000014	T	T	T
0.558050000000015	0.249160000000034	0.351170000000033	T	T	T
0.811529999999976	0.249850000000021	0.342570000000020	T	T	T
0.727769999999996	0.249859999999982	0.938479999999984	T	T	T
0.893389999999966	0.251500000000001	0.950440000000004	T	T	T
0.943480000000010	0.752299999999982	0.861649999999974	T	T	T
0.690959999999969	0.751040000000033	0.840820000000008	T	T	T
0.774529999999986	0.749560000000024	0.442349999999976	T	T	T
0.610059999999972	0.751060000000025	0.447139999999974	T	T	T
0.943319999999999	0.475540000000023	0.516950000000014	T	T	T
0.818210000000005	0.333799999999965	0.322099999999989	T	T	T
0.804299999999978	0.632910000000025	0.685800000000004	T	T	T
0.917169999999987	0.417400000000007	0.423149999999997	T	T	T
0.893000000000007	0.550440000000018	0.553379999999971	T	T	T
0.967120000000013	0.639400000000020	0.453560000000031	T	T	T
0.978630000000026	0.632790000000000	0.552360000000002	T	T	T
0.068429999999993	0.491160000000007	0.400440000000032	T	T	T
0.991030000000021	0.606450000000024	0.399039999999994	T	T	T
0.934660000000009	0.679000000000020	0.424529999999972	T	T	T
0.957459999999975	0.667780000000005	0.606630000000027	T	T	T
0.039299999999972	0.490009999999981	0.436660000000034	T	T	T
0.014600000000015	0.595700000000008	0.579470000000006	T	T	T

Figure S17 ZnFe-IS

Structure files (CONTCAR) involved in this work:

Si O Al Zn Fe H C

1.0000000000000000

20.0219999999999985 0.0000000000000000 0.0000000000000000

0.0000000000000000 19.8990000000000009 0.0000000000000000

0.0000000000000000 0.0000000000000000 13.3829999999999991

93 193 3 1 1 6 2

Selective dynamics

Direct

0.4229141193706922 0.0581534253114713 0.6490883143545297 T T T

0.3061591895854937 0.0285490877315067 0.7953985143611695 T T T

0.2822829973217841 0.0581866244201676 0.0169621793247954 T T T

0.1228348547737962 0.0614968416342992 0.0118088705959296 T T T

0.0683700970143451 0.0293656397713282 0.8004650033206943 T T T

0.1818380154606187 0.0582197250249544 0.6637155556435087 T T T

0.4204982208842057 0.8262553328236513 0.6704443534606123 T T T

0.3043870563273366 0.8696060584116362 0.8092387262831741 T T T

0.2669173036003142 0.8291518364719338 0.0277058555912679 T T T

0.1121638398493219 0.8261575318656958 0.0149120558832933 T T T

0.0655622330909704 0.8721343650055945 0.8006507526907991 T T T

0.1827388874976745 0.8272064711239483 0.6735010810291313 T T T

0.0777387886656615 0.9407465813805596 0.1507226375868297 T T T

0.1958565103404133 0.9705261852915278 0.2951467236913694 T T T

0.2190347202077511 0.9381761106196899 0.5172787819413354 T T T

0.3794576662811682 0.9338168861891456 0.5139301459438398 T T T

0.4345633808561756 0.9680667819613205 0.3019089301309648 T T T

0.3208515997519272 0.9398636032784443 0.1640788287713477 T T T

0.0822746189466202 0.1715565707042623 0.1666103577048148 T T T

0.1962436893577899 0.1296993477633967 0.3094548198863199 T T T

0.2334839982370460 0.1696220399004464 0.5262974920665656 T T T

0.3880367997912376 0.1727119896052550 0.5101327464606782 T T T

0.4365196029240395 0.1264831692551449 0.2972111903265679 T T T

0.3170254809553860 0.1705646619388137 0.1727968488868664 T T T

0.5779701803020146 0.5566433678554417 0.3544270488557958 T T T

0.6883621655319484 0.5272514404627661 0.1992176261526062 T T T

0.7162768134119057 0.5649309965087036 0.9835484362554100 T T T

0.8747887399072807 0.5709845029868799 0.9827830383695015 T T T

0.8090474483570232 0.5516776102427172 0.3372105055344648 T T T

0.5739631897578196 0.3274578403827699 0.3285017871082655 T T T

0.6926476728839248 0.3737950861085103 0.1902671787244752 T T T

0.7327368600462897 0.3279456496277147 0.9776151336476210 T T T

0.8876682635192243 0.3253312867538249 0.9901138760814550 T T T

0.9431979023267744 0.3739847812128743 0.1887124346325499 T T T

0.9210009342223657 0.4452232603130109 0.8564172289933035 T T T

0.8011435077814669 0.4740679608516351 0.7151862227454726 T T T

0.7776402920773891 0.4354167215287180 0.4907388411965417 T T T

0.6193703810140216 0.4288589631067155 0.4870590011404379 T T T

0.5687308213355284 0.4675946694869145 0.7006791814501224 T T T

0.6775153960504529 0.4460199978867399 0.8510931680781182 T T T

0.9189348955733799 0.6777657517784730 0.8238639209795473 T T T

0.7658613714732551 0.6687932867520860 0.4598859019210707 T T T

0.6118353170048021 0.6728341676581510 0.4889370444093710 T T T

0.5614519408734582 0.6261163144234958 0.7007435301897560 T T T

0.6767952739934474 0.6736750165016172 0.8232844076129620 T T T

Structure files (CONTCAR) involved in this work:

0.5792605816883920	0.9437164736262482	0.3568773955153862	T	T	T
0.6977525297955789	0.9719913546792035	0.2117091437979508	T	T	T
0.7217180308554505	0.9383877966089764	0.9901430858905407	T	T	T
0.8820427989146633	0.9340559193936776	0.9946998153427211	T	T	T
0.9336900021385944	0.9700188693741069	0.2052070963940177	T	T	T
0.8218088931277845	0.9453614855396272	0.3500356193671564	T	T	T
0.5794892826780982	0.1728867317970153	0.3278131534604932	T	T	T
0.6978669845647341	0.1300453627894099	0.1910007134590828	T	T	T
0.7334095386758390	0.1707026733848843	0.9709560486049816	T	T	T
0.8882044500885407	0.1730119846219356	0.9822927032508908	T	T	T
0.9364713353298907	0.1283067266671241	0.1970899102117495	T	T	T
0.8193098152266373	0.1736235073465640	0.3266232268174296	T	T	T
0.9240527235768708	0.0539170656216527	0.8544498218907043	T	T	T
0.8040082357205466	0.0261482491660908	0.7056228001358740	T	T	T
0.7824244285715306	0.0661925866973087	0.4891643707369698	T	T	T
0.6217293392173858	0.0689951933926177	0.4896306163679598	T	T	T
0.5678100385239758	0.0320141715910361	0.6989283502693197	T	T	T
0.6809471045142453	0.0547751295314740	0.8439093720598480	T	T	T
0.9228138842985758	0.8293031094526927	0.8356821420508255	T	T	T
0.8031697232855051	0.8682038114814443	0.6923966511774193	T	T	T
0.7689080594815879	0.8263904965701968	0.4763728066732731	T	T	T
0.6141364538515848	0.8265579533381904	0.4916007961433811	T	T	T
0.5640890989731669	0.8747799096340274	0.7000460356684580	T	T	T
0.6803965264980029	0.8322950077687810	0.8307362498107775	T	T	T
0.4233269159170631	0.4416999805436737	0.6441885108178889	T	T	T
0.3052859141621339	0.4701014425348558	0.7902306593716806	T	T	T
0.2788353033924233	0.4401400295583275	0.0118743232040226	T	T	T
0.1213857960146780	0.4356930331214209	0.0135478431509595	T	T	T
0.0650875282121384	0.4694141405771021	0.8014999870566041	T	T	T
0.1786227555165754	0.4419077262895491	0.6586626897417439	T	T	T
0.4183748400158349	0.6724753026648237	0.6662187155584723	T	T	T
0.3031918985844869	0.6279750633351842	0.8057514347244180	T	T	T
0.2676043156659253	0.6697045607093279	0.0245107836490044	T	T	T
0.1135712851568672	0.6725586326552399	0.0096258122123255	T	T	T
0.0631620473353588	0.6279233287680849	0.7979332101258021	T	T	T
0.1814644808470232	0.6689154464651900	0.6699571132091435	T	T	T
0.0795552207217675	0.5574404765326070	0.1471308550451446	T	T	T
0.1980049104906202	0.5256080598447483	0.2897248142801593	T	T	T
0.2172018545443715	0.5593882181126077	0.5137211604085240	T	T	T
0.3768874360533536	0.5654566418932504	0.5121704317486898	T	T	T
0.4307912918195548	0.5283262705918147	0.3018889597983411	T	T	T
0.3226514964934039	0.5559575235207032	0.1557327251812989	T	T	T
0.0863195455563057	0.3237780162773791	0.1620859225989112	T	T	T
0.1966561742324857	0.3676459363386708	0.3077042825652431	T	T	T
0.2323542967052726	0.3289868244009720	0.5257883564409206	T	T	T
0.3863910225517251	0.3264891334941449	0.5064514364009927	T	T	T
0.4320027889653634	0.3711165839693513	0.2929548602130687	T	T	T
0.3145422846620854	0.3286273231292736	0.1685744718103178	T	T	T
0.3577498472128561	0.0657674798009407	0.7203593051658064	T	T	T
0.3144436407748936	0.0610235123538785	0.9057834637016775	T	T	T
0.2023231585691446	0.0461054033989425	0.0103708230919401	T	T	T
0.0939867575821177	0.0687959996932055	0.8995125965437649	T	T	T
0.1051208240934955	0.0599465997767614	0.7024011267912549	T	T	T

Structure files (CONTCAR) involved in this work:

0.2297943417580318	0.0395347597219426	0.7578768664397296	T	T	T
0.3602854257383384	0.8256956878995765	0.7515231782945246	T	T	T
0.3062095115276883	0.8497169503579562	0.9263897636151879	T	T	T
0.1892062283296784	0.8523187140445425	0.0183186457458752	T	T	T
0.0847310177118092	0.8311730699080500	0.9016130208590485	T	T	T
0.1052775694773258	0.8387807522588270	0.7065268620234088	T	T	T
0.2304797950695456	0.8531233528119521	0.7644364534895546	T	T	T
0.3224422124374037	0.9485368491319341	0.7956340663147603	T	T	T
0.0873048510514522	0.9502252622299299	0.8128638197074858	T	T	T
0.4323264822196267	0.1269167935153290	0.5851645601007308	T	T	T
0.4151785427878555	0.9953948159869456	0.5724247128795549	T	T	T
0.3965538713283251	0.8631008582234786	0.5683426640640910	T	T	T
0.2009079025662962	0.1320407326514007	0.6216742930183208	T	T	T
0.1886083227101654	0.0023151977149364	0.5762062332650721	T	T	T
0.1986110188230346	0.8680354162537087	0.5713028442594943	T	T	T
0.9887694617187752	0.0396690475591600	0.7844599606856019	T	T	T
0.9855981591629822	0.8672009344911816	0.7816187986451524	T	T	T
0.1437065719059681	0.9336822779523345	0.2204453138722904	T	T	T
0.1879907136094851	0.9375945374528066	0.4053191200377455	T	T	T
0.2994840803018009	0.9459346414501826	0.5133288063257264	T	T	T
0.4078386773903478	0.9296000648893655	0.4011094563458263	T	T	T
0.3971681406008118	0.9375152926782614	0.2043043096120737	T	T	T
0.2720053626118867	0.9593912934488704	0.2568712110329057	T	T	T
0.1405788744352346	0.1730363814189646	0.2506169678878589	T	T	T
0.1921547812454076	0.1495200294662250	0.4265240536609567	T	T	T
0.3108810436553625	0.1465796134642436	0.5123041419488300	T	T	T
0.4166618865426737	0.1678334248051909	0.3974008448161411	T	T	T
0.3947790310554494	0.1576258766688088	0.2032174942156454	T	T	T
0.2705060431713733	0.1470651298740788	0.2667198596394900	T	T	T
0.1795059482019045	0.0504426278593733	0.2956540370734164	T	T	T
0.4176932412871683	0.0477564498353990	0.3121780458783895	T	T	T
0.0669797696334186	0.8703651253402613	0.0909049001764788	T	T	T
0.0852355917073913	0.0003414580856687	0.0687127266593847	T	T	T
0.1082408208508824	0.1315929730569484	0.0686200427448506	T	T	T
0.3014895722968911	0.8659879088015675	0.1221196149280680	T	T	T
0.3154617306997111	0.9953401892538682	0.0757534630507879	T	T	T
0.2981562346559356	0.1286064841016545	0.0728650492894061	T	T	T
0.5139454314943985	0.9552803146980211	0.2870517775471128	T	T	T
0.5161783627662311	0.1340505485431700	0.2766449754468699	T	T	T
0.6379965057517043	0.5658079231025068	0.2747743641897702	T	T	T
0.6948621447158715	0.5734158154162843	0.1000489035768942	T	T	T
0.7958583063763907	0.5508321687807720	0.9721143844993078	T	T	T
0.8971368746712403	0.5812756891628691	0.0969501947016218	T	T	T
0.8857845033950728	0.5422261665728313	0.3071940985596717	T	T	T
0.7613741881619631	0.5214979414698684	0.2521877726558265	T	T	T
0.6394187471047131	0.3331598249883510	0.2594660990923914	T	T	T
0.6912652160654232	0.3390049885747190	0.0800235572424833	T	T	T
0.8103233403844878	0.3506415137631271	0.9926600814150285	T	T	T
0.9173951238252652	0.3216980806187159	0.1028108618870314	T	T	T
0.9055749817880713	0.3568734765362730	0.2938492228631467	T	T	T
0.7655211579735948	0.3716979170434419	0.2392772263407823	T	T	T
0.6642079656922837	0.4509719322594738	0.1771844801556521	T	T	T
0.9300305652921597	0.4492035542570003	0.1516640611326305	T	T	T

Structure files (CONTCAR) involved in this work:

0.5672057561084501	0.6268027787753214	0.4142262103132648	T	T	T
0.5948323787637085	0.4983176677383362	0.4355271137316444	T	T	T
0.5835792431387685	0.3647399492430179	0.4360087763402921	T	T	T
0.7919128354521383	0.6303524581824107	0.3599234620149581	T	T	T
0.7956127488255192	0.5128464583998672	0.4476743989540540	T	T	T
0.8266359393620186	0.3829073379216262	0.4360381709587432	T	T	T
0.0128346153206212	0.5559012041822825	0.2262749794053709	T	T	T
0.0229612347840418	0.3630107534051982	0.2077560757980664	T	T	T
0.8555025359066807	0.4366491171436350	0.7851145590081212	T	T	T
0.7957876264381526	0.4350196472836526	0.6085794013148509	T	T	T
0.6997119787441266	0.4209875535443378	0.4708171454346685	T	T	T
0.6011248779147554	0.4294512545309108	0.6046378873634858	T	T	T
0.6038444083886065	0.4397411172310225	0.8016355226169790	T	T	T
0.7283186253208329	0.4754445857062536	0.7661942048877015	T	T	T
0.8639918944579846	0.6837518024988499	0.7378917661574058	T	T	T
0.8139777082644323	0.6432122861736943	0.5527852536317065	T	T	T
0.6894895415524448	0.6473054597632359	0.4862129756513842	T	T	T
0.5831121878114091	0.6674643924674674	0.6012806304460266	T	T	T
0.5980590166767561	0.6585545702150963	0.7976211322103834	T	T	T
0.7217295495451185	0.6523363345686293	0.7284755640095613	T	T	T
0.8259838965166632	0.5506660934356190	0.6892273450328446	T	T	T
0.5816980808393462	0.5476183219311007	0.6874751847137637	T	T	T
0.9307344379670536	0.3767367112290507	0.9207635417193616	T	T	T
0.9164776543882627	0.5101015591122751	0.9288186375051819	T	T	T
0.8895951914208741	0.6399510397856579	0.9219910848133442	T	T	T
0.7007482966016756	0.3723220914290402	0.8877108859175384	T	T	T
0.6755063448251616	0.4995615046810726	0.9423288127010900	T	T	T
0.6964000350326797	0.6326770535632844	0.9242864211296778	T	T	T
0.4896171333762460	0.4512868017104689	0.7118850171720438	T	T	T
0.4808360502123951	0.6319059241379346	0.7150984780656624	T	T	T
0.6445173537544245	0.9362943691602581	0.2860903622060721	T	T	T
0.6959894828654912	0.9337468273520996	0.1047770162757282	T	T	T
0.8023251552328965	0.9466015401966678	0.9852135267577262	T	T	T
0.9043057046354336	0.9279908350974189	0.1107268805472883	T	T	T
0.8978061746265285	0.9457024511329565	0.3077012339273926	T	T	T
0.7722420143613372	0.9650842552815690	0.2584489722111301	T	T	T
0.6415093007479631	0.1727950790169447	0.2503693144711866	T	T	T
0.6957937336745732	0.1538444065314606	0.0752790916026688	T	T	T
0.8110855436904317	0.1470299106879689	0.9796294157790051	T	T	T
0.9160116765777829	0.1677514378572899	0.0955516245628973	T	T	T
0.8965711066608271	0.1584443169658415	0.2923866973229393	T	T	T
0.7713804945175629	0.1426300447391767	0.2381748857912233	T	T	T
0.6785754857931657	0.0507325858112146	0.1989152257761328	T	T	T
0.9197079125293340	0.0489737193896089	0.1839007751929696	T	T	T
0.5694333169435047	0.8747271032182475	0.4204099381474461	T	T	T
0.5856573299271013	0.0057396439544800	0.4350655750220304	T	T	T
0.6008958404475934	0.1378377944268101	0.4327460580277125	T	T	T
0.8059648348226732	0.8703278426589868	0.3912863094606909	T	T	T
0.8153699177086038	0.9990566760751474	0.4404231226318030	T	T	T
0.8050418364594466	0.1334498133708119	0.4309348863570281	T	T	T
0.0130440518632404	0.9552194207498307	0.2200597637301088	T	T	T
0.0164123936219191	0.1373036170807256	0.2155703112947864	T	T	T
0.8578743313169922	0.0543663023089683	0.7852599912659538	T	T	T

Structure files (CONTCAR) involved in this work:

0.8078402149282549	0.0710733072247734	0.6044906089989289	T	T	T
0.7016962723288446	0.0577220450472355	0.4853578769637289	T	T	T
0.5963691697767867	0.0748970634160108	0.6045532123520803	T	T	T
0.6049353564348338	0.0533150047624919	0.8018468050210513	T	T	T
0.7296111557776404	0.0314342094382386	0.7531238265785440	T	T	T
0.8590522443746471	0.8335383706781936	0.7620754256467706	T	T	T
0.8065788860663066	0.8326715332740521	0.5832689964261142	T	T	T
0.6917782843053730	0.8511575839031219	0.4876548507201223	T	T	T
0.5875437344316382	0.8288722516689573	0.6059201680799188	T	T	T
0.6040699137609783	0.8520125270950559	0.8000206918812431	T	T	T
0.7293707384609056	0.8568260183465584	0.7402535713089533	T	T	T
0.8189809565452597	0.9477722025524266	0.6799501986479011	T	T	T
0.5796456715053622	0.9528495687702345	0.6742003046486674	T	T	T
0.9327652681391887	0.1267719445570093	0.9076624035149805	T	T	T
0.9202389606091164	0.9965782322054084	0.9410999859598685	T	T	T
0.9039131876684194	0.8642207889654804	0.9416160409382377	T	T	T
0.6979833867003645	0.1306015466210932	0.8797480526428311	T	T	T
0.6878102424309896	0.0037907052815194	0.9381535703398114	T	T	T
0.7000303470927969	0.8696784626677974	0.9342234194697293	T	T	T
0.4888828890497435	0.0469279093162226	0.7170626717567544	T	T	T
0.4845662310315880	0.8641359427081625	0.7193850549184641	T	T	T
0.3584124132615522	0.4337231475893100	0.7164285079789922	T	T	T
0.3070103915977327	0.4333213593516750	0.8986079916545727	T	T	T
0.1993205598696796	0.4590755949940687	0.0122204433653134	T	T	T
0.0913668694105576	0.4317983105125882	0.9017479085360386	T	T	T
0.1032970823830541	0.4403021788714683	0.7034974430560270	T	T	T
0.2298246524504567	0.4642608698659806	0.7465783494961289	T	T	T
0.3567920324652508	0.6725372019800767	0.7448400676167647	T	T	T
0.3053424208208093	0.6521626938834089	0.9209402186377521	T	T	T
0.1900625410607096	0.6452995365431562	0.0155947052101115	T	T	T
0.0868166751851516	0.6696492467376056	0.8961022495716950	T	T	T
0.1037902573262033	0.6566578759391991	0.7012885947319677	T	T	T
0.2287579879903821	0.6392941609040490	0.7591067079538835	T	T	T
0.3242085643014199	0.5492500756678329	0.7993231870306134	T	T	T
0.0809703388693645	0.5490226125668426	0.8139427803826670	T	T	T
0.4322716126658210	0.3745783259092332	0.5762911744474412	T	T	T
0.4166611073836597	0.5061010027929014	0.5700183823050005	T	T	T
0.3939846954077204	0.6375746706325724	0.5623636938859674	T	T	T
0.1973358847324952	0.3674409699404254	0.6188254835429300	T	T	T
0.1805881753480943	0.4959872363267405	0.5672435385729145	T	T	T
0.1959274435758060	0.6300197348614963	0.5651837774768131	T	T	T
0.9860349678829335	0.4551287522254556	0.7837004735561433	T	T	T
0.9839251222826113	0.6367369659118485	0.7796737449617772	T	T	T
0.1453724435573963	0.5641687769598246	0.2161191653455474	T	T	T
0.1919155955218706	0.5614242112758822	0.3981500626473677	T	T	T
0.2973836081619157	0.5492994816402760	0.5198573040469552	T	T	T
0.4000121979030095	0.5689904025776432	0.3965301831689233	T	T	T
0.3980581439566498	0.5574995004763776	0.1994620585053667	T	T	T
0.2728688876351844	0.5339403645094980	0.2466450350501174	T	T	T
0.1440946818622709	0.3219400404812640	0.2469750671170663	T	T	T
0.1921143519712591	0.3482287661229270	0.4245870544738704	T	T	T
0.3095157471773282	0.3532464510837231	0.5138264108673526	T	T	T
0.4107477484775435	0.3276814138722097	0.3908850264679016	T	T	T

Structure files (CONTCAR) involved in this work:

0.3923246275666826	0.3443826571530528	0.1943924527060991	T	T	T
0.2714186029746761	0.3530680157918122	0.2656729502254783	T	T	T
0.1774428770088577	0.4468615597066449	0.2938860892773871	T	T	T
0.4130450915217202	0.4491522967667066	0.3147856572273026	T	T	T
0.0682164161105199	0.6242970560136442	0.0812274051110221	T	T	T
0.0785715008914568	0.4905387205571099	0.0797178125241002	T	T	T
0.1146705344283955	0.3620100803522816	0.0630469401704397	T	T	T
0.3031118997138535	0.6303133686052063	0.1161587343681281	T	T	T
0.3183919906809596	0.5015193480094503	0.0656337139598576	T	T	T
0.2910443734629815	0.3694388569602803	0.0693568484441209	T	T	T
0.5106060787549529	0.5385513259236502	0.2935324408132395	T	T	T
0.5110616677515624	0.3621769499052573	0.2706435311830786	T	T	T
0.4394316554495391	0.7493302465633467	0.6421505397276741	T	T	T
0.1958625353700276	0.7480342791475746	0.6516798773567601	T	T	T
0.2716987780221372	0.7491110640077274	0.0473241844519441	T	T	T
0.1080611074523977	0.7484351804678078	0.0518610507183381	T	T	T
0.0667855843510670	0.2478378326752912	0.1308857798091045	T	T	T
0.3040497937511438	0.2492604965650101	0.1474523257480262	T	T	T
0.2282529391487971	0.2494335294666723	0.5472443959760639	T	T	T
0.3920536341455381	0.2501375558923791	0.5477352269403190	T	T	T
0.5578436709513055	0.2494650672606501	0.3525693065989687	T	T	T
0.8069384869241908	0.2519182514825042	0.3427301630914523	T	T	T
0.7282626569175602	0.2498450941072503	0.9442997285037142	T	T	T
0.8929174014004728	0.2501596962703478	0.9431036951071180	T	T	T
0.9437102453134915	0.7522528792401965	0.8586646635101594	T	T	T
0.6863333445213555	0.7526363910583377	0.8499818670407816	T	T	T
0.7723531925012727	0.7484128302378823	0.4410535809564106	T	T	T
0.6076395658446025	0.7500212708645181	0.4509163811919846	T	T	T
0.9355369044417076	0.4960633178680274	0.5120119929967359	T	T	T
0.8211939926977043	0.3356681200040076	0.3218379949337494	T	T	T
0.8009141922488549	0.6376349029418564	0.6866429154488297	T	T	T
0.9239242680699433	0.5299931565635496	0.1919792865048104	T	T	T
0.8678249721167001	0.5569030089986738	0.5485016386517748	T	T	T
0.9352910560098572	0.4034652459548690	0.4319414310958542	T	T	T
0.9836289151561340	0.6432749398709808	0.3035343221102370	T	T	T
1.0000760653377390	0.5700944936064709	0.3796599719140678	T	T	T
0.0683769361597531	0.6167517749364358	0.3254620787028024	T	T	T
0.9667826107485583	0.4867585589374576	0.5664904187587654	T	T	T
0.0635914222473790	0.4167825771913442	0.4659832580050802	T	T	T
0.0448512583980627	0.3283869031352243	0.4552414873424386	T	T	T
0.0166868838801279	0.6001251180106396	0.3156971201939427	T	T	T
0.0233503631801407	0.3793083755693046	0.4568134511155048	T	T	T

Figure S17 ZnFe-TS

Si O Al Zn Fe H C

1.0000000000000000

20.0219999999999985 0.0000000000000000 0.0000000000000000

0.0000000000000000 19.8990000000000009 0.0000000000000000

0.0000000000000000 0.0000000000000000 13.3829999999999991

93 193 3 1 1 6 2

Selective dynamics

Direct

0.4227591374173915 0.0579996186531521 0.6484522498002492 T T T

0.3060199280618564 0.0281059675501332 0.7946629240586249 T T T

Structure files (CONTCAR) involved in this work:

0.2822549904871323	0.0571802422326229	0.0163600259142634	T	T	T
0.1228669245932005	0.0606803666645862	0.0113146716616249	T	T	T
0.0684832567172569	0.0287850233053191	0.8002440822672450	T	T	T
0.1816018212678177	0.0582032321878515	0.6632938791584185	T	T	T
0.4205098374529984	0.8264000929371270	0.6708325714425740	T	T	T
0.3042471795159275	0.8691333594579884	0.8091881668673920	T	T	T
0.2671485786130219	0.8285523094342578	0.0281747463115735	T	T	T
0.1124583216915609	0.8249002287093038	0.0157745880231683	T	T	T
0.0659470775351844	0.8716252429755066	0.8015383280355051	T	T	T
0.1824246405086881	0.8267907693044579	0.6729161953349251	T	T	T
0.0776603264239675	0.9400995283477572	0.1501956619603330	T	T	T
0.1956964246231235	0.9705296054120738	0.2945873792199618	T	T	T
0.2186629441019857	0.9381691165622600	0.5169189436164894	T	T	T
0.3789943410793605	0.9335823370223520	0.5139326231210244	T	T	T
0.4344785351677795	0.9675171721280591	0.3025219834281681	T	T	T
0.3209081958724169	0.9393211035557458	0.1641052632141013	T	T	T
0.0827451210783117	0.1718358473935168	0.1652151898961950	T	T	T
0.1961316475427208	0.1297079324986476	0.3085846235549106	T	T	T
0.2329592537203947	0.1695857686563552	0.5257286518501783	T	T	T
0.3875204187721571	0.1726745773420438	0.5100133747981511	T	T	T
0.4362123692078170	0.1259825829351903	0.2975514627885022	T	T	T
0.3171453471309770	0.1697832893887787	0.1718570153312037	T	T	T
0.5794791061363325	0.5552761647492436	0.3537238622104860	T	T	T
0.6899288635356871	0.5284402912839259	0.1981137372530912	T	T	T
0.7164232294771383	0.5643119226495762	0.9812043357615432	T	T	T
0.8742860680772827	0.5699088383113361	0.9858525416740763	T	T	T
0.8117342037473042	0.5486704129956514	0.3396446544802353	T	T	T
0.5737629393070904	0.3277140994887799	0.3292456940163295	T	T	T
0.6945704431149333	0.3739521705170889	0.1937242756239613	T	T	T
0.7319304073587096	0.3270306906545440	0.9788786133385280	T	T	T
0.8862051454459049	0.3242538440190687	0.9875370749139754	T	T	T
0.9406161524151597	0.3735137446630492	0.1817194053997013	T	T	T
0.9220129776897250	0.4450563545147620	0.8590490640091263	T	T	T
0.8003669237910743	0.4731373801016055	0.7197266253566406	T	T	T
0.7786466223381452	0.4344717595544370	0.4941277705012657	T	T	T
0.6213445106778630	0.4275265651991275	0.4875744823764677	T	T	T
0.5681638955855123	0.4674692135279734	0.7004382534237292	T	T	T
0.6747380060222721	0.4440727269073020	0.8526037040114455	T	T	T
0.9194980828906800	0.6771972182350008	0.8274334344794647	T	T	T
0.7684734735225299	0.6676667380770978	0.4600278160174660	T	T	T
0.6133848274056182	0.6714876924523050	0.4875407372017646	T	T	T
0.5619246862917808	0.6260338172810472	0.7003780005517806	T	T	T
0.6752795509429176	0.6752233444497523	0.8242946091938603	T	T	T
0.5792958191609663	0.9431787183142668	0.3578357877784332	T	T	T
0.6980919346219444	0.9720526912279713	0.2137748368364685	T	T	T
0.7215673928417817	0.9394460431750550	0.9912427984953417	T	T	T
0.8818359719616593	0.9343017649678422	0.9954315723665002	T	T	T
0.9337701542799749	0.9702804908139778	0.2060011319175606	T	T	T
0.8223754854298753	0.9443548564326510	0.3511948802819135	T	T	T
0.5791638963090999	0.1730064099893188	0.3275404884450225	T	T	T
0.6978824218852240	0.1304851557233883	0.1922338762633313	T	T	T
0.7331565633275332	0.1694921827634512	0.9711544704136680	T	T	T
0.8878460803412802	0.1721820403011012	0.9810275892416990	T	T	T

Structure files (CONTCAR) involved in this work:

0.9365526783312905	0.1288151495421883	0.1964428087794387	T	T	T
0.8201418173109580	0.1740551321273812	0.3280581987521071	T	T	T
0.9242918407135603	0.0533070174508517	0.8542066748843797	T	T	T
0.8038517580619219	0.0255087178507656	0.7063229152313953	T	T	T
0.7826802545067311	0.0651868727773796	0.4894878169307745	T	T	T
0.6219527348697984	0.0690094868955004	0.4892097351474399	T	T	T
0.5678847757109806	0.0319881545361364	0.6978591320588600	T	T	T
0.6804596904253153	0.0547556782194383	0.8439498994278726	T	T	T
0.9230417293073583	0.8288985954778945	0.8376059509814189	T	T	T
0.8033618101394617	0.8672832208101217	0.6939930945673904	T	T	T
0.7700137736829505	0.8252919681706430	0.4772629693994521	T	T	T
0.6147906228195690	0.8254905705576463	0.4921088763816575	T	T	T
0.5642932138038225	0.8751578748105733	0.6992739197784610	T	T	T
0.6797064209061084	0.8330239225827327	0.8325161606000121	T	T	T
0.4233662117617132	0.4425120241682284	0.6394219271679759	T	T	T
0.3055930515110608	0.4698826033285797	0.7868360772185801	T	T	T
0.2822969509865738	0.4385752082211588	0.0068294222848462	T	T	T
0.1248712887383778	0.4352584726967534	0.0076944184318034	T	T	T
0.0657487559631798	0.4693489865421137	0.7992895025282166	T	T	T
0.1787133991933441	0.4426877173175769	0.6557991388179424	T	T	T
0.4189260618212503	0.6726512480260377	0.6634513674000853	T	T	T
0.3028578603614486	0.6278578560656196	0.8028266708211085	T	T	T
0.2685533214136360	0.6693411855642387	0.0223021075603253	T	T	T
0.1140437184269090	0.6709576656179426	0.0103110683706532	T	T	T
0.0636727328952211	0.6279720700151868	0.7983791751611194	T	T	T
0.1806783817979018	0.6685262593611009	0.6677663108568492	T	T	T
0.0767712939132671	0.5551114107288500	0.1470815813075525	T	T	T
0.1986492666781637	0.5265908147584913	0.2853230750382033	T	T	T
0.2186244422775862	0.5601363522678792	0.5110964954760628	T	T	T
0.3779055980119570	0.5665317002600628	0.5092660141634204	T	T	T
0.4307893175573314	0.5271773403243087	0.3007857819198225	T	T	T
0.3246157021589384	0.5546833260849910	0.1514171203507777	T	T	T
0.0865497407932844	0.3246028181228870	0.1557799653770221	T	T	T
0.1964337232792411	0.3679590200914399	0.3051067331030960	T	T	T
0.2315321042835622	0.3288209452104017	0.5237368186685982	T	T	T
0.3855859066906347	0.3260909479155504	0.5050119664706817	T	T	T
0.4314104344420292	0.3705061815354053	0.2927071292339025	T	T	T
0.3151787612787690	0.3277896481057172	0.1656883542362979	T	T	T
0.3577703724602803	0.0654950509587623	0.7200058433790122	T	T	T
0.3145523495194141	0.0601299285887409	0.9052743454860068	T	T	T
0.2023006247130444	0.0450645918346331	0.0094879763907423	T	T	T
0.0937225612937148	0.0685484780029499	0.8992168160395425	T	T	T
0.1049205605834401	0.0597132990753677	0.7021682906405174	T	T	T
0.2297175023953794	0.0397435613096895	0.7573207227713673	T	T	T
0.3608880492634532	0.8251974613218070	0.7528326779546537	T	T	T
0.3057350523132538	0.8502092433801428	0.9266038437506949	T	T	T
0.1893721430937386	0.8516317885512229	0.0199321701334974	T	T	T
0.0855307340932587	0.8307968169184685	0.9021721562587832	T	T	T
0.1051144322878708	0.8384606349851296	0.7067452678698006	T	T	T
0.2307101477331245	0.8521592936634901	0.7635767790939124	T	T	T
0.3219900149576846	0.9480697570260069	0.7941031011264947	T	T	T
0.0878280606411090	0.9498087827498953	0.8128696002074779	T	T	T
0.4320069190235602	0.1269333565592384	0.5848306199411236	T	T	T

Structure files (CONTCAR) involved in this work:

0.4150638633833347	0.9953278135614601	0.5716440948306708	T	T	T
0.3956258097762941	0.8630692589373921	0.5691320923810758	T	T	T
0.2002888564446448	0.1321002162886057	0.6210746548294316	T	T	T
0.1883020001380011	0.0023593829920383	0.5757953206195632	T	T	T
0.1981708462971301	0.8681270177726954	0.5710341797698295	T	T	T
0.9887842358861066	0.0386862694758682	0.7840864718989178	T	T	T
0.9857893806652641	0.8668860867246611	0.7836853141124387	T	T	T
0.1435833578506858	0.9336010426890005	0.2200892154878860	T	T	T
0.1877213653685867	0.9378958128979031	0.4049277254723767	T	T	T
0.2991225575646702	0.9460516166382853	0.5130042043474076	T	T	T
0.4075703220531292	0.9286431399377885	0.4012644295163070	T	T	T
0.3972524735483153	0.9375077849683785	0.2044822138227981	T	T	T
0.2719257502968460	0.9593211386771731	0.2565844967170831	T	T	T
0.1406459779076098	0.1735084430640114	0.2498940117321338	T	T	T
0.1920085368845383	0.1493718010962747	0.4257040621117179	T	T	T
0.3104037577844970	0.1465388033001286	0.5122837051182260	T	T	T
0.4160917731726975	0.1677904128290921	0.3972279586955476	T	T	T
0.3947377433905687	0.1564501244758989	0.2028899980086360	T	T	T
0.2704050619318171	0.1470960990781704	0.2659807573924005	T	T	T
0.1793034113692719	0.0505108456575147	0.2944797204806862	T	T	T
0.4178638073396346	0.0472400396895733	0.3135922962580893	T	T	T
0.0669096460093684	0.8695139487604587	0.0911009920603297	T	T	T
0.0850104714540419	0.9995605519251974	0.0678118260631489	T	T	T
0.1087488184405432	0.1307733330078925	0.0684021283287350	T	T	T
0.3020082768745588	0.8652497928186605	0.1226647148674360	T	T	T
0.3155033263862769	0.9944783280960617	0.0753221289001745	T	T	T
0.2980560442204404	0.1275968778640141	0.0723019404950935	T	T	T
0.5139269427471965	0.9545734773563412	0.2881256069080766	T	T	T
0.5158869152437211	0.1338914661213166	0.2770658321935790	T	T	T
0.6377421593038256	0.5664348868685873	0.2714788885552888	T	T	T
0.6959655641827879	0.5734203168523606	0.0979637274502165	T	T	T
0.7956752095292269	0.5495415470392432	0.9675543890626883	T	T	T
0.8914733958575162	0.5796180355374271	0.1020291196663519	T	T	T
0.8883439887570939	0.5264417741570566	0.3142467955026641	T	T	T
0.7629782096950750	0.5252837033951873	0.2519454242200906	T	T	T
0.6396422939290763	0.3344702565986202	0.2612661982827197	T	T	T
0.6948973281610136	0.3374562977621842	0.0849441662958673	T	T	T
0.8095263164469014	0.3513178271455361	0.9854906598525927	T	T	T
0.9119821436852470	0.3183820474857217	0.1026264186700042	T	T	T
0.9075275386259303	0.3595027742691339	0.2930555529679885	T	T	T
0.7665569600697012	0.3719496919158247	0.2458265487454881	T	T	T
0.6677189858370709	0.4513439125100656	0.1778067771183669	T	T	T
0.9219383046532603	0.4472953952716578	0.1461008305268101	T	T	T
0.5679155907867548	0.6250496330819819	0.4144179578067050	T	T	T
0.6015660937938837	0.4973521900856788	0.4328002192222531	T	T	T
0.5835045776288296	0.3644158512934220	0.4372567810317265	T	T	T
0.8015278418831411	0.6284768104894144	0.3642774726481590	T	T	T
0.7933409538717683	0.5124340161557903	0.4504249676138113	T	T	T
0.8313323183237329	0.3861237648693867	0.4370804727936473	T	T	T
0.0121432372531455	0.5464504979546875	0.2168377736253934	T	T	T
0.0209591943432047	0.3638308106502252	0.1950924913554305	T	T	T
0.8560649148820594	0.4366989275835105	0.7881410134471738	T	T	T
0.7974176774410510	0.4354212394771373	0.6114747051443752	T	T	T

Structure files (CONTCAR) involved in this work:

0.7018007716844303	0.4153198863881191	0.4745189044138507	T	T	T
0.6019508749205146	0.4303081889930664	0.6045578065889877	T	T	T
0.6013927614681236	0.4385292430629735	0.8021554046886678	T	T	T
0.7267993035027578	0.4702323484399099	0.7671850645582285	T	T	T
0.8639661584299687	0.6833305397315337	0.7419744546309682	T	T	T
0.8130697538697552	0.6429156462242298	0.5574808892779117	T	T	T
0.6912387729036912	0.6459000151823193	0.4795377718574101	T	T	T
0.5862991566877311	0.6657615691651686	0.6007520419674457	T	T	T
0.5968537883122578	0.6594426745649267	0.7979801530777130	T	T	T
0.7201402834373019	0.6565901563305520	0.7280547137437786	T	T	T
0.8222824256210687	0.5510796134226411	0.6964141537044444	T	T	T
0.5822740633571349	0.5474052141593131	0.6896979140636607	T	T	T
0.9319423108207102	0.3757624307434886	0.9220735047805219	T	T	T
0.9175327332691670	0.5094809307309173	0.9321791294266598	T	T	T
0.8908707781375531	0.6388971728672624	0.9255864938820897	T	T	T
0.6951234134310015	0.3703186852769611	0.8922462292233226	T	T	T
0.6742492752046765	0.4994791720720845	0.9412458252920933	T	T	T
0.6963741753454475	0.6321855818783307	0.9224974866075404	T	T	T
0.4889736956531376	0.4513613008322663	0.7088149567130859	T	T	T
0.4812795876770813	0.6318746567496726	0.7122973405805140	T	T	T
0.6445682099177575	0.9358307100559979	0.2870208198904864	T	T	T
0.6960468302712325	0.9350963434803844	0.1059412799148311	T	T	T
0.8021592658971574	0.9473226077090284	0.9855228213323342	T	T	T
0.9036281482359706	0.9287266772085001	0.1116453336538797	T	T	T
0.8982610305899709	0.9456475785131097	0.3086876505724797	T	T	T
0.7725725358963286	0.9641337392847513	0.2599950869918701	T	T	T
0.6407793871296006	0.1736101171327979	0.2492908623501979	T	T	T
0.6960218220650535	0.1515145989159301	0.0753841703919261	T	T	T
0.8108674324563759	0.1456921930273579	0.9783341383354639	T	T	T
0.9153925843438238	0.1674276705803820	0.0944652074742567	T	T	T
0.8969630764591932	0.1597004114243709	0.2915577549886882	T	T	T
0.7709777439512417	0.1458580169131166	0.2392630015654321	T	T	T
0.6796403537417650	0.0511713044640292	0.2037971331488901	T	T	T
0.9197090689418341	0.0493958321283279	0.1856759432276358	T	T	T
0.5701482181443335	0.8740958285809477	0.4214644496410042	T	T	T
0.5856266975321317	0.0055597013637704	0.4355182686585000	T	T	T
0.6013659698590708	0.1378353218516251	0.4320187865075670	T	T	T
0.8069846011287799	0.8691423244554063	0.3920704705777090	T	T	T
0.8153437467187551	0.9975216831216094	0.4421932869137005	T	T	T
0.8063116961392214	0.1318966660848023	0.4306269823548786	T	T	T
0.0130922865444642	0.9553310526054872	0.2196117571415665	T	T	T
0.0164066633133559	0.1384623000777894	0.2141644498969071	T	T	T
0.8579314211690565	0.0539942258714590	0.7853544689121045	T	T	T
0.8075662916715992	0.0703215816707190	0.6050047345369514	T	T	T
0.7019328642685592	0.0576325411881747	0.4844804936341405	T	T	T
0.5968690576546083	0.0754254759867603	0.6042578409002921	T	T	T
0.6046239654784933	0.0526065279685433	0.8014230071127995	T	T	T
0.7294717927746462	0.0312184600364605	0.7537361837745726	T	T	T
0.8595125291943045	0.8328951431008133	0.7633374954103808	T	T	T
0.8069314345125338	0.8319568548668473	0.5846372092762938	T	T	T
0.6926484417545079	0.8493723846948517	0.4876942948878285	T	T	T
0.5883791600677819	0.8281150446611053	0.6065904787676001	T	T	T
0.6039478326476997	0.8536390427334306	0.8001675882933953	T	T	T

Structure files (CONTCAR) involved in this work:

0.7296863459225845	0.8552821848520201	0.7419723635295086	T	T	T
0.8186208893041297	0.9469863692042902	0.6816364785962302	T	T	T
0.5798512175476447	0.9530114683964338	0.6716889491095960	T	T	T
0.9330811783014608	0.1263802129912921	0.9068439212541712	T	T	T
0.9203983387663817	0.9964501629541007	0.9414713762536444	T	T	T
0.9034372050403451	0.8642332848683024	0.9429983739965450	T	T	T
0.6970836679296283	0.1308580813462878	0.8791209068135194	T	T	T
0.6874820950560847	0.0047262672232251	0.9392187789604036	T	T	T
0.6993282556462302	0.8709456620908899	0.9354284162691967	T	T	T
0.4889897842451520	0.0468383344791406	0.7159285426441155	T	T	T
0.4847600138088757	0.8648019517250352	0.7184164566699419	T	T	T
0.3574282991047446	0.4352298444537662	0.7092932135141500	T	T	T
0.3110725664420840	0.4315472748524480	0.8936888550398424	T	T	T
0.2031767348169360	0.4567902855746646	0.0035500472138833	T	T	T
0.0941491410245629	0.4293395752971864	0.8957788654521284	T	T	T
0.1023101254266464	0.4426687374896042	0.6977760256638968	T	T	T
0.2293962700634171	0.4635704789468817	0.7452253370113374	T	T	T
0.3564639253738658	0.6714530148738392	0.7402021553237870	T	T	T
0.3053143053374612	0.6536123581210539	0.9170851095460349	T	T	T
0.1912029553901026	0.6449255539596729	0.0153447248834951	T	T	T
0.0886020129413502	0.6697777473170337	0.8953383023802742	T	T	T
0.1032279981440525	0.6559921913940160	0.7001004087613021	T	T	T
0.2284670739531217	0.6385741573315350	0.7560158161445452	T	T	T
0.3237089448182444	0.5490264055188466	0.7982010493067608	T	T	T
0.0808806270469281	0.5487859810161672	0.8137747741458056	T	T	T
0.4321683417231185	0.3749624479081348	0.5724759754015054	T	T	T
0.4189400504356290	0.5069798598506448	0.5649850456114631	T	T	T
0.3965727002669826	0.6386795274458389	0.5580007038415991	T	T	T
0.1959741617277729	0.3677746617035987	0.6159576014734436	T	T	T
0.1821835385669471	0.4960535975121692	0.5636254889967763	T	T	T
0.1949910936886878	0.6300230652640245	0.5625692428036958	T	T	T
0.9861199373809989	0.4547389217625038	0.7838730120900543	T	T	T
0.9841267329927278	0.6367283094634261	0.7813753294272976	T	T	T
0.1446098583481511	0.5638599829362714	0.2145378604168120	T	T	T
0.1963355741350106	0.5621283727364839	0.3946838947798858	T	T	T
0.2987313707855070	0.5508810409779509	0.5220593316327256	T	T	T
0.3987000128916989	0.5696906030897334	0.3926215084535806	T	T	T
0.3999888334131725	0.5555962614048130	0.1966393630345152	T	T	T
0.2735296502916351	0.5331977845516397	0.2406664754509310	T	T	T
0.1407139026106579	0.3248273986334629	0.2460509576381904	T	T	T
0.1916560315414959	0.3470853020186227	0.4217034274055932	T	T	T
0.3087644331580503	0.3530139512340398	0.5124120289831570	T	T	T
0.4095739384241877	0.3260590217244848	0.3892786982563694	T	T	T
0.3926380027918311	0.3437748820139918	0.1935182605754586	T	T	T
0.2702834960836137	0.3517383548536164	0.2612329383699167	T	T	T
0.1791712667425434	0.4474450975436723	0.2937485810497794	T	T	T
0.4117872700655598	0.4483174459068447	0.3153378002859487	T	T	T
0.0683692335966599	0.6226037023317417	0.0791238280420399	T	T	T
0.0847131754810274	0.4909564139861506	0.0718690562408202	T	T	T
0.1178902407614325	0.3612650013255941	0.0580005192736549	T	T	T
0.3064709543093853	0.6291803610879868	0.1111200135375591	T	T	T
0.3214661280333144	0.4999053992560806	0.0614856842352374	T	T	T
0.2938208058388803	0.3679510276434955	0.0650769044046517	T	T	T

Structure files (CONTCAR) involved in this work:

0.5111713080080436	0.5351953434581797	0.2968229090572931	T	T	T
0.5108347508011473	0.3625407578321084	0.2717922126203827	T	T	T
0.4402042840698598	0.7497738990965572	0.6420051846203434	T	T	T
0.1951450273355227	0.7477256658950762	0.6500941629371113	T	T	T
0.2730203678144056	0.7485846587207303	0.0469923769270605	T	T	T
0.1086610013656003	0.7472872979914829	0.0520040365640895	T	T	T
0.0678237592178475	0.2478866006991239	0.1277027653442576	T	T	T
0.3049502228134144	0.2483370310438544	0.1452754368621232	T	T	T
0.2275123283892160	0.2494158019934535	0.5464781558423236	T	T	T
0.3913517067519540	0.2501110826153096	0.5477668440221842	T	T	T
0.5576170412208271	0.2496146410325824	0.3523532845305842	T	T	T
0.8097028458877961	0.2523940406580142	0.3487454766452586	T	T	T
0.7279850783511859	0.2488622070745667	0.9466268815297202	T	T	T
0.8917927295977330	0.2491826458379331	0.9405500221106107	T	T	T
0.9438123481596842	0.7519595360668140	0.8615594324716020	T	T	T
0.6839398323152942	0.7535673805100529	0.8547322619220161	T	T	T
0.7746522451172707	0.7472327470800482	0.4417871598158644	T	T	T
0.6082503131745761	0.7489633662317714	0.4510750946209631	T	T	T
0.9274185743775801	0.4912840356117481	0.5288186727658962	T	T	T
0.8236612979222773	0.3356626435681821	0.3255015621854469	T	T	T
0.7996698198559367	0.6389420674364380	0.6917410204894762	T	T	T
0.9285136748567311	0.5284179324526924	0.1909194559771956	T	T	T
0.8628251554445137	0.5570797468415296	0.5564607936557135	T	T	T
0.9305049016894985	0.4307759396341378	0.4043361877364742	T	T	T
0.9846428823520182	0.6096713329499817	0.3801305732041996	T	T	T
0.0296934516927258	0.5430449526460563	0.4529590159006679	T	T	T
0.0782995440143028	0.6034579828414121	0.3722475415276836	T	T	T
0.9561798146809107	0.4786826842702200	0.5847144854027158	T	T	T
0.0558477908173688	0.4299417750744549	0.4788777145218059	T	T	T
0.0546457170459717	0.4176845533379410	0.3442873073105170	T	T	T
0.0310710309203017	0.5855935311310786	0.4018949834247537	T	T	T
0.0242687744988224	0.4249006488882034	0.4117483672752535	T	T	T

Figure S17 ZnFe-FS

Si O Al Zn Fe H C

1.0000000000000000

20.0219999999999985 0.0000000000000000 0.0000000000000000

0.0000000000000000 19.8990000000000009 0.0000000000000000

0.0000000000000000 0.0000000000000000 13.3829999999999991

93 193 3 1 1 6 2

Selective dynamics

Direct

0.4234721263150058	0.0583922075822620	0.6476192062936607	T	T	T
0.3059479100656803	0.0279298934569006	0.7928097312165532	T	T	T
0.2826872102618561	0.0580327477540328	0.0148066294867135	T	T	T
0.1233776898361897	0.0611094209240880	0.0115112550457105	T	T	T
0.0689229355517202	0.0297460070799589	0.8002654645570964	T	T	T
0.1810868441083865	0.0578813521395004	0.6606954992863339	T	T	T
0.4203185982823366	0.8265404541976622	0.6687849184733815	T	T	T
0.3048684345846722	0.8691618867379111	0.8086986347546748	T	T	T
0.2675752199263718	0.8291526991182683	0.0271245377453639	T	T	T
0.1132131482819773	0.8253770288048538	0.0132172484556849	T	T	T
0.0660880878800441	0.8725244950819464	0.7997137570793584	T	T	T
0.1830313949644695	0.8274705959966997	0.6723915612351470	T	T	T

Structure files (CONTCAR) involved in this work:

0.0782012676844742	0.9402090102841550	0.1490322246039524	T	T	T
0.1964342952479052	0.9713382042866429	0.2934232959613284	T	T	T
0.2189935526970401	0.9385907581077935	0.5157415822770169	T	T	T
0.3790221773355311	0.9347591896983697	0.5133873422688778	T	T	T
0.4341752850722779	0.9681505646381841	0.3017090135680764	T	T	T
0.3216127450242879	0.9410144037742137	0.1614234612487342	T	T	T
0.0831350721399669	0.1719098159421012	0.1652962121158126	T	T	T
0.1963198491266491	0.1300980183241967	0.3092016979435959	T	T	T
0.2333216084342615	0.1709340715845832	0.5261070653995490	T	T	T
0.3880111958563845	0.1734933914329108	0.5097028607136331	T	T	T
0.4361492138208661	0.1265589234442823	0.2968991039442697	T	T	T
0.3169737808870133	0.1699478106568452	0.1716113059321641	T	T	T
0.5770724596607044	0.5556559749041203	0.3536004281552836	T	T	T
0.6906107207988526	0.5259294616419714	0.2007497567641076	T	T	T
0.7142488457866096	0.5665598851112684	0.9842094897998460	T	T	T
0.8717330965873493	0.5714295760738082	0.9867315410672650	T	T	T
0.8110721813943865	0.5483153741212979	0.3437502632981383	T	T	T
0.5734412539938103	0.3276062489275027	0.3301452699277995	T	T	T
0.6944619805325473	0.3718623929501443	0.1926449941275882	T	T	T
0.7301194755703215	0.3264213986731181	0.9797079196290445	T	T	T
0.8846252602358909	0.3252950861584399	0.9929991124214822	T	T	T
0.9411076496954109	0.3754969785166253	0.1857494135219263	T	T	T
0.9205202209412365	0.4451708372880964	0.8608641477147284	T	T	T
0.7990628623624739	0.4717741287698947	0.7207106079277117	T	T	T
0.7739238678359038	0.4352369969077984	0.4957301301672772	T	T	T
0.6167964343701380	0.4284822058374819	0.4885789363522293	T	T	T
0.5676704429692164	0.4683257589756172	0.7019686459794773	T	T	T
0.6739995140518436	0.4460987343380780	0.8568361075418819	T	T	T
0.9202075121816983	0.6771248133267908	0.8299842764642118	T	T	T
0.7694050175792584	0.6685381428766796	0.4614035215397761	T	T	T
0.6141902437302922	0.6722345215125449	0.4857689485506246	T	T	T
0.5615050547440459	0.6266769854465738	0.6980408635270844	T	T	T
0.6729573161462645	0.6740465033563722	0.8266432707746575	T	T	T
0.5793200530247198	0.9441087140214951	0.3578064075901316	T	T	T
0.6992580478542674	0.9728435178381222	0.2136725483571008	T	T	T
0.7217859389895064	0.9376458319623089	0.9917324934405872	T	T	T
0.8821169335670455	0.9340632874121374	0.9950734433084848	T	T	T
0.9341629409956235	0.9693109186049974	0.2052782560266993	T	T	T
0.8234532680226072	0.9457784291292433	0.3527892183416527	T	T	T
0.5789280768332181	0.1728168140034772	0.3284841127402985	T	T	T
0.6987601817466111	0.1315551463765398	0.1926539881107748	T	T	T
0.7329690932869042	0.1702862321915015	0.9715935761694845	T	T	T
0.8876606171453968	0.1728713537257862	0.9831605913632517	T	T	T
0.9375666352299984	0.1275005761775664	0.1967952165845848	T	T	T
0.8217493351424511	0.1737661477922686	0.3287900549391633	T	T	T
0.9241510878062701	0.0540487255462406	0.8553502852528976	T	T	T
0.8035989255567755	0.0255042393380473	0.7069437018591502	T	T	T
0.7825620538233045	0.0663697782439076	0.4902067737671232	T	T	T
0.6219546680407002	0.0691103431875418	0.4899005366810422	T	T	T
0.5683734670248546	0.0317986923384361	0.6987553130854355	T	T	T
0.6803765462240481	0.0533951620414145	0.8461788081968002	T	T	T
0.9238225907196932	0.8295713347597742	0.8361604857020732	T	T	T
0.8033271358520718	0.8679601393109474	0.6939771095794276	T	T	T

Structure files (CONTCAR) involved in this work:

0.7707234498921963	0.8257876529184696	0.4774756002664705	T	T	T
0.6155154973181980	0.8261334098145865	0.4911596296710046	T	T	T
0.5643244317051193	0.8747369664431099	0.6987856588558481	T	T	T
0.6797357119272515	0.8326667331744310	0.8319731424559834	T	T	T
0.4234499309000626	0.4438676044912224	0.6391021164015603	T	T	T
0.3043388247428625	0.4709758850106597	0.7857224899075362	T	T	T
0.2816137272113886	0.4377868835368222	0.0049008398177561	T	T	T
0.1237342697659212	0.4360743213969272	0.0096624541817759	T	T	T
0.0654965126297564	0.4700210171613588	0.8001239985438759	T	T	T
0.1776098530402334	0.4446060680827025	0.6537742710724983	T	T	T
0.4185921879446357	0.6728243837532661	0.6586947001343032	T	T	T
0.3026317048698668	0.6287060027527591	0.8008336827995868	T	T	T
0.2693040178642297	0.6709326045211719	0.0189179933520979	T	T	T
0.1151386464330044	0.6716191831777197	0.0059777637853131	T	T	T
0.0638008236298740	0.6286101155066308	0.7956603500129146	T	T	T
0.1808273746233803	0.6686849301723461	0.6658243202776339	T	T	T
0.0746650503809471	0.5573905204076129	0.1464310958334970	T	T	T
0.1978449079348842	0.5279068842037674	0.2827154359466887	T	T	T
0.2197297899878561	0.5611620281387598	0.5096779022741188	T	T	T
0.3780282088987910	0.5663215857928594	0.5073724664807596	T	T	T
0.4294809036682286	0.5275014675585307	0.2974698712445634	T	T	T
0.3239130874331982	0.5543475802038418	0.1458641464824109	T	T	T
0.0861172627061088	0.3247147090779799	0.1571606460211984	T	T	T
0.1965774677016715	0.3694171226696078	0.3043708619277157	T	T	T
0.2319192808617664	0.3298868703145568	0.5232912097664072	T	T	T
0.3863511082655891	0.3269976106867821	0.5045917533493497	T	T	T
0.4321792727856150	0.3702546110405882	0.2909673401885141	T	T	T
0.3150887019249898	0.3281350391964175	0.1650001310740320	T	T	T
0.3580885050347559	0.0651284808516814	0.7184608945399498	T	T	T
0.3124834614392866	0.0621840802708231	0.9022937300762464	T	T	T
0.2027237742254298	0.0447705372660011	0.0120088637548756	T	T	T
0.0955595131147647	0.0691956762271468	0.8987060239697127	T	T	T
0.1048349023147038	0.0604016363265467	0.7015133440598007	T	T	T
0.2299298840853537	0.0372846522816469	0.7529155288077015	T	T	T
0.3607508048142994	0.8251671559697952	0.7507368771765308	T	T	T
0.3071923734280836	0.8488966612533567	0.9255834894701558	T	T	T
0.1900371521484828	0.8524870555730619	0.0161610571820868	T	T	T
0.0852126765385169	0.8314399604822795	0.9002255655780266	T	T	T
0.1056233931962843	0.8399291402069864	0.7049592522771124	T	T	T
0.2310583200478878	0.8531358589578585	0.7632715528009181	T	T	T
0.3232657785470300	0.9481769089957582	0.7957769164566626	T	T	T
0.0876897482360417	0.9506634205719946	0.8123733729345023	T	T	T
0.4324318767049068	0.1274840029627484	0.5842978324126014	T	T	T
0.4168607902040449	0.9957355200108041	0.5704550090794754	T	T	T
0.3954505474759445	0.8638922824396029	0.5676634088629164	T	T	T
0.2005780396040497	0.1320577501432618	0.6202046813568806	T	T	T
0.1857567776077278	0.0027173878498911	0.5716668927497655	T	T	T
0.1994922991141599	0.8684694230633221	0.5703913221206930	T	T	T
0.9891346004957139	0.0401008683685861	0.7860142340384435	T	T	T
0.9860062433942166	0.8675134857815879	0.7807388091945926	T	T	T
0.1444043472626422	0.9347107006265601	0.2185033755628115	T	T	T
0.1905024267067127	0.9360777382044810	0.4023248429359014	T	T	T
0.2993663790225184	0.9488696397975024	0.5155399119689338	T	T	T

Structure files (CONTCAR) involved in this work:

0.4060590789313693	0.9294910161515597	0.3998900674631002	T	T	T
0.3976537466292244	0.9381582121390603	0.2030779484535235	T	T	T
0.2723767212368194	0.9631328756712135	0.2525274806805508	T	T	T
0.1413300144122247	0.1738050812310823	0.2493612615488754	T	T	T
0.1925446614652679	0.1520435822398444	0.4253932818243729	T	T	T
0.3107452206952667	0.1479093577203963	0.5124675909497737	T	T	T
0.4162160433668321	0.1682671089642354	0.3967191367537924	T	T	T
0.3947771358299570	0.1573544829226404	0.2023860316629975	T	T	T
0.2706542042318691	0.1457019902743939	0.2653354149394961	T	T	T
0.1783494200066642	0.0508862617687946	0.2985378085059482	T	T	T
0.4176076600112693	0.0478653656748913	0.3125470311702651	T	T	T
0.0681826187963406	0.8697799470591928	0.0894471661716181	T	T	T
0.0843873342057307	0.0004344510695594	0.0674647383126461	T	T	T
0.1091736645157231	0.1315186942173084	0.0678401314302381	T	T	T
0.3015466556373725	0.8669791891678912	0.1213325540391590	T	T	T
0.3181174376780593	0.9953497394629608	0.0711654167412055	T	T	T
0.2986015500152129	0.1282873111109617	0.0712077532942285	T	T	T
0.5137096282970874	0.9551445074772077	0.2885696447317559	T	T	T
0.5159534371096268	0.1340513277871629	0.2766322018916212	T	T	T
0.6373917265361523	0.5622499004131890	0.2739497476418916	T	T	T
0.6999158925545923	0.5730456401176880	0.1033629119898262	T	T	T
0.7930598426537612	0.5564301157293449	0.9594418588673306	T	T	T
0.8830540424625309	0.5775148005819832	0.1049330114946102	T	T	T
0.8872960383673837	0.5260140645131850	0.3174598568814357	T	T	T
0.7617823930961327	0.5214956966225974	0.2592843587263936	T	T	T
0.6411768881471294	0.3350295366841610	0.2662777427926242	T	T	T
0.6910887896845909	0.3335578838190359	0.0851412420730113	T	T	T
0.8074581068165578	0.3511100952297799	0.9908055587924984	T	T	T
0.9102453494415379	0.3200289450197201	0.1087432556601020	T	T	T
0.9084762989617483	0.3636489900965021	0.2994596451422421	T	T	T
0.7681448454227803	0.3690670273041244	0.2394081901774947	T	T	T
0.6689374224776813	0.4494751028459673	0.1749910278829193	T	T	T
0.9238891416558501	0.4488143960556097	0.1478353522755206	T	T	T
0.5685773099662697	0.6267882579481300	0.4116639829387621	T	T	T
0.5927132938647360	0.4979033328115411	0.4364984697970261	T	T	T
0.5801899658094075	0.3644182323426775	0.4386802233989806	T	T	T
0.8024237239565215	0.6284034325154717	0.3664767376631001	T	T	T
0.7919373534215135	0.5135639128989705	0.4556497073092700	T	T	T
0.8249891980351071	0.3866835088242526	0.4360120585751742	T	T	T
0.0087280146832972	0.5531853806186059	0.2135506867063455	T	T	T
0.0208685866020882	0.3631213142841915	0.2002523363182036	T	T	T
0.8562350693419601	0.4349912595164236	0.7863260075905696	T	T	T
0.7902083663537655	0.4326293868861630	0.6139647026621001	T	T	T
0.6971889679389606	0.4194900372735991	0.4705867082055100	T	T	T
0.6011075010361929	0.4295843686440907	0.6069480549224419	T	T	T
0.6011886782645416	0.4409406413183763	0.8044637963079170	T	T	T
0.7273784211386131	0.4733514438476471	0.7741046476546700	T	T	T
0.8616195267201633	0.6806553897146406	0.7489495120084629	T	T	T
0.8130821219558956	0.6441965401044881	0.5604417636768464	T	T	T
0.6920298989312428	0.6465616831621248	0.4790491260481067	T	T	T
0.5871061040215054	0.6661121879691798	0.5988994832877881	T	T	T
0.5947130367470893	0.6610261206594720	0.7962535344149456	T	T	T
0.7191445362763649	0.6492470888206469	0.7349432832300861	T	T	T

Structure files (CONTCAR) involved in this work:

0.8230044223004229	0.5487566350939589	0.6939812495241513	T	T	T
0.5821936899130880	0.5480211551213883	0.6885911304378677	T	T	T
0.9297386295680548	0.3769358070478707	0.9267372719438092	T	T	T
0.9134708557616843	0.5099447507169013	0.9327176909960649	T	T	T
0.8959913492850528	0.6404116395414642	0.9321767005248306	T	T	T
0.6943042638972881	0.3718393900728013	0.8946447320052423	T	T	T
0.6727103285967390	0.5004218050667419	0.9469899599973467	T	T	T
0.6878257097758219	0.6342155960360193	0.9304251394276158	T	T	T
0.4883924840628511	0.4524175923428499	0.7102985884958503	T	T	T
0.4807602725963502	0.6320361965457076	0.7078509327436674	T	T	T
0.6446089945134694	0.9383491247123760	0.2868216844877159	T	T	T
0.6984642553066037	0.9335897326864855	0.1075267660899344	T	T	T
0.8022955579623174	0.9453901490162819	0.9826955167148392	T	T	T
0.9026261737988707	0.9277730792373649	0.1118467492850734	T	T	T
0.8990205383294839	0.9464177436876180	0.3090777114476596	T	T	T
0.7730528900619160	0.9655269305252059	0.2623653063620101	T	T	T
0.6414550726474829	0.1729357891869790	0.2519518665214813	T	T	T
0.6961066561703477	0.1554604903906724	0.0770834450201559	T	T	T
0.8106252245191321	0.1466331843633456	0.9802251214152802	T	T	T
0.9157193792747934	0.1673428579826205	0.0962088321027708	T	T	T
0.8981109180020099	0.1565892410382830	0.2932963274219537	T	T	T
0.7717521996675607	0.1465900293187790	0.2403558338939724	T	T	T
0.6815865581634761	0.0518024341896652	0.1992687023623404	T	T	T
0.9210598390245677	0.0483369607195697	0.1830953164894875	T	T	T
0.5708708973526785	0.8745132802530603	0.4203008368728441	T	T	T
0.5850460281921971	0.0057444869960245	0.4369374745633032	T	T	T
0.5999782537294517	0.1379036176173095	0.4337178274352636	T	T	T
0.8083533453142322	0.8706599559300341	0.3942594425226975	T	T	T
0.8171418514169021	0.9995122399787360	0.4432878057134819	T	T	T
0.8062376443348594	0.1336151575416422	0.4325509000762995	T	T	T
0.0133505892195951	0.9537777746861654	0.2186405454167089	T	T	T
0.0173461332931281	0.1374511067238698	0.2143667041124272	T	T	T
0.8583170456274537	0.0536359752976113	0.7852716684752454	T	T	T
0.8054047688696478	0.0715225674194279	0.6066652154188027	T	T	T
0.7019372056333391	0.0580393017189021	0.4819245037151553	T	T	T
0.5986830980382317	0.0750533793666556	0.6058256325020794	T	T	T
0.6047209346106538	0.0518524897987898	0.8028864179040801	T	T	T
0.7297854286928572	0.0296386006703357	0.7566274759393034	T	T	T
0.8593465906273370	0.8338050875078495	0.7637599817915597	T	T	T
0.8066322365957164	0.8311084234589189	0.5857475961192053	T	T	T
0.6933665326645018	0.8500891893483987	0.4869904769535815	T	T	T
0.5888888637553591	0.8284484945132642	0.6055198220775500	T	T	T
0.6037732480635857	0.8526013146146374	0.7996183000187975	T	T	T
0.7296908820027573	0.8572384825150507	0.7427138635939901	T	T	T
0.8187826498108027	0.9474870989754227	0.6791695349521704	T	T	T
0.5797728279507330	0.9527989725927400	0.6724997164016326	T	T	T
0.9321842159158422	0.1274445339011244	0.9075162580058626	T	T	T
0.9199734102893591	0.9974847166569776	0.9430889000218615	T	T	T
0.9057024518720459	0.8648802307224118	0.9421088621985032	T	T	T
0.6971032710134291	0.1293296911363306	0.8817979735826952	T	T	T
0.6867086945533879	0.0029676251307433	0.9410854052602609	T	T	T
0.6984668722596271	0.8691281134295917	0.9365930110987013	T	T	T
0.4895557600305895	0.0476038247809606	0.7156501336521861	T	T	T

Structure files (CONTCAR) involved in this work:

0.4847635539153840	0.8642406393129571	0.7170166827092876	T	T	T
0.3567687017623135	0.4377551359086352	0.7075585910836267	T	T	T
0.3078539174460063	0.4298301114482423	0.8904908845697374	T	T	T
0.2024892140910349	0.4563015506768190	0.0072424604776827	T	T	T
0.0948946093464361	0.4307782869851597	0.8965076810487036	T	T	T
0.1014795149435638	0.4436587137531062	0.6976940777793719	T	T	T
0.2285841284110759	0.4661889758354059	0.7424301223966711	T	T	T
0.3555161952247374	0.6702312599857773	0.7339576562775247	T	T	T
0.3063589915325591	0.6587990383536534	0.9127717850244074	T	T	T
0.1923419885801919	0.6456035093169455	0.0103131184814887	T	T	T
0.0898888702416415	0.6717038251670759	0.8907154108649633	T	T	T
0.1030760670939682	0.6547018056832342	0.6958392220202076	T	T	T
0.2278941269497366	0.6380532285056988	0.7545392676640796	T	T	T
0.3228799761673290	0.5496237453854332	0.8024859381824513	T	T	T
0.0802255240753152	0.5495408226270244	0.8137335832369647	T	T	T
0.4323350578239313	0.3759886027895591	0.5728494691110989	T	T	T
0.4206368937804714	0.5079717670205803	0.5635473090988716	T	T	T
0.3974237819012064	0.6394149363275569	0.5523388795910208	T	T	T
0.1957255967468109	0.3698205291099275	0.6140116937734436	T	T	T
0.1811165043364249	0.4981347498712153	0.5618542255826167	T	T	T
0.1968034459227443	0.6317099429625608	0.5599759580480769	T	T	T
0.9856295890590121	0.4547334689637949	0.7875063152053098	T	T	T
0.9840338511983108	0.6374286187809755	0.7797752332611154	T	T	T
0.1417455895504048	0.5652459139525409	0.2160091566130543	T	T	T
0.2004852754805271	0.5635422946640434	0.3921410147349915	T	T	T
0.2994124977390574	0.5499721781609777	0.5249347374094760	T	T	T
0.3959148161796918	0.5683360976547036	0.3896580872480456	T	T	T
0.3985371014584357	0.5551138349807664	0.1933166214181677	T	T	T
0.2712592310490509	0.5328631567706503	0.2326316375406069	T	T	T
0.1417146754744760	0.3252063368187989	0.2452298666342307	T	T	T
0.1925198809056899	0.3473482781872799	0.4205572390846283	T	T	T
0.3093482101255398	0.3535043837456100	0.5116501112672626	T	T	T
0.4108202316553801	0.3270729349089455	0.3890492517738980	T	T	T
0.3928461425719265	0.3427606743876448	0.1927962283793351	T	T	T
0.2705077809184927	0.3543532646601993	0.2595124779725532	T	T	T
0.1782397883932583	0.4487004207072022	0.2941845363407309	T	T	T
0.4130423406106080	0.4482130383660465	0.3121605245467193	T	T	T
0.0693519871191264	0.6228314040275346	0.0733891270810484	T	T	T
0.0831518587024856	0.4910823464862633	0.0746233014305869	T	T	T
0.1151146352937612	0.3616671712104549	0.0582160347673330	T	T	T
0.3073800387238378	0.6290919239343853	0.1055715656330274	T	T	T
0.3222937530907599	0.4996147313476750	0.0558354454932694	T	T	T
0.2947388665632102	0.3674540722381072	0.0632506872084306	T	T	T
0.5094345827110900	0.5388050512694812	0.2931025785362200	T	T	T
0.5115998747148619	0.3618054303622449	0.2692780514858051	T	T	T
0.4397392705307478	0.7501082135038241	0.6386864914580255	T	T	T
0.1950463001768166	0.7481931096296162	0.6508727870714802	T	T	T
0.2729255290522851	0.7494593874306116	0.0486672262556447	T	T	T
0.1099677996554743	0.7476870929589693	0.0489007778621915	T	T	T
0.0670431207130076	0.2480267026608516	0.1291440735758323	T	T	T
0.3035868280296842	0.2485697723715016	0.1468268660715679	T	T	T
0.2277483975494760	0.2506439194679046	0.5483752797884116	T	T	T
0.3923966864289628	0.2509493450663375	0.5471414064974709	T	T	T

Structure files (CONTCAR) involved in this work:

0.5573017680779391	0.2494777833696007	0.3526349908519494	T	T	T
0.8140866314875549	0.2525732978540032	0.3479985924176808	T	T	T
0.7275262639513355	0.2490946600388267	0.9425148391687587	T	T	T
0.8914915601621675	0.2504707629736699	0.9454326103053060	T	T	T
0.9445884243402846	0.7526579792879917	0.8593887968907640	T	T	T
0.6852858071241308	0.7529168496935368	0.8503253614381965	T	T	T
0.7757265325286570	0.7478914998838593	0.4409396649334828	T	T	T
0.6094484192034652	0.7497383844777596	0.4496661076041356	T	T	T
0.9212312320194948	0.4844805136416280	0.5295503522997597	T	T	T
0.8232310508992474	0.3361751748998335	0.3247849228741800	T	T	T
0.7987585906423432	0.6364043946714831	0.6949257699195703	T	T	T
0.9261662037729069	0.5302801736021895	0.1927334303707080	T	T	T
0.8623029708415693	0.5573044340292700	0.5558817961720296	T	T	T
0.9221895392207865	0.4319638149849437	0.4076414565517709	T	T	T
1.0175118719938414	0.5419766943956088	0.3839938368440824	T	T	T
0.0412826857431137	0.5246560743664215	0.5108111404110464	T	T	T
0.0965140809044205	0.5094080200280506	0.4103257527708794	T	T	T
0.9484799546513631	0.4693775069665976	0.5857722586785882	T	T	T
0.0306010463074522	0.4017133755219804	0.4836647936430596	T	T	T
0.0337900593289895	0.4124599070242646	0.3488106488220544	T	T	T
0.0439673193243445	0.5068515088285031	0.4334809523678669	T	T	T
0.0202888411591458	0.4359310210732348	0.4205642247576180	T	T	T

Figure S17 ZnCo-IS

Si O Al Co Zn H C

1.0000000000000000

20.0219999999999985 0.0000000000000000 0.0000000000000000

0.0000000000000000 19.8990000000000009 0.0000000000000000

0.0000000000000000 0.0000000000000000 13.3829999999999991

93 193 3 1 1 6 2

Selective dynamics

Direct

0.4239975813757759	0.0570718644036710	0.6474677250265244	T	T	T
0.3047509019273306	0.0263985321565240	0.7921842008048373	T	T	T
0.2827171330917331	0.0593433206293836	0.0135679210525702	T	T	T
0.1234525123888992	0.0608422579234144	0.0112384918600878	T	T	T
0.0705239747846424	0.0290970359710286	0.7999825132207791	T	T	T
0.1804696942471035	0.0549977713480665	0.6556057650974015	T	T	T
0.4206877184667970	0.8262110525134596	0.6679963987009752	T	T	T
0.3043247343215387	0.8681228079766424	0.8095308906501998	T	T	T
0.2664117158088847	0.8270303565428362	0.0277586888062853	T	T	T
0.1117108000542677	0.8252175021852683	0.0141004162766784	T	T	T
0.0661373220548484	0.8721401906646329	0.7998483585835919	T	T	T
0.1829555251438545	0.8278314443275845	0.6714758977435245	T	T	T
0.0769740999296629	0.9411066048558734	0.1481118800709227	T	T	T
0.1972693796343928	0.9716562246399241	0.2912794750670181	T	T	T
0.2194879640663992	0.9370345954310305	0.5131028400894528	T	T	T
0.3793471566038723	0.9342617257479072	0.5129910052702440	T	T	T
0.4329240236124534	0.9682089388211641	0.3006953539438193	T	T	T
0.3223397293580046	0.9423041670603621	0.1557812560808673	T	T	T
0.0818655877841961	0.1708059858421653	0.1653411186648518	T	T	T
0.1966903424064029	0.1300689095817115	0.3094785801950646	T	T	T
0.2338855841320210	0.1707420639830700	0.5264321607727294	T	T	T
0.3882944982518608	0.1729770422134174	0.5105950837198573	T	T	T

Structure files (CONTCAR) involved in this work:

0.4367363209487250	0.1265461775503786	0.2977036748228868	T	T	T
0.3178422377328763	0.1698663626880061	0.1718511401799536	T	T	T
0.5768382435442717	0.5560514380367613	0.3564573883475124	T	T	T
0.6897189397104532	0.5254560352414610	0.2016748261869986	T	T	T
0.7159274843690282	0.5669247452794359	0.9868276587790910	T	T	T
0.8754661297459604	0.5718861274060894	0.9851347932871365	T	T	T
0.8090919148194353	0.5534934316981299	0.3409557247207967	T	T	T
0.5749961695218246	0.3274871313583160	0.3304691702961042	T	T	T
0.6953666654888747	0.3714414168345294	0.1919105428289008	T	T	T
0.7318925436475950	0.3271273190458492	0.9791446574886559	T	T	T
0.8865591268735151	0.3258801315997881	0.9949759574098985	T	T	T
0.9438373820660251	0.3738013850470390	0.1931963052084776	T	T	T
0.9207164717507765	0.4442884708936913	0.8586759606586977	T	T	T
0.8010564913017471	0.4725156928279969	0.7176439895242114	T	T	T
0.7760183951054069	0.4379044304480888	0.4918318237272765	T	T	T
0.6182509306749109	0.4290686195551728	0.4889786456410386	T	T	T
0.5693015060522737	0.4683524716285392	0.7017238092045085	T	T	T
0.6770385003752608	0.4470443175756953	0.8551745291102241	T	T	T
0.9194359784918748	0.6783374799785632	0.8262490843613556	T	T	T
0.7671823511033775	0.6692905759417240	0.4643311049560528	T	T	T
0.6129762218454278	0.6734468415718389	0.4896096611050255	T	T	T
0.5610072176883162	0.6265289774921708	0.6999688376282576	T	T	T
0.6752370266350215	0.6730610951992436	0.8254662064133266	T	T	T
0.5784681506255206	0.9445574667963152	0.3582383675847000	T	T	T
0.6991128695644838	0.9731029405761231	0.2145015925588643	T	T	T
0.7216124948035215	0.9366625484407307	0.9926931909841974	T	T	T
0.8819548716777554	0.9341929246611057	0.9952277558761160	T	T	T
0.9328087683018934	0.9704982514224156	0.2061704416479702	T	T	T
0.8232847174973479	0.9459728496738254	0.3549951488558913	T	T	T
0.5795698364288169	0.1727517340208565	0.3296910246689441	T	T	T
0.6991655042708799	0.1314243701906141	0.1929613168991838	T	T	T
0.7335271252645038	0.1710793432692526	0.9720644568335927	T	T	T
0.8880645731748170	0.1734058696745537	0.9843687610750392	T	T	T
0.9361999766395903	0.1287301692652155	0.1993384626977962	T	T	T
0.8203098097707258	0.1742816625650303	0.3307608149517284	T	T	T
0.9250735807771632	0.0548797291098368	0.8566517547663115	T	T	T
0.8041887107768821	0.0267535465549211	0.7089337810218564	T	T	T
0.7824088040074650	0.0661183262249416	0.4916194953163903	T	T	T
0.6220858344655334	0.0689195448190219	0.4905064849625763	T	T	T
0.5690030923729478	0.0313062659598327	0.6996371010903606	T	T	T
0.6804108004956453	0.0532674655807285	0.8485874750378674	T	T	T
0.9240677753170601	0.8302726425183861	0.8369042122183072	T	T	T
0.8031528635375105	0.8696058161508176	0.6963747994637906	T	T	T
0.7700799209203253	0.8269665335778363	0.4800309494646398	T	T	T
0.6153404163225200	0.8269038780083622	0.4918728972982319	T	T	T
0.5643854013296266	0.8743134591567855	0.6998450498801102	T	T	T
0.6796027755228655	0.8323995687970720	0.8329045318053347	T	T	T
0.4236356472375915	0.4429898514202941	0.6428537831737634	T	T	T
0.3036497382255195	0.4711893101781089	0.7881586182995217	T	T	T
0.2791874993044510	0.4379775409417750	0.0089903833198930	T	T	T
0.1219220345404034	0.4355142522500163	0.0120835135160616	T	T	T
0.0653394472183693	0.4697758969410825	0.7994515982145635	T	T	T
0.1773990998925553	0.4440721127527176	0.6532492014591991	T	T	T

Structure files (CONTCAR) involved in this work:

0.4179963502086112	0.6720624667942321	0.6631710629385507	T	T	T
0.3020742651242887	0.6287287621044766	0.8049569523004033	T	T	T
0.2664657373554711	0.6697369685253804	0.0236543618201502	T	T	T
0.1123905809873874	0.6715897788034704	0.0083308656425983	T	T	T
0.0622014219121122	0.6286360605227218	0.7952020070714053	T	T	T
0.1811062084453957	0.6694163383682022	0.6679318533456517	T	T	T
0.0795473873078805	0.5561241935189577	0.1467986385740078	T	T	T
0.1993276395620713	0.5239985111810748	0.2877534569611074	T	T	T
0.2172093239121256	0.5607788302999726	0.5112649438708959	T	T	T
0.3761378115983133	0.5653456107929125	0.5105601118945734	T	T	T
0.4294702615323713	0.5281799895964412	0.3002432515037545	T	T	T
0.3232100611299711	0.5528992123089608	0.1501779248606717	T	T	T
0.0868659986474744	0.3231852244376103	0.1580523284836659	T	T	T
0.1974195579124319	0.3665264930552081	0.3063279600967219	T	T	T
0.2324896290233481	0.3281249565242901	0.5245897098769873	T	T	T
0.3866170805043852	0.3266965967821370	0.5056824604167860	T	T	T
0.4332623863616756	0.3706291344661301	0.2922333219399718	T	T	T
0.3156911790033277	0.3283280990032182	0.1675449569617671	T	T	T
0.3584212836961336	0.0614107028812251	0.7182098661099784	T	T	T
0.3068234220574978	0.0657650824335304	0.8983062301916892	T	T	T
0.2028508981227038	0.0454028098424582	0.0197088120138985	T	T	T
0.1005027587963287	0.0689420415973925	0.8959888123496801	T	T	T
0.1048117670453771	0.0577426245125207	0.6986971037266310	T	T	T
0.2302276423581530	0.0316590465656758	0.7451710304250240	T	T	T
0.3600678611340424	0.8264075050728011	0.7481393469626308	T	T	T
0.3050192871933443	0.8410732640021208	0.9234786641067732	T	T	T
0.1889360142007612	0.8509562766350476	0.0177044537212517	T	T	T
0.0847914570841267	0.8304997911024967	0.9004576347842935	T	T	T
0.1055680495484220	0.8393091365234114	0.7050569317042223	T	T	T
0.2307956268317637	0.8553684122645060	0.7610605523479931	T	T	T
0.3231184084242318	0.9474476726740714	0.8068387704068292	T	T	T
0.0884807313970273	0.9498738887503595	0.8136469915945777	T	T	T
0.4320729369016834	0.1271024154313656	0.5861698853091443	T	T	T
0.4184266667805988	0.9953343086181018	0.5681681050710636	T	T	T
0.3977820856631130	0.8631773881663343	0.5654083866302287	T	T	T
0.2002693107722027	0.1295531562865896	0.6175087240023156	T	T	T
0.1831691574201617	0.0015149832022409	0.5639121329663219	T	T	T
0.1981103883800010	0.8674539305936475	0.5679358258640893	T	T	T
0.9907480062972456	0.0404361997941780	0.7890122685100853	T	T	T
0.9861089596338791	0.8679278112499268	0.7804799959876516	T	T	T
0.1431460430623445	0.9367581351516430	0.2177623406881597	T	T	T
0.1958972434068572	0.9322000710022509	0.3974238730040328	T	T	T
0.2996522231148582	0.9480135519968993	0.5213325538444090	T	T	T
0.4024926963237285	0.9295222206550231	0.3974861792703693	T	T	T
0.3975361005499376	0.9390706727952868	0.2005115197588864	T	T	T
0.2716573883689857	0.9662580600454886	0.2438653017887995	T	T	T
0.1414089738755381	0.1715961973545584	0.2471673838367305	T	T	T
0.1935555086576934	0.1564242609914623	0.42370444331437389	T	T	T
0.3110889202624941	0.1470897999547227	0.5123346131076375	T	T	T
0.4169471657289018	0.1678625792564029	0.3979369519656747	T	T	T
0.3955706199032976	0.1580043647004520	0.2034277813746137	T	T	T
0.2708381550039719	0.1437794370261925	0.2636084372211293	T	T	T
0.1787695940614915	0.0505153651668240	0.3056768393653645	T	T	T

Structure files (CONTCAR) involved in this work:

0.4171933156433711	0.0480094551182806	0.3121495907272404	T	T	T
0.0670925656147815	0.8697672661943290	0.0904577071206046	T	T	T
0.0831106825811085	0.9994853545258890	0.0636022706219311	T	T	T
0.1057183617939068	0.1306480274277418	0.0665210141378383	T	T	T
0.3022601335890491	0.8677679459054712	0.1174145993211971	T	T	T
0.3208842648143605	0.9956395166476215	0.0638117923798820	T	T	T
0.3010698908649641	0.1290104748125386	0.0700260772157166	T	T	T
0.5124195912995686	0.9546040152093436	0.2895836987351197	T	T	T
0.5165637440703487	0.1336666478658342	0.2781144106851743	T	T	T
0.6375422155154259	0.5610756493298579	0.2773799148492159	T	T	T
0.6964937336861403	0.5734740516840865	0.1044184208459257	T	T	T
0.7957159309008627	0.5563260585740638	0.9714095848024329	T	T	T
0.8968074670336171	0.5795236316760597	0.1000936738278024	T	T	T
0.8859809452526625	0.5437738301024890	0.3116826168225262	T	T	T
0.7619962580348506	0.5211920896734941	0.2571065835584404	T	T	T
0.6419948267301461	0.3338530043268931	0.2648240308538775	T	T	T
0.6912074243258777	0.3346266948480090	0.0830975830006382	T	T	T
0.8091746356951931	0.3511841801831052	0.9938086895112435	T	T	T
0.9141661510040016	0.3219182654056678	0.1091123098394320	T	T	T
0.9095568962907509	0.3553472995187940	0.3013653031522316	T	T	T
0.7691468870036614	0.3682404811454231	0.2377300343814832	T	T	T
0.6685399527397309	0.4489500044947051	0.1757414747198276	T	T	T
0.9288593821708416	0.4487049401524675	0.1569249787539368	T	T	T
0.5691690312986798	0.6273985392464602	0.4140143949309228	T	T	T
0.5901901342371708	0.4978882081958010	0.4393523220727753	T	T	T
0.5831767392984031	0.3641460678744492	0.4388716438318210	T	T	T
0.7923193300784610	0.6322198854189568	0.3626508121393480	T	T	T
0.7946423866461103	0.5161183852912656	0.4524734914003322	T	T	T
0.8257577552552868	0.3886136663109553	0.4329024673384591	T	T	T
0.0137737700376992	0.5546549059730167	0.2277285394537871	T	T	T
0.0240255122248779	0.3625473508140930	0.2047516184486515	T	T	T
0.8562404070220386	0.4340747488451265	0.7852183284940365	T	T	T
0.7923538629630118	0.4347163316555184	0.6103037724182457	T	T	T
0.6984315909913663	0.4238032571709814	0.4685159026344414	T	T	T
0.6031040243366267	0.4289179301371542	0.6076924861912303	T	T	T
0.6034726943962317	0.4425049493570994	0.8046432040825533	T	T	T
0.7292036201531488	0.4751593853082274	0.7712260883845463	T	T	T
0.8611199829595807	0.6832287491750021	0.7453272524295564	T	T	T
0.8151474134120884	0.6424542508218913	0.5569479047918070	T	T	T
0.6906619863738890	0.6479630948712585	0.4901485857758763	T	T	T
0.5829282501524352	0.6684800398747162	0.6012121462034741	T	T	T
0.5965679412976408	0.6590212259255955	0.7977431893834384	T	T	T
0.7208684306621626	0.6480363397764227	0.7332825476951726	T	T	T
0.8270314377781104	0.5490119439210389	0.6920384760878630	T	T	T
0.5820393479310049	0.5482492619720293	0.6860670100039654	T	T	T
0.9305617767569054	0.3772572644625815	0.9264934385533554	T	T	T
0.9144661716236121	0.5100551010159134	0.9288769679299581	T	T	T
0.8951418276522175	0.6409438005245576	0.9276809052090040	T	T	T
0.6981367028472649	0.3727624939210234	0.8921621233765141	T	T	T
0.6763223736322727	0.5006311854628164	0.9462627409270923	T	T	T
0.6920314041671968	0.6343095158070950	0.9297047263262269	T	T	T
0.4900402487611557	0.4518860876222795	0.7106289845836569	T	T	T
0.4802108920423543	0.6314935990673242	0.7127981847936038	T	T	T

Structure files (CONTCAR) involved in this work:

0.6434417888875109	0.9392330319155592	0.2866316601827812	T	T	T
0.7000263256849063	0.9326914319059606	0.1092399755845921	T	T	T
0.8021030046520858	0.9437723015040503	0.9805189144058436	T	T	T
0.9012054425221655	0.9291365027599298	0.1125934479504496	T	T	T
0.8985745076066515	0.9461558250590983	0.3099215296809398	T	T	T
0.7721406194284788	0.9665213088456479	0.2659448284831276	T	T	T
0.6418665529880838	0.1723127878218188	0.2529568290796589	T	T	T
0.6973061582343948	0.1572740866195858	0.0783128084890769	T	T	T
0.8111429994121052	0.1468438914051189	0.9792475619026189	T	T	T
0.9148685710842990	0.1679774058209027	0.0980898628762464	T	T	T
0.8973038772606831	0.1591303480984888	0.2953073256577934	T	T	T
0.7720407743413884	0.1446321480811718	0.2417539341471152	T	T	T
0.6812635130567034	0.0516737966397335	0.1967759971182848	T	T	T
0.9189046952759634	0.0495693053954894	0.1863187707978841	T	T	T
0.5703791072671571	0.8750636101894441	0.4211164369914044	T	T	T
0.5839048072979841	0.0064392010364147	0.4370018062907632	T	T	T
0.6004939382762262	0.1382074006989438	0.4353101166061183	T	T	T
0.8083779211773667	0.8706676259481541	0.3959614652020672	T	T	T
0.8180125439922811	0.9991916348706641	0.4463004808996631	T	T	T
0.8061205344054798	0.1331213929190594	0.4340500949259172	T	T	T
0.0123110192011513	0.9553816981010609	0.2175544781970134	T	T	T
0.0163116566616286	0.1374097067056133	0.2163822128526209	T	T	T
0.8599435168106523	0.0555974390894808	0.7851370063213824	T	T	T
0.8042755473683122	0.0722596509258259	0.6082828974786502	T	T	T
0.7018892462402522	0.0568460687131098	0.4814820370279775	T	T	T
0.5995370858335958	0.0744641007634288	0.6068418054125165	T	T	T
0.6050418557302575	0.0513379289197882	0.8039663337507903	T	T	T
0.7308788389165052	0.0301172577668505	0.7601318926856374	T	T	T
0.8587748847557006	0.8350520033409423	0.7665396332410539	T	T	T
0.8060767764495488	0.8329704705214684	0.5881255252383962	T	T	T
0.6928368760924709	0.8520057065208883	0.4881200552944872	T	T	T
0.5887332717633180	0.8283616355816918	0.6062692205856542	T	T	T
0.6034195118472159	0.8517287560914468	0.8007416937009575	T	T	T
0.7294272748264597	0.8597386883541903	0.7451851355896191	T	T	T
0.8199098033620396	0.9487843743664528	0.6816312579707051	T	T	T
0.5803324533752485	0.9522621354919985	0.6737788381177829	T	T	T
0.9334882271959505	0.1277886018729186	0.9099801470496502	T	T	T
0.9194135009344118	0.9978496145133017	0.9434823824517647	T	T	T
0.9078098220438622	0.8650901500040930	0.9439571626388495	T	T	T
0.6962570671148492	0.1293536968280588	0.8843085661504729	T	T	T
0.6863650763940992	0.0023122008009685	0.9430723180106800	T	T	T
0.6971015686554042	0.8679812199906615	0.9388188717870857	T	T	T
0.4900019754303361	0.0467399741579081	0.7156889684844742	T	T	T
0.4847081423036529	0.8637782320013805	0.7175878279184698	T	T	T
0.3585164834361944	0.4369408019083685	0.7149712196838046	T	T	T
0.3022447360990608	0.4302081438511765	0.8933052562834778	T	T	T
0.2000483766226794	0.4581232890915972	0.0164853378377950	T	T	T
0.0951546057690139	0.4335278749309623	0.8984596848408007	T	T	T
0.1024293900923921	0.4412555665917227	0.6999159722161444	T	T	T
0.2295072543564932	0.4678841970955672	0.7391156657642678	T	T	T
0.3557860095015667	0.6708313453910494	0.7405486369959554	T	T	T
0.3036767417301302	0.6580981419284512	0.9176496447151354	T	T	T
0.1891407202194389	0.6448949452716033	0.0130368924610915	T	T	T

Structure files (CONTCAR) involved in this work:

0.0852112401446680	0.6689691682182937	0.8949840126641109	T	T	T
0.1033205584020065	0.6579568254994335	0.6994558125165257	T	T	T
0.2279599696146182	0.6381292055491304	0.7562802752932246	T	T	T
0.3224682576876258	0.5496825744197471	0.8065753284755296	T	T	T
0.0797119046000017	0.5496525921655017	0.8099238287763421	T	T	T
0.4315746296074613	0.3752162085156827	0.5761536816632207	T	T	T
0.4179009580619689	0.5067568264772562	0.5671297185912928	T	T	T
0.3947693134995600	0.6378926287283803	0.5581682660302738	T	T	T
0.1966527624030202	0.3698491815368268	0.6135636288163155	T	T	T
0.1775211685443103	0.4978294887415378	0.5612581632028175	T	T	T
0.1950628976395663	0.6314274376786492	0.5620729438325168	T	T	T
0.9861960089448295	0.4536158412683489	0.7864597419142739	T	T	T
0.9830017024284654	0.6378501713867739	0.7761797715723309	T	T	T
0.1460401875672641	0.5618148736032862	0.2144170938166575	T	T	T
0.1968136789698947	0.5637551874605892	0.3936029605052089	T	T	T
0.2969450604952291	0.5491083223210118	0.5246425529746611	T	T	T
0.3953685506921120	0.5679857258956531	0.3932508476059256	T	T	T
0.3979757071267794	0.5561310339174240	0.1962310359821683	T	T	T
0.2729410519154588	0.5284952813086983	0.2391189271043332	T	T	T
0.1458804270673386	0.3224877967899005	0.2410329293783966	T	T	T
0.1925300471056387	0.3415044856548239	0.4209448510709373	T	T	T
0.3094321229858568	0.3529732678095751	0.5111761346116096	T	T	T
0.4119404277467583	0.3276052515665698	0.3905655807101688	T	T	T
0.3936395224439187	0.3433196165386199	0.1938410893396986	T	T	T
0.2724733290141989	0.3552715932587946	0.2631555223418562	T	T	T
0.1773200475103868	0.4460113808123442	0.3003546970591478	T	T	T
0.4139344116336163	0.4486213466293522	0.3132282928905313	T	T	T
0.0679873352809425	0.6228805190086302	0.0806745871880495	T	T	T
0.0780916472374655	0.4894838078822832	0.0783762261739420	T	T	T
0.1133333113467357	0.3608278378918742	0.0575329174713119	T	T	T
0.3025412541163462	0.6269651219960971	0.1111990050329220	T	T	T
0.3215339845045801	0.4990595224561198	0.0589525559551336	T	T	T
0.2931461732031700	0.3674555310059620	0.0662265815015550	T	T	T
0.5090016807332777	0.5409120725920810	0.2951028820279537	T	T	T
0.5126529231085958	0.3622413823029392	0.2709793312146749	T	T	T
0.4390820939598903	0.7490788078132087	0.6403688624224974	T	T	T
0.1965803948642825	0.7485067086610745	0.6517414273969524	T	T	T
0.2699460585734561	0.7479040517876252	0.0556697020173442	T	T	T
0.1065617502688465	0.7474561561639889	0.0507112496541756	T	T	T
0.0667840991643397	0.2470645220151144	0.1292238192818941	T	T	T
0.3038741321213564	0.2488038685767484	0.1495089731744796	T	T	T
0.2295367318277760	0.2496765213369895	0.5548243653436183	T	T	T
0.3925343679380786	0.2505085996284705	0.5476890793583549	T	T	T
0.5580332810524438	0.2495088374117760	0.3532022601590408	T	T	T
0.8085005795709569	0.2523540755091268	0.3501161953905393	T	T	T
0.7288417276174126	0.2497299188388649	0.9417393795727513	T	T	T
0.8927115411787655	0.2509611078907125	0.9471711478733820	T	T	T
0.9449161227190311	0.7530688349695434	0.8581425184186281	T	T	T
0.6864828784298095	0.7524140338136495	0.8476864624090634	T	T	T
0.7740384651519274	0.7488635544237201	0.4459414458131077	T	T	T
0.6094081639600112	0.7504470822788837	0.4505729797226042	T	T	T
0.9330263395683706	0.4891239498074954	0.5178769324282170	T	T	T
0.8235315191256899	0.3353749537988105	0.3255005963774757	T	T	T

Structure files (CONTCAR) involved in this work:

0.8004237897956825	0.6357389371505769	0.6908264965144718	T	T	T
0.9241884518338386	0.5297545186778064	0.1964724295679034	T	T	T
0.9275093416391615	0.4170127245126165	0.4163161230647350	T	T	T
0.8679848654424355	0.5543212252081853	0.5520027473496417	T	T	T
0.9884310445489261	0.6360626631179533	0.3205519140092568	T	T	T
0.0043162410272206	0.5570005249680677	0.3830466530817156	T	T	T
0.9608774918543849	0.4744968245209109	0.5736441479118101	T	T	T
0.0727488042086131	0.6061450377248754	0.3341227346031567	T	T	T
0.0446786057173022	0.4311259337908371	0.4805879890089514	T	T	T
0.0368288604098626	0.3611426155700204	0.3904501178981814	T	T	T
0.0205362138441317	0.5915083373366334	0.3239575065954312	T	T	T
0.0119165746068783	0.4033955626828489	0.4282507236231193	T	T	T

Figure S17 ZnCo-TS

Si O Al Co Zn H C

1.0000000000000000

20.0219999999999985 0.0000000000000000 0.0000000000000000

0.0000000000000000 19.8990000000000009 0.0000000000000000

0.0000000000000000 0.0000000000000000 13.3829999999999991

93 193 3 1 1 6 2

Selective dynamics

Direct

0.4240386843057620	0.0567007171092800	0.6465131041726916	T	T	T
0.3044536069955807	0.0255433325703835	0.7908484330263210	T	T	T
0.2829320357689778	0.0583319815016219	0.0125585417660983	T	T	T
0.1236123598593646	0.0603772821074396	0.0107499392206842	T	T	T
0.0705794339465720	0.0283217871039458	0.7996848335911447	T	T	T
0.1798620091793600	0.0548492793923083	0.6546826677509077	T	T	T
0.4207667334348023	0.8262644563694352	0.6671525390507657	T	T	T
0.3042371444733721	0.8669506707956758	0.8088564547450278	T	T	T
0.2671346706720379	0.8262461311911740	0.0276134174309755	T	T	T
0.1126283418450320	0.8238345437744422	0.0138985413792934	T	T	T
0.0665557648644777	0.8714814610409021	0.8000107816335001	T	T	T
0.1825452755294478	0.8269014314818773	0.6703177883959873	T	T	T
0.0776101146851121	0.9401314105411139	0.1471368372551185	T	T	T
0.1975683148277891	0.9713606771427328	0.2902609990371314	T	T	T
0.2190745455065924	0.9370739883607588	0.5125826800732953	T	T	T
0.3787152123250547	0.9344207138483536	0.5123256970758026	T	T	T
0.4327571140065833	0.9678009214041808	0.3007546693639291	T	T	T
0.3226720392461909	0.9416638926386406	0.1551970980728962	T	T	T
0.0822727082660164	0.1711523517942548	0.1636849946907479	T	T	T
0.1967150463615769	0.1297403812931333	0.3079945046251487	T	T	T
0.2333684971312403	0.1704727305052331	0.5254504822005602	T	T	T
0.3878939412075352	0.1728988402723276	0.5107426592769694	T	T	T
0.4364980337252065	0.1261587783335354	0.2980675430647641	T	T	T
0.3181590546737831	0.1689557591769399	0.1706936833373811	T	T	T
0.5776670615863549	0.5550492065761684	0.3545407351600440	T	T	T
0.6905772054852712	0.5259919678524367	0.2011058636392591	T	T	T
0.7162696243914527	0.5666137737800945	0.9846106631894315	T	T	T
0.8739331297468449	0.5717879630136252	0.9893742680498637	T	T	T
0.8113119342577476	0.5485809954280656	0.3457363697074490	T	T	T
0.5739060743258017	0.3275143381930803	0.3306155473522073	T	T	T
0.6951976460013870	0.3715214047809242	0.1929929084772293	T	T	T
0.7304354525917068	0.3263587975867021	0.9790684107184969	T	T	T

Structure files (CONTCAR) involved in this work:

0.8846895149493256	0.3246145432343852	0.9930505894315534	T	T	T
0.9408059689736982	0.3749069072608941	0.1839134761533810	T	T	T
0.9217628437521265	0.4451787794161974	0.8638647006517184	T	T	T
0.8011840518283966	0.4717582842708931	0.7216751035599913	T	T	T
0.7770451307406199	0.4359584352945043	0.4972116912310847	T	T	T
0.6198483993114103	0.4277872897911884	0.4890158337374196	T	T	T
0.5687752013492802	0.4685759076092794	0.7009559270888975	T	T	T
0.6752280025289772	0.4462246222204521	0.8559607528768367	T	T	T
0.9208436299716799	0.6770349247046894	0.8320711585260785	T	T	T
0.7711650677760341	0.6687152633016000	0.4631527140775094	T	T	T
0.6158266634074478	0.6722300414629626	0.4865565308948509	T	T	T
0.5622393746198965	0.6267616299429336	0.6975690711006710	T	T	T
0.6734803315603471	0.6734192175672176	0.8268888084023646	T	T	T
0.5785484418980761	0.9442417108649849	0.3589287111880194	T	T	T
0.6996263790440964	0.9731614608200013	0.2157143103632717	T	T	T
0.7213419932116056	0.9369563180641415	0.9935166260811749	T	T	T
0.8816303828438192	0.9336634635347056	0.9957057938847639	T	T	T
0.9336674919115049	0.9697410799570926	0.2054830302257151	T	T	T
0.8244320600056646	0.9461131252393691	0.3553527657747275	T	T	T
0.5791178997221429	0.1727213894600140	0.3298860410873281	T	T	T
0.6993469237187974	0.1321993299668251	0.1940846963966550	T	T	T
0.7328570090043013	0.1702733983865867	0.9721695466536473	T	T	T
0.8875137723019489	0.1725364504064547	0.9831563159791059	T	T	T
0.9368263834869909	0.1279297487525048	0.1975187285932503	T	T	T
0.8219625907936793	0.1746724528892388	0.3313669546446708	T	T	T
0.9248949843028725	0.0535496601708854	0.8562754491164114	T	T	T
0.8036774719129395	0.0252402015401123	0.7084814566969083	T	T	T
0.7825475967991408	0.0664196035095032	0.4913978673567365	T	T	T
0.6222805871589191	0.0688352622187877	0.4902852834423776	T	T	T
0.5692561012333726	0.0307866522162776	0.6987926742868920	T	T	T
0.6800483735572767	0.0526346358812744	0.8486292216452445	T	T	T
0.9243557159013794	0.8295272370864193	0.8374789234207289	T	T	T
0.8032866853835695	0.8678892127783425	0.6961857855979110	T	T	T
0.7715697135153867	0.8258102055238551	0.4791517787619954	T	T	T
0.6164959699205304	0.8258786369386953	0.4911634692062148	T	T	T
0.5650379207698666	0.8739378627640026	0.6985212053758475	T	T	T
0.6793349544181121	0.8322726486284914	0.8337695487606160	T	T	T
0.4238387651950783	0.4438186406015455	0.6384137085231196	T	T	T
0.3037740974937220	0.4709695027196308	0.7843481458113450	T	T	T
0.2826024725198709	0.4361931387499148	0.0038115217891525	T	T	T
0.1252410612738197	0.4347728766243056	0.0073539090078545	T	T	T
0.0662218666666292	0.4692731105368279	0.7990618956575091	T	T	T
0.1766502484941791	0.4441641403232167	0.6509336130271643	T	T	T
0.4183557754684538	0.6723491017725326	0.6595216455977012	T	T	T
0.3022402882992773	0.6287928776594945	0.8021288789500001	T	T	T
0.2676295693655522	0.6691233498766086	0.0214285116770276	T	T	T
0.1132904101660200	0.6699636539549851	0.0084651171750090	T	T	T
0.0633173830083129	0.6279309420805356	0.7962069648717595	T	T	T
0.1803729629937913	0.6684993010715236	0.6652608364705149	T	T	T
0.0749248780488407	0.5539379621799639	0.1461102799720780	T	T	T
0.1977388456811058	0.5249756805401984	0.2834854273322275	T	T	T
0.2180928137545906	0.5604149698877386	0.5085924551509085	T	T	T
0.3761597184787479	0.5658397993964734	0.5081693007984736	T	T	T

Structure files (CONTCAR) involved in this work:

0.4283870671909632	0.5268023046201477	0.2998876974296357	T	T	T
0.3238413282682300	0.5512797890075984	0.1463444755109400	T	T	T
0.0861765837722685	0.3241278312589291	0.1538837734902397	T	T	T
0.1961566741246626	0.3670903149349952	0.3042555354931735	T	T	T
0.2317201914196014	0.3278932673496277	0.5233156440489182	T	T	T
0.3858315735002643	0.3263042889013444	0.5050637855549232	T	T	T
0.4317715279986564	0.3697729724983029	0.2922710092969667	T	T	T
0.3154676781486189	0.3273212138846972	0.1640316911306079	T	T	T
0.3585763286478194	0.0603997552471946	0.7174177438101659	T	T	T
0.3066600973272538	0.0646833821268349	0.8971295273826388	T	T	T
0.2029848898232278	0.0450083894551447	0.0193317229643808	T	T	T
0.1004862483334885	0.0683065864485816	0.8955627204398823	T	T	T
0.1043406238858026	0.0575877214500703	0.6983710492732734	T	T	T
0.2300186379638063	0.0315869179099419	0.7437295037136586	T	T	T
0.3608626831458844	0.8256928001123284	0.7483703462190519	T	T	T
0.3055200537338637	0.8411805575030521	0.9233129759613997	T	T	T
0.1897004885405555	0.8502901557346761	0.0177700587814178	T	T	T
0.0857254260398789	0.8299245232827994	0.9002155757084592	T	T	T
0.1053471171435854	0.8388803585467978	0.7044918261365705	T	T	T
0.2309873497772181	0.8528224249889115	0.7603550908889454	T	T	T
0.3221575141329089	0.9464636841232178	0.8046088285559760	T	T	T
0.0890683328894215	0.9492907440680100	0.8130937809521120	T	T	T
0.4318866652767507	0.1271494738560323	0.5862188952775780	T	T	T
0.4185705741352883	0.9955127275535678	0.5662851493955894	T	T	T
0.3969216762498848	0.8635886811025094	0.5654354994188708	T	T	T
0.1993461280043794	0.1294449460340223	0.6163388767800290	T	T	T
0.1822011121965279	0.0014237545374987	0.5629236016334703	T	T	T
0.1980454677561073	0.8675780370736773	0.5677267498923753	T	T	T
0.9906858419837040	0.0392157228263455	0.7890207665138476	T	T	T
0.9863400248672105	0.8676452590326861	0.7817602948707976	T	T	T
0.1438620113886814	0.9360551228978189	0.2166107935395665	T	T	T
0.1960374741412728	0.9322434259485504	0.3966655778560250	T	T	T
0.2991806449013913	0.9487557587215263	0.5212415286826371	T	T	T
0.4016027803979641	0.9288224576603635	0.3967520403769787	T	T	T
0.3979886234100069	0.9392084332576210	0.1998004975974026	T	T	T
0.2721139954458776	0.9661529231157105	0.2432269768834587	T	T	T
0.1417903525468856	0.1719214567277468	0.2456301454910706	T	T	T
0.1935412152099756	0.1559106851484405	0.4223259075703444	T	T	T
0.3107083177545170	0.1469618545053356	0.5123451449384669	T	T	T
0.4166259016773795	0.1677079837439359	0.3980685983208516	T	T	T
0.3957474488152579	0.1573790960870533	0.2033021107754323	T	T	T
0.2709630545394966	0.1432036232388934	0.2624343391385520	T	T	T
0.1785327860752324	0.0502539729727559	0.3038237922645804	T	T	T
0.4172369461650903	0.0476155764215263	0.3129649643677654	T	T	T
0.0677193969762099	0.8689541092472962	0.0894357026754786	T	T	T
0.0832273512734660	0.9992181132412332	0.0634830816106577	T	T	T
0.1059522637939088	0.1306089148104488	0.0651798161485323	T	T	T
0.3029115128828246	0.8669465416262128	0.1175857682409932	T	T	T
0.3209756966409694	0.9945521740407564	0.0626003491795773	T	T	T
0.3019090310014154	0.1278161676547448	0.0689963182432840	T	T	T
0.5123210154843499	0.9540035459163563	0.2907124439441998	T	T	T
0.5163811157063819	0.1333065466817428	0.2785098500363947	T	T	T
0.6351760064145637	0.5624358274299316	0.2704527929683485	T	T	T

Structure files (CONTCAR) involved in this work:

0.7017516372866670	0.5726299881215777	0.1036945536197674	T	T	T
0.7953145518471064	0.5575341878130565	0.9606011634856105	T	T	T
0.8849195163341100	0.5777281835618999	0.1077480182420889	T	T	T
0.8867854783896627	0.5249735269258831	0.3178027583134900	T	T	T
0.7602777562929606	0.5222411138604183	0.2634065945012420	T	T	T
0.6408884288814081	0.3346388992788829	0.2649176026972883	T	T	T
0.6922976901519746	0.3335802992844710	0.0851709724295572	T	T	T
0.8078139726862956	0.3510267384259078	0.9892601558878197	T	T	T
0.9093220062010227	0.3183350603383523	0.1092112368933929	T	T	T
0.9098654113307147	0.3627448354162381	0.2983977791433903	T	T	T
0.7683917948848870	0.3684198354639179	0.2413520669622855	T	T	T
0.6700925103262048	0.4492428658790272	0.1752452415903714	T	T	T
0.9207271927174949	0.4474839243074900	0.1460410074162877	T	T	T
0.5702891106747199	0.6259688164740815	0.4135460431138981	T	T	T
0.5969975968224113	0.4971379539786792	0.4354601733958274	T	T	T
0.5828195753325640	0.3640116424924751	0.4390659495060567	T	T	T
0.8044039887883802	0.6289087187548590	0.3680040552559230	T	T	T
0.7928026082652077	0.5148159640489824	0.4584838062292944	T	T	T
0.8291583306935474	0.3897993351411790	0.4346967763126124	T	T	T
0.0101706143121008	0.5466533780969649	0.2152847229698226	T	T	T
0.0210181082354113	0.3640218501177231	0.1940357528564425	T	T	T
0.8569115170964302	0.4356356494033179	0.7904435862825108	T	T	T
0.7954077450410624	0.4321518639434235	0.6147070788276062	T	T	T
0.7005128038860188	0.4178940039995040	0.4734973089660341	T	T	T
0.6030966994981687	0.4294109964132554	0.6070524015028456	T	T	T
0.6019998046338180	0.4424369265246581	0.8044454197241399	T	T	T
0.7283843105430874	0.4726070982828923	0.7719925582671212	T	T	T
0.8606927827968083	0.6804876980712444	0.7537722991721625	T	T	T
0.8150917156851644	0.6444669550369835	0.5619605734411277	T	T	T
0.6937375847532109	0.6466342284037581	0.4804379167896301	T	T	T
0.5885274867627410	0.6672351990974497	0.5997396629423259	T	T	T
0.5951728448250307	0.6599325312857532	0.7969089176477332	T	T	T
0.7195812310224994	0.6485215352443768	0.7350595787133818	T	T	T
0.8250554660912698	0.5486486114446975	0.6939832694693761	T	T	T
0.5828507318951415	0.5482057799480914	0.6860913670891656	T	T	T
0.9308783156046092	0.3766330798617690	0.9291427774724176	T	T	T
0.9156003704198568	0.5101175360486954	0.9356008574320172	T	T	T
0.8989864735484010	0.6408081734086500	0.9358173071472977	T	T	T
0.6943118994675739	0.3716464468757495	0.8940252823579219	T	T	T
0.6755614939111599	0.5001997027131626	0.9465324500518518	T	T	T
0.6889004781515967	0.6338639456045826	0.9307831790359671	T	T	T
0.4895127554618725	0.4522431874421404	0.7081161455931035	T	T	T
0.4814256406548247	0.6318148795363470	0.7064455655845191	T	T	T
0.6435715859012840	0.9395882939205019	0.2873492991288534	T	T	T
0.6996648775335690	0.9332776941749640	0.1100436745500101	T	T	T
0.8018020395605037	0.9441445658385291	0.9816173941318536	T	T	T
0.9011715756741498	0.9280829760917724	0.1129238878080014	T	T	T
0.8995641321473237	0.9468569976922221	0.3100337986428831	T	T	T
0.7727183148521313	0.9653469772554187	0.2664513834004550	T	T	T
0.6413843132689049	0.1728032514790512	0.2530073172758831	T	T	T
0.6970541658204268	0.1564802216487624	0.0787310051105954	T	T	T
0.8105103332381347	0.1461628355757388	0.9791030373527987	T	T	T
0.9147043780126988	0.1675210720486777	0.0968045137631621	T	T	T

Structure files (CONTCAR) involved in this work:

0.8980066935518946	0.1572153170206874	0.2944642537080126	T	T	T
0.7718204455118265	0.1480646427613018	0.2428161304684603	T	T	T
0.6831018525401549	0.0522277313561703	0.1998440225629106	T	T	T
0.9202093198055528	0.0487698168069928	0.1838133460982168	T	T	T
0.5712821736965465	0.8744707515308840	0.4214150883530747	T	T	T
0.5838525154485599	0.0061926024255462	0.4376772996530799	T	T	T
0.6005118211085949	0.1381814219649782	0.4353145985023142	T	T	T
0.8104742562591325	0.8710010088271873	0.3976772943964232	T	T	T
0.8189172137326278	1.0001725286033447	0.4455426436200026	T	T	T
0.8063420692954280	0.1340131792105219	0.4347119017162843	T	T	T
0.0129727921938541	0.9542252114959449	0.2168672550792395	T	T	T
0.0167027649080717	0.1377393211611392	0.2148145169423759	T	T	T
0.8599099821734522	0.0533489327247564	0.7844606975084706	T	T	T
0.8035776567266698	0.0716287002952419	0.6085356580704168	T	T	T
0.7021314801346609	0.0569085357977193	0.4800513976530846	T	T	T
0.6003938767278503	0.0744455526087851	0.6068869404299140	T	T	T
0.6048199503283617	0.0504713085612247	0.8036610873622021	T	T	T
0.7307159311937290	0.0288857910372848	0.7607425964987139	T	T	T
0.8595959513044646	0.8340048343163045	0.7657412521616768	T	T	T
0.8060116394374992	0.8302899294090669	0.5885308043794374	T	T	T
0.6941807961336514	0.8504044571535997	0.4863151706837401	T	T	T
0.5903597645946888	0.8275000994844863	0.6058707673542044	T	T	T
0.6035372233985542	0.8519964969532201	0.8002506197257283	T	T	T
0.7298887893556188	0.8577961622152682	0.7458949825980187	T	T	T
0.8186938909088137	0.9473012980985233	0.6797845178509864	T	T	T
0.5809445087865560	0.9518910382247492	0.6720218378566423	T	T	T
0.9326863659719378	0.1269688377967936	0.9085207054412822	T	T	T
0.9193786893817375	0.9972452167286293	0.9441140937642727	T	T	T
0.9065621922510975	0.8645466505105827	0.9438312305469015	T	T	T
0.6956997922210411	0.1288622577422162	0.8840215453659322	T	T	T
0.6858674217407634	0.0024915690982077	0.9440049096164015	T	T	T
0.6968140490803252	0.8684594472610917	0.9392326072984261	T	T	T
0.4902420462615467	0.0461537381897503	0.7142955292523422	T	T	T
0.4853125683465661	0.8636187975711093	0.7156167052918878	T	T	T
0.3575714738935389	0.4384732889969638	0.7077246912279371	T	T	T
0.3065558335932506	0.4287963036287996	0.8882892853872874	T	T	T
0.2037576802057106	0.4556938721187310	0.0086440695019642	T	T	T
0.0981797735234934	0.4296428126440021	0.8933318601202158	T	T	T
0.1008293277345229	0.4430958091620751	0.6956259423336985	T	T	T
0.2287464740928125	0.4664142411647330	0.7378656026337919	T	T	T
0.3568536287439904	0.6699418069271538	0.7377825663396308	T	T	T
0.3040512793266515	0.6588284389749288	0.9142567198499287	T	T	T
0.1905633383943326	0.6441610727339960	0.0124426054490471	T	T	T
0.0879250025868522	0.6696713304160666	0.8933860586427130	T	T	T
0.1029787153770267	0.6556915291695716	0.6978442192622729	T	T	T
0.2283818906363893	0.6384412840842025	0.7530857014691722	T	T	T
0.3216785317223625	0.5494763473830643	0.8040314308344425	T	T	T
0.0806041715816271	0.5488784075528905	0.8123252376558935	T	T	T
0.4319465181867658	0.3756701527320913	0.5725321426794391	T	T	T
0.4200842754117437	0.5077290641366288	0.5625950333152875	T	T	T
0.3949662450565868	0.6387742086190098	0.5542468538332050	T	T	T
0.1944428493004076	0.3694109962743802	0.6112724225908981	T	T	T
0.1780723018160024	0.4972107899300139	0.5580091593102297	T	T	T

Structure files (CONTCAR) involved in this work:

0.1947609386550677	0.6306449161505469	0.5595002209459841	T	T	T
0.9863731208170607	0.4539488035822456	0.7896693813870406	T	T	T
0.9836259715509150	0.6368743253620756	0.7794330835656792	T	T	T
0.1425866932413522	0.5614076457638446	0.2141384179636462	T	T	T
0.1999396938994283	0.5638685180429716	0.3906124868697536	T	T	T
0.2975947810717489	0.5487472756825091	0.5262394170751662	T	T	T
0.3931655284725232	0.5682927450262932	0.3901483921740863	T	T	T
0.3982990880164850	0.5536540961264467	0.1946242183355302	T	T	T
0.2710738292298613	0.5276840692587947	0.2321577633057810	T	T	T
0.1405372277403083	0.3247032306908225	0.2436859549710000	T	T	T
0.1929870973051294	0.3408895833322673	0.4186120453253087	T	T	T
0.3087996471023035	0.3528171132972504	0.5118441637458685	T	T	T
0.4100956739655981	0.3257522181849307	0.3893903191283350	T	T	T
0.3928750442470881	0.3427277870276964	0.1933596328935398	T	T	T
0.2697042186005452	0.3542947532568053	0.2567800543847041	T	T	T
0.1772354416990110	0.4465506022386023	0.3009149991190218	T	T	T
0.4120789509929035	0.4474562274540366	0.3147466053087202	T	T	T
0.0679430788062024	0.6212907042316778	0.0770762525284099	T	T	T
0.0832420688524842	0.4896158104849028	0.0704804504755538	T	T	T
0.1167298987301110	0.3600994146564263	0.0552329795645060	T	T	T
0.3057541549217072	0.6257414946727208	0.1063507219347241	T	T	T
0.3243767771313709	0.4970667813470103	0.0553760628022927	T	T	T
0.2960204995827823	0.3653273747001814	0.0606757489556750	T	T	T
0.5083055426620473	0.5379963227292299	0.2987672247093648	T	T	T
0.5114132176085840	0.3621298418922352	0.2716750549833871	T	T	T
0.4393880233759229	0.7494889874502522	0.6378750836254706	T	T	T
0.1949745737741989	0.7477388814732827	0.6484034082306365	T	T	T
0.2716388602416716	0.7471404899638535	0.0548193152706299	T	T	T
0.1080831801378747	0.7463269780913990	0.0503983549385778	T	T	T
0.0666125456372133	0.2473776924729769	0.1275825305018166	T	T	T
0.3041035246240059	0.2476268650098285	0.1473042342755819	T	T	T
0.2286602833143936	0.2494240394093520	0.5535972966534288	T	T	T
0.3920266677303125	0.2504049290591426	0.5482119680253663	T	T	T
0.5572612241213647	0.2494569386390606	0.3532377308568426	T	T	T
0.8149502337835463	0.2534422297120581	0.3520757909895259	T	T	T
0.7275560800192246	0.2489463084189275	0.9421432631462419	T	T	T
0.8914580730792117	0.2500016338706108	0.9446955574796152	T	T	T
0.9457042701720336	0.7526933826323564	0.8599151977694183	T	T	T
0.6852468152824941	0.7524053764321978	0.85064444410107294	T	T	T
0.7769206283094132	0.7480741154504408	0.4421645579352417	T	T	T
0.6108517435633729	0.7495218107109392	0.4491385208243099	T	T	T
0.9285054559561416	0.4896861118621048	0.5198015126745249	T	T	T
0.8247670029040247	0.3366558636330572	0.3258773912474405	T	T	T
0.7995848075690150	0.6360347104910107	0.6958909335128394	T	T	T
0.9264565147856541	0.5279555969746027	0.1943754916901853	T	T	T
0.9226687763079822	0.4314957492851698	0.4023257227646760	T	T	T
0.8659079552423067	0.5574167206831927	0.5565835688689853	T	T	T
-0.0005953815312800	0.6452520149245802	0.3684215131585298	T	T	T
0.9979015492184091	0.5672384461993014	0.4480947308530143	T	T	T
0.9536382186880282	0.4702971383564886	0.5752270317344598	T	T	T
0.0800602930369073	0.6044859313644371	0.4071252749040211	T	T	T
0.0405316001650717	0.4553474118636521	0.4558078833659222	T	T	T
0.0351469208024281	0.3903806457378628	0.3545162287333144	T	T	T

Structure files (CONTCAR) involved in this work:

0.0257931083261684 0.6064614827141271 0.4098787505707184 T T T
0.0094761184345161 0.4261139719742015 0.4037122030471111 T T T

Figure S17 ZnCo-FS

Si O Al Co Zn H C

1.0000000000000000

20.0219999999999985 0.0000000000000000 0.0000000000000000

0.0000000000000000 19.8990000000000009 0.0000000000000000

0.0000000000000000 0.0000000000000000 13.3829999999999991

93 193 3 1 1 6 2

Selective dynamics

Direct

0.4234843367951977 0.0577180804639877 0.6473798938099853 T T T
0.3055506107033278 0.0272137696820659 0.7929879953028787 T T T
0.2827435869845187 0.0591292653500127 0.0144544544828643 T T T
0.1230656116390584 0.0618593567412909 0.0108911012944159 T T T
0.0691157528216415 0.0293920053669144 0.7995105976439694 T T T
0.1810467902890592 0.0564210735984963 0.6589132261287699 T T T
0.4207261690869693 0.8264541943573336 0.6687687864161737 T T T
0.3047036978573914 0.8684161784887768 0.8094580153092492 T T T
0.2671283695257192 0.8280435941064846 0.0278546998489485 T T T
0.1127228587850051 0.8252849411715448 0.0135304210974472 T T T
0.0659972463681970 0.8720321594813040 0.7997149224607701 T T T
0.1830538501510681 0.8271294240856445 0.6723117363717173 T T T
0.0780533402929667 0.9407994440422178 0.1483247733562068 T T T
0.1965627181360171 0.9709682619823051 0.2930116963139217 T T T
0.2191558625681308 0.9372372780649908 0.5147032871753544 T T T
0.3792697123585114 0.9343132294197112 0.5127319434847970 T T T
0.4338984635254804 0.9679507753199766 0.3010840710052882 T T T
0.3215638542770087 0.9414909240711103 0.1598609172174169 T T T
0.0826529520212848 0.1719687404620227 0.1648814176564878 T T T
0.1966306164221421 0.1296084315312554 0.3087960682344019 T T T
0.2336396550659718 0.1706257515545180 0.5258429866797373 T T T
0.3882857265695069 0.1733214182849291 0.5102973757804999 T T T
0.4366997701105750 0.1263267274694251 0.2976945128178499 T T T
0.3177317125435983 0.1698062576990788 0.1721154777233553 T T T
0.5772995156856755 0.5553693120316391 0.3550983363192938 T T T
0.6913288968152773 0.5257002723365357 0.2018416222301120 T T T
0.7146369476336524 0.5666573158349333 0.9860742728260055 T T T
0.8727551383132424 0.5712684086482326 0.9885314342020995 T T T
0.8113832073944991 0.5484065813853084 0.3445345517555334 T T T
0.5737654110593527 0.3275145128552731 0.3304766040886502 T T T
0.6953778538743800 0.3714712932507386 0.1932259445456957 T T T
0.7305127510227888 0.3262088839836712 0.9801688253644552 T T T
0.8850475316381536 0.3251148517462939 0.9938126301663555 T T T
0.9416239057527355 0.3750962803828318 0.1872029692738477 T T T
0.9205451946706260 0.4448412559587587 0.8613694582427762 T T T
0.7993286537147403 0.4713619419786202 0.7209112920425392 T T T
0.7735266455765264 0.4352552489836762 0.4957698246906252 T T T
0.6164682873336297 0.4281714964941990 0.4894111273093792 T T T
0.5683949134189262 0.4681083083976276 0.7025615603615104 T T T
0.6747339641917285 0.4463324550437355 0.8579637081001020 T T T
0.9202851314367658 0.6766150968114319 0.8305032058716574 T T T
0.7700918197682679 0.6684151334680966 0.4621455010887559 T T T

Structure files (CONTCAR) involved in this work:

0.6148864930240487	0.6723373670343064	0.4865740118712583	T	T	T
0.5620132932612715	0.6263787939120133	0.6982041601397768	T	T	T
0.6736339639154925	0.6733906277620797	0.8265726351982968	T	T	T
0.5791427725021612	0.9439876295393135	0.3573569496700152	T	T	T
0.6991925673831730	0.9726407627083540	0.2134296356692706	T	T	T
0.7219089653910034	0.9372779204967913	0.9914456304023588	T	T	T
0.8821973331250793	0.9338959172527868	0.9945237557252615	T	T	T
0.9340791814333321	0.9695759828403751	0.2047872169847781	T	T	T
0.8235275775344808	0.9455535875924327	0.3524946316747984	T	T	T
0.5794115342988546	0.1726859540316594	0.3287195375297629	T	T	T
0.6988913745884573	0.1313682224474948	0.1925004398644986	T	T	T
0.7331237712846580	0.1701067893655129	0.9714670552317501	T	T	T
0.8878274558561486	0.1728024686226311	0.9836473115433856	T	T	T
0.9373631228383781	0.1276733219704029	0.1973387356166661	T	T	T
0.8215112747055165	0.1736799181659004	0.3292589846725306	T	T	T
0.9243773708163218	0.0541638216251704	0.8552367060183937	T	T	T
0.8038655344538289	0.0253976192453972	0.7073124134115135	T	T	T
0.7825104334188544	0.0658120868532292	0.4902755051468904	T	T	T
0.6220207880349631	0.0688438101764410	0.4896587234676714	T	T	T
0.5684733748298199	0.0313509690701146	0.6985748705949913	T	T	T
0.6804031339978664	0.0530362993181341	0.8460778148411946	T	T	T
0.9238355974857472	0.8289491794748947	0.8362843748227772	T	T	T
0.8037138902765971	0.8678449081080708	0.6942803530350699	T	T	T
0.7710883687607858	0.8258277240532804	0.4775230699923488	T	T	T
0.6158900175423142	0.8261484835896190	0.4911616102883659	T	T	T
0.5647829621586283	0.8743436415948391	0.6989838864930539	T	T	T
0.6801745708569690	0.8321768798555461	0.8318987202306349	T	T	T
0.4239657045252265	0.4436389756305846	0.6406019218244897	T	T	T
0.3050372399768257	0.4707064492934689	0.7878955424697759	T	T	T
0.2817001476765688	0.4376628074567194	0.0066701030595949	T	T	T
0.1241542453853347	0.4362815900194144	0.0110630775026307	T	T	T
0.0655399365190375	0.4695662662281485	0.8018046898090815	T	T	T
0.1781556248817253	0.4437482040578634	0.6563162465047844	T	T	T
0.4185757165608177	0.6725806407965218	0.6610931201116054	T	T	T
0.3031237967649356	0.6286492905741168	0.8042219249311207	T	T	T
0.2679861605771480	0.6702225013317374	0.0221797378674930	T	T	T
0.1137757442184925	0.6714839102465980	0.0089563896861195	T	T	T
0.0634598161115730	0.6281179889120192	0.7976456281674612	T	T	T
0.1813754580798049	0.6684352744703277	0.6683532819148890	T	T	T
0.0753980212498828	0.5569143100050137	0.1494193368860758	T	T	T
0.1980216145784077	0.5266082678665713	0.2859876084275841	T	T	T
0.2198053524376468	0.5601680604406046	0.5120735963862573	T	T	T
0.3781106263256530	0.5659731436529354	0.5092481815865768	T	T	T
0.4300277918317614	0.5280432097791500	0.2991054325375429	T	T	T
0.3233092953314287	0.5535588314340317	0.1490706186311588	T	T	T
0.0866678816418139	0.3248328384171446	0.1586829272562756	T	T	T
0.1962850137834053	0.3685633569400126	0.3071442954371731	T	T	T
0.2320907196064989	0.3290732776542191	0.5256299661610493	T	T	T
0.3863802575955698	0.3269199233911732	0.5056079696750967	T	T	T
0.4324209251359067	0.3706510575443486	0.2921635063815664	T	T	T
0.3147782085853169	0.3283059012520340	0.1672126189056513	T	T	T
0.3580627938539711	0.0633539079394008	0.7182545073442648	T	T	T
0.3109595289611958	0.0635570701073851	0.9010804154519727	T	T	T

Structure files (CONTCAR) involved in this work:

0.2026080479872567	0.0468010226508615	0.0143278767400379	T	T	T
0.0967682571078920	0.0689922403762675	0.8971554226271066	T	T	T
0.1048672733344693	0.0590987118306195	0.7000025678851716	T	T	T
0.2299343040337799	0.0354384025952979	0.7508370046039250	T	T	T
0.3607480559855645	0.8257103120779377	0.7499576294901862	T	T	T
0.3065386491277197	0.8451440618426576	0.9251145266609710	T	T	T
0.1897275593509941	0.8518951149271892	0.0167471859075478	T	T	T
0.0853166060416802	0.8308224000701209	0.9001085458280716	T	T	T
0.1056583358630253	0.8396028619593071	0.7049058984286535	T	T	T
0.2310534306253283	0.8535298446496978	0.7626488363944388	T	T	T
0.3230250328426882	0.9476747957095490	0.8006581303182770	T	T	T
0.0871922843678844	0.9502270209359379	0.8126190108126585	T	T	T
0.4322352990688185	0.1274800377303536	0.5856970296126307	T	T	T
0.4170160549720749	0.9958535165966899	0.5686833830529469	T	T	T
0.3967926339785312	0.8637163648472526	0.5670574006953090	T	T	T
0.2006052495806194	0.1305240203764018	0.6184941644452983	T	T	T
0.1852925169055815	0.0015257819137682	0.5694533681981926	T	T	T
0.1992505340784385	0.8673146201203638	0.5695654037946687	T	T	T
0.9894051088453469	0.0406283596706095	0.7857803846881600	T	T	T
0.9859664264239171	0.8668148072011655	0.7806453332673567	T	T	T
0.1442624471303550	0.9350869665213403	0.2176825179669931	T	T	T
0.1915596904765866	0.9340914529308110	0.4008610586445250	T	T	T
0.2994851307332488	0.9477102397710224	0.5164318597940658	T	T	T
0.4051984769080811	0.9289416544001580	0.3986489238155577	T	T	T
0.3975474455294006	0.9388031721150475	0.2017539866099663	T	T	T
0.2722385949166157	0.9637313982903749	0.2507633006015240	T	T	T
0.1419876343998052	0.1725642039180222	0.2471384722135557	T	T	T
0.1931303265740461	0.1538909584541341	0.4240315603091385	T	T	T
0.3110366660510806	0.1476138679661159	0.5119198423307258	T	T	T
0.4170943293715836	0.1679976416324876	0.3977065909146875	T	T	T
0.3954858537152716	0.1575983740672452	0.2033626508390981	T	T	T
0.2710805671422624	0.1436748944767564	0.2642996038158927	T	T	T
0.1781838878090056	0.0503234078853431	0.3014901714202916	T	T	T
0.4177563267448818	0.0477016306241350	0.3129310077385231	T	T	T
0.0676515696072288	0.8704635674890328	0.0886613962662096	T	T	T
0.0843187563315720	0.0009278603613682	0.0666288235480375	T	T	T
0.1067323665710866	0.1323343247498241	0.0656770030838422	T	T	T
0.3017621846078185	0.8672985998638069	0.1201281352970183	T	T	T
0.3180235915196256	0.9956963651458217	0.0693456357456338	T	T	T
0.3005649688078867	0.1291113568326296	0.0703553983406745	T	T	T
0.5133768539080942	0.9544424821340118	0.2882679811270642	T	T	T
0.5165154309575070	0.1334242467692840	0.2774866529415221	T	T	T
0.6386309297269271	0.5608250160577368	0.2770835360121461	T	T	T
0.6988889561518555	0.5735634767056067	0.1048689521151025	T	T	T
0.7937480946989759	0.5564363559280849	0.9639518223681204	T	T	T
0.8858797287056859	0.5779762943799390	0.1063297492340232	T	T	T
0.8881917338940001	0.5267297777824955	0.3200282261630361	T	T	T
0.7633075034119177	0.5217693080827652	0.2584576396302838	T	T	T
0.6416052893545920	0.3352306013311658	0.2668301614097741	T	T	T
0.6914632292514939	0.3332362600338946	0.0856271397011487	T	T	T
0.8078729943584618	0.3507698059714027	0.9916790012510253	T	T	T
0.9108622220988967	0.3200421570935624	0.1095718920670882	T	T	T
0.9099926039681855	0.3627560193885384	0.3014865786598769	T	T	T

Structure files (CONTCAR) involved in this work:

0.7691399564220250	0.3682816290653563	0.2395266399164072	T	T	T
0.6702793126801152	0.4492358816875289	0.1754686695502879	T	T	T
0.9236407757438717	0.4487083509644151	0.1511771033735112	T	T	T
0.5693404966505213	0.6267215638686060	0.4127038832938606	T	T	T
0.5908497429049201	0.4974803489302367	0.4385450747850279	T	T	T
0.5802847541286839	0.3638853680251964	0.4394150199740605	T	T	T
0.8026379343203942	0.6285202269239781	0.3666866674616277	T	T	T
0.7917955043759494	0.5137980522180590	0.4561044839647779	T	T	T
0.8243507993722867	0.3870253311641505	0.4360925442307362	T	T	T
0.0103587944155968	0.5511694365589085	0.2182957235225195	T	T	T
0.0215696718238398	0.3638702135111134	0.2007288014686888	T	T	T
0.8563941465519054	0.4344044559346320	0.7866187180703478	T	T	T
0.7889133028385323	0.4324519979142941	0.6143828158666792	T	T	T
0.6967209968001570	0.4204631853401964	0.4696307520755058	T	T	T
0.6018566999239836	0.4286702872347400	0.6081564316649720	T	T	T
0.6019113352483227	0.4416204639212318	0.8055464217682994	T	T	T
0.7281027691214889	0.4739655699851258	0.7755153813052656	T	T	T
0.8614714863770101	0.6802281866838977	0.7499616213353029	T	T	T
0.8142215931829145	0.6435637770372681	0.5604769120073135	T	T	T
0.6927465928713270	0.6466683377501000	0.4804863267924008	T	T	T
0.5875793727755815	0.6665445356847661	0.5996572482393960	T	T	T
0.5953274740752114	0.6600328913518825	0.7968732855305642	T	T	T
0.7195996365416895	0.6484295022075587	0.7346597729421063	T	T	T
0.8239183694716802	0.5481710175892789	0.6938924822254149	T	T	T
0.5825825584817058	0.5477424308080080	0.6874618579769755	T	T	T
0.9300867117285458	0.3767586500962845	0.9274999939731197	T	T	T
0.9134409588107820	0.5094392455204365	0.9336514182111633	T	T	T
0.8965216274622054	0.6400048707665958	0.9329980164519167	T	T	T
0.6949508256843040	0.3718810069200336	0.8951498058530827	T	T	T
0.6735439129094615	0.5002979181196865	0.9486075638045144	T	T	T
0.6889028173788282	0.6339530455977179	0.9306003275591720	T	T	T
0.4891761459246765	0.4519007459341181	0.7112189613679901	T	T	T
0.4813006104520022	0.6316941253649073	0.7083303751807865	T	T	T
0.6443198167554214	0.9381024754721016	0.2861673036276390	T	T	T
0.6987134059539162	0.9333541241477307	0.1073002186031795	T	T	T
0.8024065565644662	0.9454904932033706	0.9821153010109075	T	T	T
0.9026918419010580	0.9279617814644439	0.1113303881953953	T	T	T
0.8990022209836934	0.9464109737609347	0.3084953558811916	T	T	T
0.7728882609823740	0.9654020233845441	0.2624835432279242	T	T	T
0.6416346558127196	0.1728397136523842	0.2516953341828589	T	T	T
0.6962670889563521	0.1552365875338168	0.0769155737439582	T	T	T
0.8108248226945088	0.1465568628111301	0.9801735075618546	T	T	T
0.9155250086344415	0.1677321925851879	0.0969481520048280	T	T	T
0.8979372913204757	0.1564277336009064	0.2940018864619006	T	T	T
0.7717996999157511	0.1464631466573148	0.2404409221019516	T	T	T
0.6815749036366838	0.0516217051080181	0.1990106871414116	T	T	T
0.9207926378364690	0.0485806021467399	0.1827774090944010	T	T	T
0.5711099803395212	0.8746137580720699	0.4205991956881371	T	T	T
0.5846263020493828	0.0061188497646381	0.4356888140509786	T	T	T
0.6009258996043098	0.1381230500986870	0.4340169015501291	T	T	T
0.8086124496955098	0.8703408050216587	0.3937335817062663	T	T	T
0.8173643627477329	0.9990949877853685	0.4432911663019707	T	T	T
0.8056965646538244	0.1332362636365438	0.4327102438593313	T	T	T

Structure files (CONTCAR) involved in this work:

0.0133455800357041	0.9544545168317425	0.2181250719071771	T	T	T
0.0171538834473664	0.1377722769588103	0.2151748974523561	T	T	T
0.8584401188023418	0.0542885741744860	0.7853697963584496	T	T	T
0.8054639191008782	0.0710284436486163	0.6066531790382438	T	T	T
0.7019278081908101	0.0569610346578686	0.4821752736796736	T	T	T
0.5984467906084880	0.0746078896248177	0.6054474164071203	T	T	T
0.6047911136796775	0.0518421428447918	0.8025179446963225	T	T	T
0.7299727648299390	0.0292147696772046	0.7567314619743917	T	T	T
0.8594091207290246	0.8328975235712183	0.7638066471135314	T	T	T
0.8070725325653514	0.8316272481284191	0.5856271437139154	T	T	T
0.6937320815032303	0.8501717092811312	0.4868173709502169	T	T	T
0.5893116008922216	0.8281739907612282	0.6055821845874120	T	T	T
0.6041778528462545	0.8521602362262785	0.7998316184121598	T	T	T
0.7299513555392527	0.8571678708786596	0.7426473532376819	T	T	T
0.8197262408367104	0.9473418794132268	0.6805591083191960	T	T	T
0.5803715701871339	0.9523622093326568	0.6726470658769396	T	T	T
0.9325415533151753	0.1271911133675157	0.9084822942270373	T	T	T
0.9203119337927211	0.9969670017928217	0.9420331772046934	T	T	T
0.9055816228078365	0.8644596758229915	0.9420459232452860	T	T	T
0.6973081435336346	0.1289189473800947	0.8818684167730774	T	T	T
0.6863611452978140	0.0023026206654054	0.9407060962169749	T	T	T
0.6989927882280303	0.8684346052706329	0.9366883466413600	T	T	T
0.4895299700428148	0.0465656588295346	0.7153317813946244	T	T	T
0.4852109370029667	0.8638880631921430	0.7173357433415586	T	T	T
0.3575269283202397	0.4377658664820950	0.7096492617873595	T	T	T
0.3088279289075407	0.4295769996695312	0.8927005167934421	T	T	T
0.2027367548224416	0.4569975897218055	0.0071975694739742	T	T	T
0.0944426277676468	0.4303772683990435	0.8985106297501567	T	T	T
0.1019878053659019	0.4430321292225214	0.6998786205329504	T	T	T
0.2292122364170721	0.4655744122711793	0.7446622510421158	T	T	T
0.3567615467775860	0.6703320823076703	0.7388493449172412	T	T	T
0.3059140232342603	0.6579233757271565	0.9167190883012127	T	T	T
0.1909623267515546	0.6454349141249103	0.0118459922236933	T	T	T
0.0875442444938195	0.6706786929921957	0.8942823808060708	T	T	T
0.1036910710460129	0.6550074864793116	0.6991843469948354	T	T	T
0.2286600470937022	0.6385729723808249	0.7572205831949870	T	T	T
0.3230805025449891	0.5494813816058701	0.8046552233310331	T	T	T
0.0803793322838047	0.5491048672567148	0.8151310380662773	T	T	T
0.4322903790486967	0.3758116661319224	0.5741184935032450	T	T	T
0.4210267509070287	0.5078654049169090	0.5653471999885572	T	T	T
0.3957632673039252	0.6390808043905666	0.5555847331989108	T	T	T
0.1962026105928013	0.3689432672728778	0.6167341136113949	T	T	T
0.1812716505193164	0.4969805835644242	0.5639104679858959	T	T	T
0.1970231301368022	0.6304919561199919	0.5631444825583685	T	T	T
0.9857724336035921	0.4545630083335792	0.7883821523364649	T	T	T
0.9838675726730889	0.6367483335967820	0.7796443761644589	T	T	T
0.1429737044918839	0.5644144384410075	0.2178924860492891	T	T	T
0.1997133812319319	0.5630952098324821	0.3948271631992665	T	T	T
0.2995226954982203	0.5486246629303504	0.5254423174260384	T	T	T
0.3970977502047320	0.5687994610722897	0.3919632581141559	T	T	T
0.3981659034012612	0.5556526119340138	0.1955437524689668	T	T	T
0.2717331107970309	0.5304307721959415	0.2365899247958028	T	T	T
0.1418460983565919	0.3243132909773553	0.2472522918065924	T	T	T

Structure files (CONTCAR) involved in this work:

0.1921819110277213	0.3458356811679044	0.4230772802856830	T	T	T
0.3093003992911150	0.3532085067097561	0.5129697104004667	T	T	T
0.4108104793207142	0.3273371911637337	0.3900449021562064	T	T	T
0.3925362097720557	0.3437189090924965	0.1941096901777261	T	T	T
0.2703474945506127	0.3543948563989360	0.2620740112683199	T	T	T
0.1771453259839055	0.4478240706937576	0.2983813104245052	T	T	T
0.4139496805667942	0.4486965376152113	0.3140254230967395	T	T	T
0.0687312413801117	0.6232373542074957	0.0784676926924783	T	T	T
0.0836331609551329	0.4915128723362726	0.0757056185960568	T	T	T
0.1165244482401730	0.3620575007051901	0.0605188345127713	T	T	T
0.3047767463335319	0.6280424479429763	0.1096827931904192	T	T	T
0.3223453596673178	0.4991384482928843	0.0585445750196566	T	T	T
0.2936796479140715	0.3672455257290341	0.0653628468271466	T	T	T
0.5098964901073120	0.5397043160651560	0.2931585783548587	T	T	T
0.5117319329202807	0.3617652070853687	0.2699736716726401	T	T	T
0.4396583197005282	0.7497240252257411	0.6397319414845598	T	T	T
0.1954546483666618	0.7477870255657026	0.6517355428112017	T	T	T
0.2717996426183619	0.7486755824760120	0.0525825497641845	T	T	T
0.1087769404553549	0.7478956596769490	0.0505611580839060	T	T	T
0.0669007980419697	0.2484578119408652	0.1302003564819023	T	T	T
0.3037160551428558	0.2486256925344801	0.1496129188132310	T	T	T
0.2283981535904029	0.2499277758375987	0.5513705526577451	T	T	T
0.3925486201204767	0.2507839005008055	0.5477413737128747	T	T	T
0.5575637683165510	0.2493254849360650	0.3523895895740864	T	T	T
0.8140698902717409	0.2524529383973214	0.3487309475310469	T	T	T
0.7277090161989703	0.2489575265367753	0.9425041621792735	T	T	T
0.8919277658616549	0.2503911641489951	0.9459819856614885	T	T	T
0.9447979397175392	0.7521280828455205	0.8598177581041055	T	T	T
0.6858022836925822	0.7523868578996556	0.8496481035422565	T	T	T
0.7762988958903853	0.7477738897373516	0.4419502464212466	T	T	T
0.6100172011174144	0.7496975846353912	0.4497123761139274	T	T	T
0.9190021609550858	0.4798722615986416	0.5293567933173833	T	T	T
0.8240762907851961	0.3361700051224774	0.3262257703869154	T	T	T
0.7993140710914837	0.6356627802672157	0.6948537608448077	T	T	T
0.9274926990559790	0.5303635166101190	0.1950930839651459	T	T	T
0.9220933359279085	0.4339663778303888	0.4040231529396912	T	T	T
0.8627256983517204	0.5557212762266682	0.5559010949299443	T	T	T
0.0036074417286640	0.5578903604113826	0.4174860218042642	T	T	T
0.0441598390462349	0.5217711848868132	0.5249557156291450	T	T	T
0.9530398367939599	0.4690688467950150	0.5790892255978485	T	T	T
0.0866803761168829	0.5327796585379013	0.4105757426840628	T	T	T
0.0368987914448098	0.4076607845496716	0.4512637323336010	T	T	T
0.0277374673839001	0.4427503947056087	0.3266215098159665	T	T	T
0.0383323498862057	0.5189105935399575	0.4435685567658278	T	T	T
0.0187560472747108	0.4507095257738303	0.4068703698673647	T	T	T

Figure S17 ZnNi-IS

Si O Al Ni Zn H C

1.0000000000000000

20.0219999999999985 0.0000000000000000 0.0000000000000000

0.0000000000000000 19.8990000000000009 0.0000000000000000

0.0000000000000000 0.0000000000000000 13.3829999999999991

93 193 3 1 1 6 2

Selective dynamics

Structure files (CONTCAR) involved in this work:

Direct

0.4237995049730356	0.0574058700512794	0.6476436859388007	T	T	T
0.3054978049672983	0.0271228516213537	0.7931968967242840	T	T	T
0.2827663130500401	0.0595803197580200	0.0143328623393532	T	T	T
0.1232213411035971	0.0615820545573296	0.0109637051042752	T	T	T
0.0697687598680621	0.0294291966416547	0.7997447114624540	T	T	T
0.1811272856958448	0.0558498801873463	0.6581656394222862	T	T	T
0.4206584454313145	0.8260767254215441	0.6682736460776927	T	T	T
0.3046721550911701	0.8685410686209923	0.8096132272630211	T	T	T
0.2666951412211674	0.8278507677628169	0.0277597241438855	T	T	T
0.1120714411793731	0.8260404332763014	0.0137920962653906	T	T	T
0.0661253716832881	0.8724848267421974	0.7996846733774878	T	T	T
0.1832531968133214	0.8277206536936098	0.6725009820666589	T	T	T
0.0772017066162972	0.9413772961157042	0.1485491625814250	T	T	T
0.1966160699582983	0.9711111054843531	0.2927481841242986	T	T	T
0.2195339150426598	0.9371166595162764	0.5143047120653681	T	T	T
0.3796410699422511	0.9341263380493411	0.5128906510363497	T	T	T
0.4336686051277715	0.9683634877756052	0.3008155425941345	T	T	T
0.3218172743154009	0.9419309879306099	0.1584772675715427	T	T	T
0.0817867818704486	0.1709743343550558	0.1658432290053102	T	T	T
0.1963548310731519	0.1297206638654635	0.3097710923535205	T	T	T
0.2339003329421550	0.1705674788064045	0.5264976967125866	T	T	T
0.3883523044741591	0.1730583185953770	0.5103412736606463	T	T	T
0.4366976229713521	0.1267226005028990	0.2974615390624230	T	T	T
0.3173590960076604	0.1701923052860698	0.1724618643555713	T	T	T
0.5769844073543350	0.5562942497230299	0.3549778742174576	T	T	T
0.6894455303008924	0.5262205392947608	0.2011519872235107	T	T	T
0.7156890248867714	0.5666170075355370	0.9856149739604166	T	T	T
0.8749411341149884	0.5717799265278818	0.9833429713221080	T	T	T
0.8099061970688143	0.5519535559181840	0.3405732269350163	T	T	T
0.5744275756029602	0.3275899924706880	0.3299204418194727	T	T	T
0.6939569463625760	0.3726247297077973	0.1912088875123320	T	T	T
0.7325714299766226	0.3273852251834277	0.9787597261107989	T	T	T
0.8875753033058654	0.3253847584571906	0.9920850159671257	T	T	T
0.9438336024459955	0.3727828362452810	0.1916017359875648	T	T	T
0.9206790733063039	0.4446070761430250	0.8572029398020783	T	T	T
0.8009680566614228	0.4732069089554740	0.7169713484397000	T	T	T
0.7772578531956745	0.4367529248829576	0.4919733683258579	T	T	T
0.6192321480861852	0.4291411866757500	0.4878143864279390	T	T	T
0.5697045447934582	0.4681925374487300	0.7010559905408250	T	T	T
0.6773124764635753	0.4468323862537845	0.8542515156902595	T	T	T
0.9195551381300987	0.6782207433124329	0.8248563029127578	T	T	T
0.7669239295723922	0.6690960722824790	0.4624612652622311	T	T	T
0.6125125752426318	0.6732567831909521	0.4883284598624359	T	T	T
0.5611409039830720	0.6264323562539171	0.6992404600920428	T	T	T
0.6747291242511158	0.6732284795789861	0.8252145179434180	T	T	T
0.5787993094352648	0.9443147941535218	0.3574893247593617	T	T	T
0.6985928503073426	0.9727254856611306	0.2133323041430953	T	T	T
0.7217666771922324	0.9370570529748595	0.9916398430410742	T	T	T
0.8820671950209829	0.9338273214734044	0.9945651416209698	T	T	T
0.9329036754508090	0.9704227260515008	0.2052515944477942	T	T	T
0.8227311167776642	0.9460064711894931	0.3531679366731019	T	T	T
0.5795046930340392	0.1729133605387532	0.3290166126133405	T	T	T

Structure files (CONTCAR) involved in this work:

0.6984546449692741	0.1307380938269157	0.1920925262399914	T	T	T
0.7334532001288666	0.1709472615212566	0.9716769811053124	T	T	T
0.8880764629141112	0.1731154988668528	0.9831657920523256	T	T	T
0.9360811369884797	0.1285666223432835	0.1980089120261020	T	T	T
0.8196509744692154	0.1737303307644060	0.3288784348722134	T	T	T
0.9247108197003543	0.0541650451117745	0.8554546882615695	T	T	T
0.8038880318302983	0.0262628555521716	0.7075010010263799	T	T	T
0.7824093469791941	0.0661934356130411	0.4906635616576487	T	T	T
0.6219703254526067	0.0690236473835213	0.4899018751009355	T	T	T
0.5686769785668947	0.0315010169255477	0.6992021864319742	T	T	T
0.6805363822468048	0.0535482915134506	0.8471444226687159	T	T	T
0.9238942802709662	0.8300721367907499	0.8356913756714067	T	T	T
0.8031213746385643	0.8688948936424126	0.6942340710413185	T	T	T
0.7696499612354565	0.8265900254167706	0.4779831258677256	T	T	T
0.6148647327407126	0.8267525562411910	0.4913333947841154	T	T	T
0.5643311020735448	0.8743823930122190	0.6995928047234419	T	T	T
0.6798777823571244	0.8322706502894252	0.8319658335401174	T	T	T
0.4237888911967985	0.4426972014433366	0.6435944657703845	T	T	T
0.3044379073275982	0.4710174963961448	0.7893913281305889	T	T	T
0.2783750992884935	0.4385561992901347	0.0103903851474259	T	T	T
0.1207426938436911	0.4356752028612325	0.0133156738398634	T	T	T
0.0650361448247153	0.4699474330732046	0.8005390810687949	T	T	T
0.1778026673983496	0.4437002959574730	0.6554209668619499	T	T	T
0.4178199422927693	0.6720823961110087	0.6635702871495376	T	T	T
0.3028806093142348	0.6286686634401074	0.8060287826245315	T	T	T
0.2666837121630496	0.6700368281423972	0.0242229989436758	T	T	T
0.1127299072959370	0.6724874147861171	0.0082469858368121	T	T	T
0.0625011306620406	0.6285851349345192	0.7957525841279492	T	T	T
0.1817754891908365	0.6692753152798058	0.6692600111390093	T	T	T
0.0790567338256475	0.5573033836293640	0.1467382908049881	T	T	T
0.1980321609686292	0.5248184717418712	0.2889515967409918	T	T	T
0.2169381455308394	0.5602846475821858	0.5123027236908521	T	T	T
0.3758798898457718	0.5651090193033598	0.5111132271012357	T	T	T
0.4294729822767136	0.5282291760184108	0.3008043835818509	T	T	T
0.3222172908009931	0.5539595724496197	0.1524141078807775	T	T	T
0.0862680774221789	0.3233295387813518	0.1614786269023098	T	T	T
0.1972511307766907	0.3672754443969661	0.3074146224896622	T	T	T
0.2324019294172119	0.3285179572074001	0.5257681355644529	T	T	T
0.3864376560369994	0.3267437399646260	0.5063455819449350	T	T	T
0.4324744558587452	0.3708570092158213	0.2927851869842601	T	T	T
0.3150805743731298	0.3287084142407390	0.1685605861589726	T	T	T
0.3582023625133082	0.0626813914506642	0.7182287804365021	T	T	T
0.3098707454047848	0.0648226084169711	0.9004359531196634	T	T	T
0.2027337323839636	0.0463367553583534	0.0157921175700187	T	T	T
0.0979639759004092	0.0693987468577071	0.8967829273810320	T	T	T
0.1050548391810192	0.0586303798045188	0.6995625945501978	T	T	T
0.2301580611700194	0.0341118494351611	0.7495233112780505	T	T	T
0.3601328020868277	0.8261416721362170	0.7486799465255591	T	T	T
0.3059478208468577	0.8430915491166868	0.9243880174329707	T	T	T
0.1892528390444693	0.8518419824204805	0.0171720192374355	T	T	T
0.0848921892753861	0.8309691894312430	0.9003168075685580	T	T	T
0.1057262998367092	0.8394725793872513	0.7051876519503640	T	T	T
0.2308264567079672	0.8550675202849524	0.7625915891861674	T	T	T

Structure files (CONTCAR) involved in this work:

0.3234109568927006	0.9477850013812751	0.8040515341130775	T	T	T
0.0883227371160992	0.9503016394160495	0.8132169468818381	T	T	T
0.4322299869692934	0.1270853951649541	0.5856169456075452	T	T	T
0.4177395625412477	0.9952859338845365	0.5692536040590486	T	T	T
0.3975200542770918	0.8631204333604785	0.5658930211431368	T	T	T
0.2009076481696822	0.1300987811746249	0.6187457975465666	T	T	T
0.1849720050332425	0.0015002363067191	0.5678277510228754	T	T	T
0.1989760311266558	0.8673648279816657	0.5692017085001012	T	T	T
0.9900405740986015	0.0401297975446255	0.7867506830327574	T	T	T
0.9861133259886168	0.8682347283016884	0.7804581429813610	T	T	T
0.1432422502339541	0.9358927895592332	0.2183569336492723	T	T	T
0.1931163612350761	0.9331476457943939	0.3999256157977367	T	T	T
0.2998336032087693	0.9475526953720973	0.5181967730490898	T	T	T
0.4045247808937750	0.9295100332888450	0.3982549633962756	T	T	T
0.3974374750454652	0.9388956917084869	0.2015058782510291	T	T	T
0.2716916518445375	0.9643472719694783	0.2481550105273025	T	T	T
0.1409388521763321	0.1716650622500267	0.2483814350276126	T	T	T
0.1931254589632179	0.1549546966159266	0.4245620932241005	T	T	T
0.3111411398309820	0.1472217522315709	0.5118805963475103	T	T	T
0.4170785666682693	0.1681122165844214	0.3977492798978015	T	T	T
0.3951463135167470	0.1581197325488724	0.2035054814540417	T	T	T
0.2705292855185110	0.1438981023154189	0.2643004575282144	T	T	T
0.1784500755029935	0.0502541648329787	0.3040113749219900	T	T	T
0.4174620353812383	0.0481052071586731	0.3121694699985678	T	T	T
0.0671539160873898	0.8704412894275630	0.0898625193551775	T	T	T
0.0839916820064522	0.0002333762655038	0.0650307591535646	T	T	T
0.1064221750536517	0.1314516815677253	0.0668190403625661	T	T	T
0.3019776097702206	0.8676385807207510	0.1188006885284950	T	T	T
0.3191030972271452	0.9960703541154118	0.0677271852254308	T	T	T
0.3002768397586226	0.1295425045045223	0.0705616441939878	T	T	T
0.5131002782474248	0.9550459996806444	0.2882302129122109	T	T	T
0.5164369894087534	0.1339606043043195	0.2772952506003189	T	T	T
0.6371797528364072	0.5632103678839604	0.2753690040923325	T	T	T
0.6973424245153017	0.5735578789093710	0.1034278644581179	T	T	T
0.7953572139255779	0.5560003073148010	0.9685721158560768	T	T	T
0.8955718792436721	0.5794410624088652	0.0985666121264129	T	T	T
0.8862315683248659	0.5415302141266320	0.3091265324132273	T	T	T
0.7612919720150326	0.5209631020287621	0.2573631626291223	T	T	T
0.6403977449741536	0.3337767991872353	0.2620994415396529	T	T	T
0.6915455596476906	0.3361537450350774	0.0821078640573743	T	T	T
0.8101181919401874	0.3506034851790360	0.9940102861869062	T	T	T
0.9175615997581635	0.3214240500860958	0.1047118700855332	T	T	T
0.9064794862732830	0.3545819591060752	0.2965766771617046	T	T	T
0.7670937641109185	0.3702386391985565	0.2392328166443757	T	T	T
0.6667491849553474	0.4500307342936117	0.1756209461024245	T	T	T
0.9311684123391196	0.4481793821944589	0.1553157679579300	T	T	T
0.5680465117869465	0.6271502418169226	0.4135930926720214	T	T	T
0.5919906418309770	0.4978859468621073	0.4369179751688838	T	T	T
0.5837107536784132	0.3643095289477447	0.4379993068759495	T	T	T
0.7938938160350937	0.6309284984166161	0.3627300725511238	T	T	T
0.7962575498276224	0.5143839917889811	0.4516733513707473	T	T	T
0.8264746057524227	0.3851049968297732	0.4359907491756250	T	T	T
0.0126069546660645	0.5562616455333020	0.2262405343808619	T	T	T

Structure files (CONTCAR) involved in this work:

0.0236598007753837	0.3616448887913121	0.2113349573653442	T	T	T
0.8558219671667455	0.4347340171540938	0.7849287611042431	T	T	T
0.7932709688127669	0.4345272383430708	0.6104262877523117	T	T	T
0.6994668842529599	0.4230936815417878	0.4684790165807596	T	T	T
0.6032741240707287	0.4294028895057467	0.6063150864153850	T	T	T
0.6038230125996050	0.4416352124175671	0.8036159542170116	T	T	T
0.7289350659582119	0.4755690299471951	0.7701668881647138	T	T	T
0.8614730398226961	0.6833013245028950	0.7436519768558362	T	T	T
0.8137829708700994	0.6434019284438055	0.5566873398955789	T	T	T
0.6901641377234826	0.6477710336613497	0.4866485123998766	T	T	T
0.5834456772261852	0.6681837145544819	0.6005249673584224	T	T	T
0.5961063280003789	0.6593672790745077	0.7971564130221285	T	T	T
0.7204287816393269	0.6487808158741001	0.7328652144504514	T	T	T
0.8263688615078816	0.5497345385791657	0.6914966519671893	T	T	T
0.5823859281204284	0.5481638782773814	0.6862532727518899	T	T	T
0.9308778582519623	0.3768075028083703	0.9229992087887859	T	T	T
0.9145879630131214	0.5097600205185638	0.9287395546157924	T	T	T
0.8948205129866337	0.6408378790027902	0.9261021082590626	T	T	T
0.6994162288670782	0.3727601565050520	0.8910053719252072	T	T	T
0.6759358236428425	0.5002306429238832	0.9456901348750932	T	T	T
0.6913350503940147	0.6339747586963690	0.9289857029890483	T	T	T
0.4904938727504670	0.4516880414310479	0.7105292951693378	T	T	T
0.4802975662257477	0.6310962556451784	0.7114337504218932	T	T	T
0.6438958858335979	0.9379629598768038	0.2862435538299019	T	T	T
0.6992041681377399	0.9327465703612163	0.1077445045766038	T	T	T
0.8022907155558341	0.9446349392573689	0.9812267004077186	T	T	T
0.9020476474658314	0.9285195176929293	0.1116018771506973	T	T	T
0.8982061951035825	0.9462421244753397	0.3087200516078216	T	T	T
0.7720913017485762	0.9667247422541525	0.2635173565922949	T	T	T
0.6418664750343792	0.1724948220392640	0.2523150247723829	T	T	T
0.6966291282737244	0.1563320504611893	0.0772803256772648	T	T	T
0.8110514592409954	0.1468157611753424	0.9795022884631384	T	T	T
0.9153503327672344	0.1681301863743333	0.0967395096269897	T	T	T
0.8968044456614629	0.1588142536659523	0.2938036330181016	T	T	T
0.7716759375884744	0.1428344581850478	0.2404441680389660	T	T	T
0.6796143597131576	0.0511721571927025	0.1966090424971709	T	T	T
0.9188323294498018	0.0494159379666532	0.1844236985160273	T	T	T
0.5698939271809597	0.8751090753594991	0.4208228534243594	T	T	T
0.5845171883657977	0.0063364031539413	0.4358897788468515	T	T	T
0.6003656634903396	0.1381944167809804	0.4345212678174981	T	T	T
0.8074587540002516	0.8707294900257776	0.3938789084501546	T	T	T
0.8173159205039968	0.9991802188321874	0.4445239093940404	T	T	T
0.8060252419881115	0.1332276889108020	0.4329883016229460	T	T	T
0.0124190067261432	0.9555449668873366	0.2177341658724298	T	T	T
0.0161596524642645	0.1370115650643442	0.2158742685122277	T	T	T
0.8591857290137996	0.0545370589091431	0.7848856472200803	T	T	T
0.8049971262191197	0.0720144916879920	0.6070952132547948	T	T	T
0.7018368838328543	0.0572473095789049	0.4819416314666894	T	T	T
0.5986868357322662	0.0745076238582562	0.6059152874342985	T	T	T
0.6049955634886732	0.0518562000046379	0.8031611389471509	T	T	T
0.7303562308883756	0.0301488586020584	0.7579911943555927	T	T	T
0.8591838044395258	0.8348051850456143	0.7641461410111584	T	T	T
0.8061104615816458	0.8323873815615761	0.5858255860726920	T	T	T

Structure files (CONTCAR) involved in this work:

0.6924336039309348	0.8515609968076102	0.4872479315446159	T	T	T
0.5885218437288557	0.8284664469608474	0.6058650266466897	T	T	T
0.6037074834309016	0.8519873113148193	0.8002403887997119	T	T	T
0.7295578920474283	0.8583278026731985	0.7432564060355672	T	T	T
0.8191438887348147	0.9482735164161573	0.6797569738768837	T	T	T
0.5799047373135722	0.9524200933597079	0.6735264453700432	T	T	T
0.9330566093263967	0.1270170182337891	0.9088681312277613	T	T	T
0.9200580894172095	0.9969242935985073	0.9421445043041018	T	T	T
0.9065240003928396	0.8643937116107628	0.9427273001896594	T	T	T
0.6968681603772656	0.1295413822686405	0.8828581144416783	T	T	T
0.6865963645537589	0.0025566495692833	0.9415458220930888	T	T	T
0.6982191534705389	0.8683415601927748	0.9371147267550171	T	T	T
0.4897250987056554	0.0469373159481316	0.7159538697853989	T	T	T
0.4847186463625330	0.8635746118486241	0.7178202326590757	T	T	T
0.3590584310387105	0.4360283952723829	0.7165269312370747	T	T	T
0.3030806169660499	0.4311616439775043	0.8954227322256233	T	T	T
0.1989953821201358	0.4578706751559353	0.0157820972940862	T	T	T
0.0931205391142321	0.4330152763972724	0.9001662533234314	T	T	T
0.1028635900408112	0.4410402003999205	0.7019375042460916	T	T	T
0.2300682859230436	0.4673201140195306	0.7410916000787992	T	T	T
0.3565121270345588	0.6714867835313288	0.7425999198607273	T	T	T
0.3047373134768753	0.6567780425374178	0.9193732004447648	T	T	T
0.1893350753379704	0.6453919492477325	0.0128012538351019	T	T	T
0.0851982521600210	0.6696149381212910	0.8951132342657480	T	T	T
0.1039444406555705	0.6574805322328202	0.7000826655101297	T	T	T
0.2285908075395850	0.6385023944839944	0.7580726693093753	T	T	T
0.3234842687985655	0.5496653484157424	0.8054679041715902	T	T	T
0.0802118678666722	0.5496939597076055	0.8117242974996410	T	T	T
0.4317892758808923	0.3751874769479671	0.5762787412712307	T	T	T
0.4173780273763085	0.5067370515542353	0.5685137801206387	T	T	T
0.3930571237897488	0.6377905358298847	0.5594731037016910	T	T	T
0.1966214272749676	0.3692942306764351	0.6158082897985921	T	T	T
0.1777367757190144	0.4974208829688478	0.5633887834899326	T	T	T
0.1961708386576457	0.6310810038359932	0.5637837606455036	T	T	T
0.9860026278054942	0.4547078161046872	0.7850900922248637	T	T	T
0.9833911895304803	0.6375804080514622	0.7758021193562479	T	T	T
0.1449993632422790	0.5629435578927494	0.2155492120579565	T	T	T
0.1945567023480278	0.5634785976040115	0.3955122079581215	T	T	T
0.2967042770438440	0.5479390204492707	0.5226754676310431	T	T	T
0.3966161107810551	0.5683564422215213	0.3944636785047398	T	T	T
0.3972365537734576	0.5565377926727326	0.1974914603161699	T	T	T
0.2720581229158786	0.5303315406805446	0.2419505035233151	T	T	T
0.1460786593769641	0.3221319393591624	0.2431648649456865	T	T	T
0.1923425298621244	0.3437187035317292	0.4227466541195551	T	T	T
0.3093735891989190	0.3532058674810931	0.5130296019380616	T	T	T
0.4109765952708545	0.3276764779548553	0.3908756022650191	T	T	T
0.3931003008296526	0.3436846211333431	0.1940836380933413	T	T	T
0.2723620229479345	0.3557943585361715	0.2646794166638303	T	T	T
0.1764060722552369	0.4465092458787953	0.2992554725404723	T	T	T
0.4131561950116220	0.4488273688049451	0.3139995506957786	T	T	T
0.0681216426137543	0.6242288260556504	0.0808920215011159	T	T	T
0.0775811304508631	0.4905148742414285	0.0789572053258483	T	T	T
0.1116903372555078	0.3617362184573153	0.0609411032025506	T	T	T

Structure files (CONTCAR) involved in this work:

0.3019682676419208	0.6281427783200161	0.1134036830546489	T	T	T
0.3195544445650285	0.4999801812285126	0.0614559690311412	T	T	T
0.2920978716451152	0.3679931806199497	0.0676264313614598	T	T	T
0.5091102684533895	0.5400474487548591	0.2942385236387952	T	T	T
0.5117204005547169	0.3623863915235586	0.2715338896980872	T	T	T
0.4390613975052494	0.7489969355980681	0.6402256271859166	T	T	T
0.1968248592477653	0.7483985646960215	0.6527450164396753	T	T	T
0.2702179457154991	0.7485238775151711	0.0540992944822120	T	T	T
0.1073193296068523	0.7483382380647939	0.0506711371551985	T	T	T
0.0665123264671505	0.2474131694680732	0.1308993575878660	T	T	T
0.3032407579911933	0.2491836874870070	0.1506632961509849	T	T	T
0.2290886280476979	0.2496856833022783	0.5534118997133235	T	T	T
0.3924432240279289	0.2504818075637756	0.5479855841614371	T	T	T
0.5578674019888205	0.2495968525801399	0.3529866320800392	T	T	T
0.8068246843248772	0.2517809894086013	0.3464809882327388	T	T	T
0.7287730181646380	0.2497784306183680	0.9424392843451213	T	T	T
0.8927533888992116	0.2503637601038046	0.9444897551490009	T	T	T
0.9450923324846517	0.7529461924683615	0.8567877467480405	T	T	T
0.6860338203671633	0.7523896299970275	0.8484513892369471	T	T	T
0.7735582105262323	0.7486783527202647	0.4428010045535041	T	T	T
0.6084814779095475	0.7503890551778090	0.4498976737349992	T	T	T
0.9370816103042712	0.4982044301234688	0.5126675743647459	T	T	T
0.8217122432486105	0.3352508377716871	0.3244343939349027	T	T	T
0.7998501432081365	0.6362984456678092	0.6902747234693875	T	T	T
0.9237654712194043	0.5292300411909894	0.1936736139773663	T	T	T
0.9305190810246410	0.4052876382300043	0.4285067142871039	T	T	T
0.8690916318381979	0.5572057385309820	0.5520403424115081	T	T	T
0.9834144463479872	0.6444341715972293	0.3015975666105566	T	T	T
0.0001437422717362	0.5720524942525086	0.3794330270327981	T	T	T
0.9672076739778094	0.4872501467120459	0.5677368099925022	T	T	T
0.0682378444292046	0.6183204750662382	0.3237078329939234	T	T	T
0.0514337344641319	0.4209763422041718	0.4921349791067596	T	T	T
0.0405792055523623	0.3399887661176690	0.4318815737996169	T	T	T
0.0165520388892175	0.6014557101241476	0.3146767061189383	T	T	T
0.0151055640210442	0.3862511361777300	0.4571196488598731	T	T	T

Figure S17 ZnNi-TS

Si O Al Ni Zn H C

1.0000000000000000

20.0219999999999985 0.0000000000000000 0.0000000000000000

0.0000000000000000 19.8990000000000009 0.0000000000000000

0.0000000000000000 0.0000000000000000 13.3829999999999991

93 193 3 1 1 6 2

Selective dynamics

Direct

0.4241794530551395	0.0566024923692435	0.6466932854829094	T	T	T
0.3040219270492367	0.0254731685917119	0.7903598851000696	T	T	T
0.2828895734720919	0.0589827265431717	0.0122795183509913	T	T	T
0.1235683108143865	0.0609543084106572	0.0111010592409636	T	T	T
0.0710072361100044	0.0284880068430539	0.7997874336601172	T	T	T
0.1795390362755123	0.0545813891171039	0.6532870290898458	T	T	T
0.4208312646274993	0.8262476196711085	0.6664622288806185	T	T	T
0.3041354556352142	0.8670132863935360	0.8084865546808182	T	T	T
0.2670618981511947	0.8262882275003023	0.0270816900494106	T	T	T

Structure files (CONTCAR) involved in this work:

0.1125204228734838	0.8243008074506953	0.0135235807180946	T	T	T
0.0664798252113655	0.8716546830911284	0.7996277795844590	T	T	T
0.1824770276487185	0.8270923198505853	0.6699897192948402	T	T	T
0.0774422215615722	0.9405617802509290	0.1471163065245422	T	T	T
0.1977980118528707	0.9715323144458655	0.2898456470106863	T	T	T
0.2191438911805269	0.9369859002560913	0.5120973695475413	T	T	T
0.3786824202322782	0.9345850375233936	0.5122350268057771	T	T	T
0.4323316886064377	0.9682343216024999	0.3003589688043440	T	T	T
0.3227299818202033	0.9421885792617576	0.1538310574743752	T	T	T
0.0818383013860824	0.1712501891029165	0.1639968370033957	T	T	T
0.1970203116715916	0.1297208039719945	0.3076707159368431	T	T	T
0.2334455341671109	0.1707075420630926	0.5251485679762421	T	T	T
0.3880169299882051	0.1729153516207757	0.5109550509467161	T	T	T
0.4367163963138935	0.1265601257982079	0.2980988552295408	T	T	T
0.3185175239014147	0.1692416094393312	0.1705395707878983	T	T	T
0.5772017700246103	0.5558737260508201	0.3541024404095676	T	T	T
0.6905182271709773	0.5253419231017752	0.2009485339576738	T	T	T
0.7165527307421529	0.5668030798951208	0.9848069590333657	T	T	T
0.8747741161187893	0.5720057591989729	0.9874684395903751	T	T	T
0.8103070525757806	0.5517332161932139	0.3432749382073604	T	T	T
0.5743907576751979	0.3275305578694135	0.3304646766919699	T	T	T
0.6952172475224072	0.3712439093614211	0.1919222319898703	T	T	T
0.7309056647030228	0.3265319870028403	0.9788489246510019	T	T	T
0.8853987275787529	0.3255789408988657	0.9956960643791766	T	T	T
0.9418467658135068	0.3752548791945206	0.1907102297887243	T	T	T
0.9214573494581809	0.4447089844015713	0.8625114610905855	T	T	T
0.8014826043435539	0.4717477472039953	0.7202217170917256	T	T	T
0.7763609276011257	0.4369463910006198	0.4951484192017171	T	T	T
0.6187233917735812	0.4288779328620647	0.4886196957706640	T	T	T
0.5685714984633327	0.4687764152074528	0.7012255053187400	T	T	T
0.6760161488233795	0.4466089708546846	0.8552340686644423	T	T	T
0.9203081046885462	0.6777152596165190	0.8294642782134143	T	T	T
0.7690245332858526	0.6691288342645473	0.4648112778217778	T	T	T
0.6143926867628213	0.6730007196571722	0.4880590345004396	T	T	T
0.5612311981872800	0.6269416807013106	0.6985105790239704	T	T	T
0.6744129255190171	0.6730708077378282	0.8258295799347397	T	T	T
0.5781255075276525	0.9444804108683970	0.3590718901976404	T	T	T
0.6993421837051101	0.9729528982262754	0.2157931997535557	T	T	T
0.7213415972033173	0.9362827847548948	0.9937817215505010	T	T	T
0.8816642125361120	0.9337590659745624	0.9958868627076470	T	T	T
0.9333928165915015	0.9699362203277758	0.2058983197919037	T	T	T
0.8241664461335383	0.9460815623295927	0.3560187324607189	T	T	T
0.5795854321488011	0.1726890950096788	0.3303402937792810	T	T	T
0.6993789586986128	0.1316273628858224	0.1938163451475360	T	T	T
0.7332234717355266	0.1705966759433301	0.9723636110214782	T	T	T
0.8879142117477773	0.1730974673640978	0.9847122952284730	T	T	T
0.9367084659506609	0.1281320745550279	0.1990652249015678	T	T	T
0.8212251989885797	0.1738824031425121	0.3315897190764148	T	T	T
0.9251734149643629	0.0543244634186632	0.8573730588878049	T	T	T
0.8041807585792285	0.0260909080920025	0.7095374949519752	T	T	T
0.7824658614051822	0.0660668439369411	0.4922136194128499	T	T	T
0.6223289971231266	0.0687349308869219	0.4907267841003732	T	T	T
0.5694093780135284	0.0307382089674948	0.6993294558035973	T	T	T

Structure files (CONTCAR) involved in this work:

0.6802253959391441	0.0524149274370289	0.8494301391665338	T	T	T
0.9243834051697748	0.8299966621776954	0.8374220592187223	T	T	T
0.8032824935042951	0.8691608364511533	0.6971185371199214	T	T	T
0.7709409329489507	0.8266132232801431	0.4802769156181956	T	T	T
0.6161714874555818	0.8264560377394710	0.4914493539766910	T	T	T
0.5649880170664638	0.8738407471432583	0.6990736916609359	T	T	T
0.6794853066474585	0.8323278924900097	0.8336533159739139	T	T	T
0.4235562704538293	0.4435225460086875	0.6399653360130281	T	T	T
0.3032908695452394	0.4713091964174444	0.7851772776732624	T	T	T
0.2810826945234217	0.4366292007967717	0.0053918888038516	T	T	T
0.1235962473045986	0.4356834937658155	0.0102380661372150	T	T	T
0.0658116365811819	0.4695268639491756	0.7995565528776083	T	T	T
0.1764889367923924	0.4442588717684565	0.6513321697338783	T	T	T
0.4179567752753461	0.6722799279842773	0.6603196672917053	T	T	T
0.3019922832673958	0.6289611445454149	0.8026070816036621	T	T	T
0.2671388004222044	0.6692874179652833	0.0217136677750413	T	T	T
0.1128448498477442	0.6705037465944613	0.0081561110398901	T	T	T
0.0626567975379208	0.6283895572571475	0.7954849688211835	T	T	T
0.1803978527976352	0.6687821244698141	0.6656897452309799	T	T	T
0.0758678750108021	0.5555935905291560	0.1481945709313539	T	T	T
0.1982093598530345	0.5247950983821148	0.2843991687598182	T	T	T
0.2174574818193295	0.5603346162973505	0.5092294361231321	T	T	T
0.3757004733497875	0.5653606328902095	0.5088499960967926	T	T	T
0.4282842477187085	0.5272757094571096	0.2997780979462965	T	T	T
0.3234517371104843	0.5515256120431591	0.1470038891365948	T	T	T
0.0860433238958267	0.3241438525441599	0.1562287893790881	T	T	T
0.1967425840407205	0.3671903023575050	0.3047285450551961	T	T	T
0.2320030598920827	0.3280563787391674	0.5238199557299272	T	T	T
0.3861391396070918	0.3264011247385813	0.5054763406259601	T	T	T
0.4322466466397379	0.3699177661092529	0.2921935983507947	T	T	T
0.3155674153863366	0.3276603248641034	0.1647945537135428	T	T	T
0.3586908544027643	0.0600680826342194	0.7175918081521042	T	T	T
0.3049655079580058	0.0653104305666672	0.8961370846610877	T	T	T
0.2029626134943729	0.0462496119436911	0.0219830280759457	T	T	T
0.1019611546226512	0.0682305967951792	0.8951594135502752	T	T	T
0.1042416195548131	0.0574433658174957	0.6978546403920520	T	T	T
0.2300407107315549	0.0307867540745592	0.7415781368905898	T	T	T
0.3605883017297413	0.8261688369586762	0.7471528218506313	T	T	T
0.3054100770393498	0.8402221492986144	0.9224680223555290	T	T	T
0.1896646372300820	0.8505034414229327	0.0171867546622564	T	T	T
0.0855478614382384	0.8300316974345828	0.8998733996119362	T	T	T
0.1052521574787801	0.8388586735651725	0.7041882642036192	T	T	T
0.2308332566080888	0.8532961882322377	0.7598718852520785	T	T	T
0.3219048754413348	0.9465752940063387	0.8058940699081554	T	T	T
0.0892343464476262	0.9493547695703844	0.8128586632434419	T	T	T
0.4318926094545956	0.1271293524673521	0.5865308731437284	T	T	T
0.4187925643950554	0.9955206871668429	0.5662012717604795	T	T	T
0.3974872820508114	0.8635673076650445	0.5644270444734187	T	T	T
0.1990298049616491	0.1292558356401523	0.6152757444768818	T	T	T
0.1814343055819453	0.0013488294490863	0.5611637150496004	T	T	T
0.1977240155891367	0.8675273876792768	0.5671070274450546	T	T	T
0.9911197183173358	0.0397996793845364	0.7905153379693619	T	T	T
0.9862878092416872	0.8679951162062691	0.7812233698169836	T	T	T

Structure files (CONTCAR) involved in this work:

0.1436055729374827	0.9364434256334773	0.2167558467761241	T	T	T
0.1973386066778465	0.9316738113011838	0.3956995176849814	T	T	T
0.2991509440216571	0.9488169027802634	0.5227571682762616	T	T	T
0.4005576242657278	0.9294872534218038	0.3961606237161821	T	T	T
0.3978621920563567	0.9397190154332079	0.1990770608023511	T	T	T
0.2719106953322582	0.9669583554589057	0.2412840534525770	T	T	T
0.1421306045168010	0.1714102354529707	0.2446225415741387	T	T	T
0.1939822419354261	0.1569019300498371	0.4214984975210205	T	T	T
0.3107817504422127	0.1470878612528571	0.5125398542238232	T	T	T
0.4167464994933319	0.1678363802438289	0.3983006168728200	T	T	T
0.3961358951634887	0.1582175440668441	0.2034512795195473	T	T	T
0.2712293039120697	0.1426032877600922	0.2616152955860575	T	T	T
0.1786851969540103	0.0502353050105117	0.3052338273087760	T	T	T
0.4169901204318786	0.0480825005983395	0.3123049589040433	T	T	T
0.0677612753981816	0.8693938974714487	0.0892217197976186	T	T	T
0.0831373705612519	0.9996365771989280	0.0634605604285728	T	T	T
0.1044287147385557	0.1311688912092355	0.0644407157663832	T	T	T
0.3030242292754948	0.8673659991052416	0.1164637110120483	T	T	T
0.3212436211167405	0.9948367679781657	0.0608854703304254	T	T	T
0.3030133490901848	0.1283247449921907	0.0683298528374052	T	T	T
0.5118486280133007	0.9541941959471154	0.2909651266481484	T	T	T
0.5166549207429000	0.1334373119150715	0.2790589495468963	T	T	T
0.6353415167536952	0.5617634363631383	0.2708779509283055	T	T	T
0.7013964012563446	0.5724755849638862	0.1037873413195152	T	T	T
0.7957460613898144	0.5574072190212751	0.9623253613096346	T	T	T
0.8891596620040531	0.5785088564436158	0.1045611948234239	T	T	T
0.8867880342005618	0.5385288074642091	0.3155693629793949	T	T	T
0.7601443220178853	0.5203588336563791	0.2630734219021367	T	T	T
0.6413790432373496	0.3344157909253757	0.2648014907781082	T	T	T
0.6914478189443869	0.3334878399428269	0.0839324530368859	T	T	T
0.8081825477635391	0.3510229365587166	0.9916353804048108	T	T	T
0.9105676993212722	0.3210868397717361	0.1116019954635360	T	T	T
0.9105575208414817	0.3577634548682987	0.3034877487273936	T	T	T
0.7688035010246580	0.3677346676346097	0.2389883354000343	T	T	T
0.6695938563812466	0.4488186243476515	0.1742009975418104	T	T	T
0.9234061080006991	0.4491185209973083	0.1565898503348773	T	T	T
0.5704853166753234	0.6270073240437802	0.4125478227523229	T	T	T
0.5941007205165730	0.4978935158047130	0.4360159230705948	T	T	T
0.5829564953597473	0.3643648234659490	0.4386681235233201	T	T	T
0.7962569252633622	0.6310561378666273	0.3651317178273283	T	T	T
0.7949240812147532	0.5151748450087089	0.4561984768892232	T	T	T
0.8265251747754483	0.3880758272014670	0.4347594263931527	T	T	T
0.0119062364503997	0.5511607864431119	0.2221694544066874	T	T	T
0.022082377226380	0.3637813757833370	0.2003922382068548	T	T	T
0.8567445886106750	0.4346493471841082	0.7889934105958656	T	T	T
0.7946228986998892	0.4329621243141118	0.6129029183944608	T	T	T
0.6993165786998623	0.4212461650446092	0.4719510633136555	T	T	T
0.6021591190034208	0.4297010006841244	0.6067475293448640	T	T	T
0.6026632705276733	0.4424624802635774	0.8039980218129705	T	T	T
0.7288641739206807	0.4735335611529617	0.7712039200298864	T	T	T
0.8605607271380693	0.6816401733765938	0.7506201656089240	T	T	T
0.8158838717081581	0.6429314817509293	0.5594475572539852	T	T	T
0.6921787088805752	0.6475728242104630	0.4879451178578839	T	T	T

Structure files (CONTCAR) involved in this work:

0.5846643317681787	0.6680465564848960	0.5998058295213536	T	T	T
0.5958391976349686	0.6599355563297722	0.7966793396161090	T	T	T
0.7204129165504740	0.6473521632717177	0.7343305332503011	T	T	T
0.8268003132937329	0.5482440444642853	0.6926076123890175	T	T	T
0.5821682081156713	0.5485153374764594	0.6862775998602060	T	T	T
0.9308224800438899	0.3771945961596507	0.9298212349916504	T	T	T
0.9155761235543788	0.5101649370564316	0.9330768517540428	T	T	T
0.8982693260019533	0.6409928686257965	0.9325205958644190	T	T	T
0.6959356971370487	0.3721538960689673	0.8930235063530776	T	T	T
0.6759498268254229	0.5005546591377974	0.9458319566888650	T	T	T
0.6897712375543475	0.6341907588590397	0.9304477707992441	T	T	T
0.4892792813642559	0.4524362744582257	0.7094343416211980	T	T	T
0.4804107730583143	0.6318434097627171	0.7094130348934486	T	T	T
0.6429864389042549	0.9396196982105365	0.2871910771669265	T	T	T
0.7001920451763775	0.9325711316184122	0.1105287411111278	T	T	T
0.8017937715600088	0.9434316815351688	0.9810755036387211	T	T	T
0.9008394678770025	0.9284038001684796	0.1132606903015516	T	T	T
0.8992304158505386	0.9468004522156859	0.3102764772514324	T	T	T
0.7721529989335165	0.9657271332377291	0.2676736701218599	T	T	T
0.6418246091870500	0.1723620345982468	0.2534502584520906	T	T	T
0.6974142583752299	0.1571292590476011	0.0790297509560377	T	T	T
0.8109494849045727	0.1467158330246293	0.9794195390051779	T	T	T
0.9146104324895060	0.1678423031384039	0.0985435089992196	T	T	T
0.8978006025782013	0.1573651037250280	0.2959288424840499	T	T	T
0.7720877709765500	0.1459139637012063	0.2426910848769299	T	T	T
0.6823786650737408	0.0517619243264539	0.1981748449962239	T	T	T
0.9200756010518569	0.0490071813504444	0.1847874472241778	T	T	T
0.5706666687727694	0.8748524076696298	0.4218360380456312	T	T	T
0.5835610930805932	0.0064495941043586	0.4377295036861700	T	T	T
0.6008414274519661	0.1382221144714361	0.4358905602781115	T	T	T
0.8102401893533746	0.8708444401127947	0.3979262745669326	T	T	T
0.8190476246797134	0.9997639514333551	0.4468043802394893	T	T	T
0.8060490165558856	0.1334644710895390	0.4351690307322640	T	T	T
0.0127544287002768	0.9543667911947614	0.2168521670016781	T	T	T
0.0166453206162460	0.1378308144530647	0.2162235479391278	T	T	T
0.8603861674574207	0.0548396343810279	0.7850899645700947	T	T	T
0.8034260187836153	0.0720947609004641	0.6092749895093401	T	T	T
0.7020855831240738	0.0562843678901880	0.4806159483733978	T	T	T
0.6004802253180804	0.0743292608868432	0.6073405334643118	T	T	T
0.6050506032286563	0.0504420559834004	0.8041306557213596	T	T	T
0.7311920943302842	0.0289573428491257	0.7617943762098953	T	T	T
0.8591668875351085	0.8346362038168967	0.7667706877353582	T	T	T
0.8056276091428057	0.8318274594957474	0.5893736647131745	T	T	T
0.6936393772372235	0.8516380324094078	0.4865668420280883	T	T	T
0.5903163259923838	0.8276136661892315	0.6062897155060512	T	T	T
0.6034315133182453	0.8516587521053595	0.8007238400780691	T	T	T
0.7297176284331331	0.8599437373567828	0.7466865711679166	T	T	T
0.8199819640948086	0.9483011728310400	0.6811321865555818	T	T	T
0.5809736619875283	0.9518069596148785	0.6728230857555306	T	T	T
0.9332622431631887	0.1275169295657914	0.9102308573945412	T	T	T
0.9190413836676006	0.9976802758850841	0.9446318293993470	T	T	T
0.9075513617009798	0.8648654862501104	0.9442571729510350	T	T	T
0.6959449631595156	0.1285863092324467	0.8849723645857760	T	T	T

Structure files (CONTCAR) involved in this work:

0.6857950668153494	0.0018844482872210	0.9444330703403767	T	T	T
0.6965234934119005	0.8676782346357957	0.9399670255119822	T	T	T
0.4903472100085863	0.0461209463261071	0.7145853330111327	T	T	T
0.4852087632377688	0.8634498375335597	0.7156636385729754	T	T	T
0.3574757182086441	0.4380267958666124	0.7098883282574806	T	T	T
0.3038965131441225	0.4293568569746261	0.8893810468070532	T	T	T
0.2022282749968901	0.4563952266489766	0.0128200228415313	T	T	T
0.0972062227517412	0.4317892974105779	0.8959268585614784	T	T	T
0.1010997571086413	0.4424145516491582	0.6972492072162300	T	T	T
0.2286764638174524	0.4676865476605180	0.7372955600599768	T	T	T
0.3559544256504160	0.6705953647350170	0.7378500451400739	T	T	T
0.3038857503622292	0.6587974662233123	0.9148896855679763	T	T	T
0.1900055265034727	0.6444770248060706	0.0117441230698547	T	T	T
0.0867155677318124	0.6695248660746639	0.8936206329513188	T	T	T
0.1028665481773680	0.6565438233763558	0.6979131214938481	T	T	T
0.2279928601224274	0.6383897251643079	0.7537263029270410	T	T	T
0.3218172941144933	0.5497319705509341	0.8045352209058126	T	T	T
0.0798103738775364	0.5493152332006708	0.8110266314504280	T	T	T
0.4318808009003624	0.3754201171373877	0.5740518858726000	T	T	T
0.4191076937524541	0.5071296621662543	0.5636887955951151	T	T	T
0.3947880698632199	0.6381343800508309	0.5552768050931761	T	T	T
0.1949470211541544	0.3696539689568616	0.6119143550650992	T	T	T
0.1769983678969114	0.4972656604712927	0.5582258287449621	T	T	T
0.1943180930956348	0.6307013190552559	0.5599186898081391	T	T	T
0.9863033678469927	0.4532737745144381	0.7886634656846176	T	T	T
0.9832409078436911	0.6375295149220840	0.7770910967544736	T	T	T
0.1440598580025031	0.5625933636377476	0.2144062179412218	T	T	T
0.1989697555277610	0.5639386742913207	0.3912775617958354	T	T	T
0.2969381737536138	0.5485145298858921	0.5263813109052656	T	T	T
0.3928162592588294	0.5678253153644148	0.3908563550261439	T	T	T
0.3979289038839141	0.5543058385464508	0.1947327503751281	T	T	T
0.2716342722468206	0.5275090069395417	0.2339188362469854	T	T	T
0.1425529997605614	0.3237606169477910	0.2430512119538776	T	T	T
0.1931729492675058	0.3414439070929553	0.4192592839537043	T	T	T
0.3090623516825728	0.3528743427370331	0.5120445817005187	T	T	T
0.4106280102931318	0.3263840023517384	0.3898970498340851	T	T	T
0.3931417052738244	0.3427473441555504	0.1934205505051324	T	T	T
0.2706790646857683	0.3551502971812726	0.2582368807547767	T	T	T
0.1769126195320200	0.4465489844589067	0.3004423884133949	T	T	T
0.4127854747629669	0.4477378344721614	0.3140100528949895	T	T	T
0.0678992780073231	0.6221301117147930	0.0782477723959091	T	T	T
0.0812189111859721	0.4901049820400639	0.0747519304131489	T	T	T
0.1145131806258743	0.3608319687808416	0.0566521662106937	T	T	T
0.3044696822820757	0.6258206073506636	0.1072872462793516	T	T	T
0.3235326727510910	0.4973917898127355	0.0559928846468672	T	T	T
0.2952214654535185	0.3657331690929115	0.0617678209684162	T	T	T
0.5079069640262954	0.5397350306785428	0.2975038258463449	T	T	T
0.5117825506337084	0.3618728112841512	0.2713411222293842	T	T	T
0.4390916382301649	0.7492886617364545	0.6376640345602627	T	T	T
0.1952702338663171	0.7479034859826028	0.6484067888060757	T	T	T
0.2711071567913500	0.7472689388205402	0.0552523892825932	T	T	T
0.1077474768612287	0.7467907649991780	0.0501883479799395	T	T	T
0.0661217870828994	0.2476590834833814	0.1289146000356287	T	T	T

Structure files (CONTCAR) involved in this work:

0.3038604521300629	0.2479853509093826	0.1481470535356051	T	T	T
0.2287332949103659	0.2495781476240138	0.5540117933241536	T	T	T
0.3921785556312287	0.2504245305217443	0.5483146030584102	T	T	T
0.5579806629113510	0.2494858800852420	0.3535707057065186	T	T	T
0.8119034861558913	0.2523707372256541	0.3514042462938745	T	T	T
0.7281048191910746	0.2491524126050909	0.9414649631416581	T	T	T
0.8925266185132849	0.2508010626332096	0.9478621898103198	T	T	T
0.9455892331412330	0.7529916119755572	0.8588111956794876	T	T	T
0.6864375475185092	0.7523108426076504	0.8479753256623794	T	T	T
0.7755671804576602	0.7486142000545001	0.4454014973666801	T	T	T
0.6105131975089682	0.7501221381578348	0.4495274070822344	T	T	T
0.9322825316801229	0.4856197740412017	0.5216996897737893	T	T	T
0.8234644006784302	0.3354714032405237	0.3258311951576375	T	T	T
0.8003352806595894	0.6353626940487218	0.6933488344555800	T	T	T
0.9267952250710187	0.5312980652333689	0.1977737634648673	T	T	T
0.9267528091105737	0.4174626321798026	0.4183795278153284	T	T	T
0.8671553595700622	0.5542039082347299	0.5535717773188384	T	T	T
0.9918551468908837	0.6464738127474734	0.3476192217344756	T	T	T
0.9986244991597878	0.5643627734594172	0.4160406207587956	T	T	T
0.9580505667423397	0.4696345065689383	0.5789799994243706	T	T	T
0.0763540178019395	0.6102115178750434	0.3755192471164324	T	T	T
0.0460899382414334	0.4481847565710252	0.4593953312112254	T	T	T
0.0385019282889779	0.3740980065923566	0.3717899838196598	T	T	T
0.0222473155904212	0.6051275743914013	0.3750123517197135	T	T	T
0.0146151822435534	0.4131633801447450	0.4169905758845120	T	T	T

Figure S17 ZnNi-FS

Si O Al Ni Zn H C

1.0000000000000000

20.0219999999999985 0.0000000000000000 0.0000000000000000

0.0000000000000000 19.8990000000000009 0.0000000000000000

0.0000000000000000 0.0000000000000000 13.3829999999999991

93 193 3 1 1 6 2

Selective dynamics

Direct

0.4236109775139318	0.0576418841208748	0.6470903715000853	T	T	T
0.3053748956483399	0.0270437390182836	0.7925306347655185	T	T	T
0.2827871248671296	0.0590859804494359	0.0140628846912840	T	T	T
0.1231866908594058	0.0616617943572653	0.0108273264772457	T	T	T
0.0692868548683462	0.0292964142921880	0.7995306805024281	T	T	T
0.1808062111580359	0.0562226239147084	0.6581117359040123	T	T	T
0.4207518625499934	0.8265369220278437	0.6684320631613555	T	T	T
0.3047097857019485	0.8682294885438228	0.8094200445661897	T	T	T
0.2672756638433218	0.8279002101036519	0.0278398884855853	T	T	T
0.1129257762806843	0.8251135705950506	0.0133908653193857	T	T	T
0.0660809159643093	0.8719838472436782	0.7996959767339916	T	T	T
0.1830355320501721	0.8271640114885286	0.6721336928075060	T	T	T
0.0781331705680394	0.9406852605859028	0.1480788650092394	T	T	T
0.1967997692217376	0.9711011893558290	0.2926080124620908	T	T	T
0.2191813433992282	0.9372550072482804	0.5143587569321174	T	T	T
0.3791949716292080	0.9344469040522289	0.5125649257208509	T	T	T
0.4338182332736960	0.9679654662008426	0.3010131189274833	T	T	T
0.3218252981493980	0.9417132081530620	0.1591486996541863	T	T	T
0.0827349143920155	0.1718832004179280	0.1646113490364651	T	T	T

Structure files (CONTCAR) involved in this work:

0.1966618095137041	0.1296711327358289	0.3087565500076735	T	T	T
0.2335402463750408	0.1708146300470057	0.5257812060052948	T	T	T
0.3882397664127902	0.1734182854151791	0.5102572115013140	T	T	T
0.4366676134841877	0.1263513440723268	0.2976606789803322	T	T	T
0.3177128434716528	0.1696732029082021	0.1719181211701407	T	T	T
0.5773616662021617	0.5551350935967416	0.3554196708739443	T	T	T
0.6916558066352148	0.5255427395798352	0.2022412446946820	T	T	T
0.7146448563253790	0.5669334899766814	0.9864385305240295	T	T	T
0.8726920489691730	0.5714683271985198	0.9894444294805705	T	T	T
0.8117915691698933	0.5475790880040964	0.3458357710481933	T	T	T
0.5737232543075966	0.3275852257118279	0.3309475453498060	T	T	T
0.6954801184279221	0.3712709900683389	0.1936563358682263	T	T	T
0.7302954226526235	0.3261504337346924	0.9806762033551015	T	T	T
0.8848119721176315	0.3251744971814974	0.9947116869457877	T	T	T
0.9416873982828714	0.3756212573756071	0.1871625514231519	T	T	T
0.9204845199835957	0.4449328868631734	0.8624523603850199	T	T	T
0.7992183063109000	0.4710720127039091	0.7217905469841601	T	T	T
0.7735867009329510	0.4347224232755367	0.4969389658422614	T	T	T
0.6164642334866000	0.4280421935062738	0.4901106343584024	T	T	T
0.5681640930367464	0.4681838648403904	0.7030710364208763	T	T	T
0.6744220615627620	0.4464029990685870	0.8586573296010241	T	T	T
0.9204527267069943	0.6765577758388691	0.8316520800502294	T	T	T
0.7706158082359447	0.6681742686127576	0.4627306628531814	T	T	T
0.6152665396530832	0.6722079548290866	0.4865400046051236	T	T	T
0.5620702260518283	0.6264593626989503	0.6982269359741308	T	T	T
0.6732743178218209	0.6735425442901728	0.8272701773013030	T	T	T
0.5791557950866882	0.9440486669932325	0.3577141917779929	T	T	T
0.6994367612653577	0.9727922240077391	0.2139423742440204	T	T	T
0.7218514367077512	0.9373784771433300	0.9918501702875436	T	T	T
0.8821377222999391	0.9339241432810311	0.9948065454193085	T	T	T
0.9341816594967971	0.9694378206965357	0.2049068551584031	T	T	T
0.8238375505817347	0.9455290364524011	0.3530520063097486	T	T	T
0.5793935380690739	0.1727307072964672	0.3287393621452956	T	T	T
0.6991514960328570	0.1316420462145883	0.1928406878911911	T	T	T
0.7331340624546036	0.1701549583099598	0.9715841816361505	T	T	T
0.8878078162271797	0.1728654279250315	0.9838140925676301	T	T	T
0.9374985024880800	0.1274765013340145	0.1973903206192217	T	T	T
0.8219486114769012	0.1737751322260663	0.3297006396458278	T	T	T
0.9244133323373870	0.0541835150482246	0.8555581968829757	T	T	T
0.8038615413010463	0.0253138269839583	0.7075741675012734	T	T	T
0.7825698577517948	0.0658479724395787	0.4904574176858532	T	T	T
0.6221171011355084	0.0688783351830746	0.4897127101463221	T	T	T
0.5686440618526059	0.0314004181469755	0.6985335027856093	T	T	T
0.6803840764690181	0.0530451459728306	0.8464413197129580	T	T	T
0.9239246464465731	0.8289874152553672	0.8365397016606513	T	T	T
0.8036950267097414	0.8677349539423587	0.6946380269230332	T	T	T
0.7714107198390144	0.8255834071327299	0.4777548146113907	T	T	T
0.6161781199285182	0.8260657240933974	0.4911976964303227	T	T	T
0.5648665548577277	0.8744237605347763	0.6988525789551522	T	T	T
0.6800155823312483	0.8323106586277251	0.8322715254419986	T	T	T
0.4237966312973932	0.4439799150822338	0.6402655075560566	T	T	T
0.3046637813049682	0.4709793946836723	0.7874998452019654	T	T	T
0.2819231329826892	0.4373587480026275	0.0062016644791741	T	T	T

Structure files (CONTCAR) involved in this work:

0.1243655872537896	0.4361520652302217	0.0109884501608739	T	T	T
0.0655279477407922	0.4695841793987881	0.8018541615670129	T	T	T
0.1777700961980383	0.4440411293125688	0.6557367581537557	T	T	T
0.4186123483708041	0.6726452060343471	0.6602999808472187	T	T	T
0.3029766796520899	0.6288747122900555	0.8036501190267622	T	T	T
0.2682320106652237	0.6703222310882135	0.0216507987304194	T	T	T
0.1140496525089611	0.6713654123737410	0.0084463789323206	T	T	T
0.0634782741056575	0.6281508410635199	0.7973570347904002	T	T	T
0.1812000481185231	0.6684595687859428	0.6677813488660409	T	T	T
0.0753876291092397	0.5568693177845393	0.1489905250285183	T	T	T
0.1981432357499646	0.5265699644182530	0.2853467665220767	T	T	T
0.2197329744010037	0.5603382862723961	0.5116564709985084	T	T	T
0.3779719846114530	0.5661250250909275	0.5087446927306591	T	T	T
0.4299250635503881	0.5279523883069346	0.2988522472508812	T	T	T
0.3236134636135177	0.5532894224667297	0.1481772771358212	T	T	T
0.0866557157266019	0.3247242015561593	0.1583594843335841	T	T	T
0.1963746117971890	0.3685368795590989	0.3067136548148205	T	T	T
0.2320390150665993	0.3291389696496821	0.5254469304298227	T	T	T
0.3863680522003630	0.3269982985248181	0.5056262878900942	T	T	T
0.4324187849338190	0.3705662013139143	0.2920875483486090	T	T	T
0.3149331168843749	0.3281783922059403	0.1668439645735856	T	T	T
0.3581734677295036	0.0629122965139723	0.7179468835092974	T	T	T
0.3103398660858522	0.0638639499115756	0.9003563567592605	T	T	T
0.2026945850674046	0.0464065213741802	0.0149144082749670	T	T	T
0.0972745002725196	0.0689481048897697	0.8969164476810078	T	T	T
0.1047531003686036	0.0589402885146402	0.6997440793828154	T	T	T
0.2299484034492020	0.0349589487930016	0.7495760729951765	T	T	T
0.3608099255973589	0.8257389172473353	0.7496550437513134	T	T	T
0.3066228110313680	0.8445196436789805	0.9248733154825963	T	T	T
0.1899020792016800	0.8517890264099021	0.0165500181108419	T	T	T
0.0854614695274784	0.8307171700204715	0.9000139190193505	T	T	T
0.1056453595252414	0.8396260862392753	0.7047481738631153	T	T	T
0.2310691673021984	0.8534176165318788	0.7625135361260863	T	T	T
0.3228778907391981	0.9475528564990019	0.8012669689525236	T	T	T
0.0873827204706671	0.9501393463831176	0.8126636446680010	T	T	T
0.4321558833922798	0.1275269671283708	0.5856279829520447	T	T	T
0.4173690148339811	0.9959051385595086	0.5680985783847069	T	T	T
0.3967231502435041	0.8638216913720447	0.5667990620611966	T	T	T
0.2003734992022480	0.1304133417813029	0.6180228130193621	T	T	T
0.1846480003355898	0.0015159175347165	0.5683161965459890	T	T	T
0.1992621834846036	0.8674081538040304	0.5694338500676247	T	T	T
0.9895325459050234	0.0404656067980943	0.7863797683368230	T	T	T
0.9860284356248157	0.8668326940672310	0.7807833374894732	T	T	T
0.1443982802087422	0.9353192142319741	0.2173662050095259	T	T	T
0.1923590443729362	0.9337075653432211	0.4001349853231713	T	T	T
0.2994706208065481	0.9481298674762205	0.5171786729489024	T	T	T
0.4046296796345512	0.9289112019641221	0.3982376531984212	T	T	T
0.3977262904687680	0.9389522136316123	0.2013942184977972	T	T	T
0.2723253804155045	0.9643417060977891	0.2495975689659177	T	T	T
0.1421059176843498	0.1725219046046073	0.2467993197425686	T	T	T
0.1931342761578606	0.1544559807294257	0.4237505332046710	T	T	T
0.3109603058139061	0.1478101688751892	0.5119482926059645	T	T	T
0.4169680561603644	0.1680630825503265	0.3976058561523319	T	T	T

Structure files (CONTCAR) involved in this work:

0.3954842689109666	0.1575052924679744	0.2032157925474694	T	T	T
0.2711057109899830	0.1434985370132496	0.2640996808351891	T	T	T
0.1781716262885315	0.0503511528451725	0.3021906829938668	T	T	T
0.4177814112213379	0.0477256450012450	0.3129834705041645	T	T	T
0.0678979799062102	0.8702296163714770	0.0886668409600665	T	T	T
0.0841398513521036	0.0007404721108955	0.0661826867100263	T	T	T
0.1068102825786883	0.1321651315648373	0.0654799056846093	T	T	T
0.3019116352352795	0.8674642015571853	0.1198317747837871	T	T	T
0.3186760143051116	0.9957046283762080	0.0682808963126788	T	T	T
0.3005649514154725	0.1290337758648163	0.0701023626330997	T	T	T
0.5133199062012774	0.9543761380150643	0.2887473075956154	T	T	T
0.5164909040984497	0.1334883937858509	0.2774970980454743	T	T	T
0.6386382522789831	0.5603894051311455	0.2772399868844541	T	T	T
0.6995064330602069	0.5735555025770408	0.1054548654044174	T	T	T
0.7937291649790295	0.5572833547500694	0.9634504834123306	T	T	T
0.8850705645212303	0.5777271733785657	0.1075518375333909	T	T	T
0.8885689397234504	0.5248236734028329	0.3206652811999075	T	T	T
0.7634922183040890	0.5217180496389205	0.2594780129990670	T	T	T
0.6416278954659013	0.3354719991991117	0.2675699654371788	T	T	T
0.6913897585371304	0.3326729711633985	0.0863616700904765	T	T	T
0.8076150318273038	0.3508357808076719	0.9921249783083093	T	T	T
0.9104333292891194	0.3199687262497049	0.1106402357482643	T	T	T
0.9097513034063813	0.3648217975895030	0.3014006331143007	T	T	T
0.7691987409315044	0.3680723356295012	0.2399426400066660	T	T	T
0.6708045620964905	0.4491258719963929	0.1752814914850560	T	T	T
0.9242448119752518	0.4487709428185060	0.1486581969455521	T	T	T
0.5696904205802175	0.6266526560194117	0.4126621545060982	T	T	T
0.5909800261907826	0.4973236059321046	0.4389395013035154	T	T	T
0.5802250275038152	0.3638446678539885	0.4399411907099162	T	T	T
0.8040310429149066	0.6278622411051172	0.3680719838542964	T	T	T
0.7919220054479306	0.5132999106501128	0.4573014335344446	T	T	T
0.8243288190774299	0.3865360488884350	0.4368668895043742	T	T	T
0.0102198616251387	0.5514856902682664	0.2176902009810671	T	T	T
0.0215522037667353	0.3636661246274540	0.2005515902064765	T	T	T
0.8563482428962703	0.4344551313045099	0.7877306927985593	T	T	T
0.7888888315252495	0.4319310791502954	0.6154760126613718	T	T	T
0.6967129866512322	0.4201988323404800	0.4707485522488674	T	T	T
0.6016175009648603	0.4286530624361665	0.6087639360436523	T	T	T
0.6015738239155087	0.4417927433740362	0.8062030311908610	T	T	T
0.7279088540030177	0.4736850209394489	0.7762566503852467	T	T	T
0.8610606388560892	0.6798320890674917	0.7520085904791537	T	T	T
0.8142048703954289	0.6436618653197496	0.5618147895720573	T	T	T
0.6931456423777449	0.6464413960888177	0.4800756363180627	T	T	T
0.5880551049019389	0.6663679880757539	0.5996674217965646	T	T	T
0.5950179892175698	0.6603417670458522	0.7970130239790159	T	T	T
0.7192970844124124	0.6484089230333873	0.7355724357567094	T	T	T
0.8234713813237968	0.5479951585722330	0.6948412014445899	T	T	T
0.5825873143252035	0.5477919939702373	0.6880526981655887	T	T	T
0.9299436145499056	0.3768833490210540	0.9286663852982826	T	T	T
0.9133190283335071	0.5096480691974050	0.9344607998614504	T	T	T
0.8975660253624199	0.6401762611630513	0.9347943231282511	T	T	T
0.6943659967118829	0.3719618557015575	0.8961715851246388	T	T	T
0.6735859997783060	0.5005337640664954	0.9490866444399716	T	T	T

Structure files (CONTCAR) involved in this work:

0.6882582946051647	0.6341731703303604	0.9314687021531217	T	T	T
0.4888430477509908	0.4522608159335184	0.7112824985352917	T	T	T
0.4813124988170757	0.6318056135410169	0.7076649074070595	T	T	T
0.6443377163567457	0.9384945368082518	0.2865258531645080	T	T	T
0.6988996257476510	0.9334880339447961	0.1078280672662886	T	T	T
0.8023383873462913	0.9453774116781315	0.9821545601860380	T	T	T
0.9024947726456348	0.9278120709415972	0.1116689652336377	T	T	T
0.8992708569741754	0.9464956572660613	0.3088721753316498	T	T	T
0.7730417605966848	0.9652487114176055	0.2631716479011079	T	T	T
0.6416435720475386	0.1729625676700824	0.2517751462184364	T	T	T
0.6964680208766983	0.1553037718935874	0.0771868883948866	T	T	T
0.8108241791246849	0.1465567233724338	0.9800495798248492	T	T	T
0.9154241352974811	0.1675678615330950	0.0971419408510620	T	T	T
0.8981948448854804	0.1558949812996113	0.2943576204664882	T	T	T
0.7719397372098810	0.1470987622690716	0.2408747173624671	T	T	T
0.6821705794354991	0.0518359683576676	0.1995683423275283	T	T	T
0.9210017216663635	0.0484003201950162	0.1826439040023295	T	T	T
0.5713576333992680	0.8745287440716880	0.4206878888241713	T	T	T
0.5845030968152364	0.0060777243729000	0.4362547547539032	T	T	T
0.6009213098415693	0.1380958383993018	0.4339885726176956	T	T	T
0.8092128434827833	0.8702665721023183	0.3944360353045394	T	T	T
0.8176459051427428	0.9991515386221781	0.4437463079716171	T	T	T
0.8058328635252082	0.1333243108987039	0.4330777440524606	T	T	T
0.0134465446308155	0.9542087611945729	0.2179835519162469	T	T	T
0.0172881411132264	0.1376581153215034	0.2149961720363620	T	T	T
0.8586110732440208	0.0541889024752511	0.7853662588243187	T	T	T
0.8052070885884268	0.0710184260193839	0.6069688777166498	T	T	T
0.7020037573644338	0.0569394731410022	0.4817725568131856	T	T	T
0.5988358868958372	0.0747646449377970	0.6056368662365911	T	T	T
0.6048192110688512	0.0517243429861479	0.8026734977757233	T	T	T
0.7300537569727978	0.0290950790073528	0.7573067403643794	T	T	T
0.8594289293718478	0.8328446653617541	0.7641611876226192	T	T	T
0.8070480090087536	0.8313255821151962	0.5861084603670581	T	T	T
0.6940492507078199	0.8499795804173601	0.4866445009152433	T	T	T
0.5896413619614819	0.8281852539892189	0.6056394935622252	T	T	T
0.6040737742956087	0.8523023566753554	0.7998930197241384	T	T	T
0.7299688964451827	0.8571278916648495	0.7431312496680571	T	T	T
0.8196754636777980	0.9472394546200521	0.6807480075190898	T	T	T
0.5805090985542791	0.9524285927634142	0.6724515486139975	T	T	T
0.9325431629672937	0.1273290901555824	0.9085215933750062	T	T	T
0.9201579738484230	0.9971646559909116	0.9426275573757227	T	T	T
0.9057522853283906	0.8645973334683222	0.9422617968645179	T	T	T
0.6971820977987978	0.1289773684511439	0.8820739476871242	T	T	T
0.6863256403685630	0.0024791073048405	0.9412752916390800	T	T	T
0.6986588169169901	0.8686345524055028	0.9370947271826769	T	T	T
0.4896787851311946	0.0466145387838063	0.7150305411154086	T	T	T
0.4852616802012024	0.8639674595512379	0.7169334542812337	T	T	T
0.3571419846619228	0.4384006081372706	0.7088852120478365	T	T	T
0.3084541315504181	0.4293603295558567	0.8919054518045135	T	T	T
0.2029959270694020	0.4567904890462278	0.0077207106276928	T	T	T
0.0950833180240246	0.4304379337472623	0.8981719644537018	T	T	T
0.1016109063541581	0.4431708258393740	0.6994649232617834	T	T	T
0.2288831622896269	0.4659735865283147	0.7440301057512833	T	T	T

Structure files (CONTCAR) involved in this work:

0.3566042704109342	0.6701192637343897	0.7376622330129126	T	T	T
0.3059074773381925	0.6589266368031068	0.9157098402796490	T	T	T
0.1912459270530395	0.6453237230928661	0.0114863137475446	T	T	T
0.0879413078551881	0.6707914307177321	0.8937119022807297	T	T	T
0.1035159173113534	0.6548946912192938	0.6986016438731832	T	T	T
0.2285108720638577	0.6384807033612231	0.7565263457737464	T	T	T
0.3227264267092985	0.5496550119945603	0.8053007201851701	T	T	T
0.0803494251650933	0.5491504307253786	0.8149646538493427	T	T	T
0.4321844580201031	0.3760141457845669	0.5740822777465800	T	T	T
0.4210831787178642	0.5080608533338075	0.5646587881977964	T	T	T
0.3960106260878566	0.6393054645471905	0.5545496154814172	T	T	T
0.1959676449320095	0.3692875914581860	0.6161117486508882	T	T	T
0.1808068129092210	0.4973207692209080	0.5633461846973079	T	T	T
0.1967893340255504	0.6307331485292099	0.5623507549629876	T	T	T
0.9857357744179022	0.4545155066383513	0.7894315739398780	T	T	T
0.9838243032894458	0.6368259426666411	0.7798856504243716	T	T	T
0.1428314796140019	0.5643854610651440	0.2177651155320258	T	T	T
0.2000236150262860	0.5630378369036000	0.3942347480870315	T	T	T
0.2994250238420697	0.5488641271804582	0.5258574311211311	T	T	T
0.3963750206531952	0.5686944083947630	0.3912369127177557	T	T	T
0.3983779078808111	0.5554578632231557	0.1950279706845748	T	T	T
0.2716922063052324	0.5303819949751215	0.2354169643108692	T	T	T
0.1419268874376537	0.3242970949060017	0.2468370168934105	T	T	T
0.1923732799209270	0.3456113390703482	0.4225779077138870	T	T	T
0.3092759102363663	0.3532242524898082	0.5129877928517558	T	T	T
0.4107468381171078	0.3273778404225772	0.3900405183448086	T	T	T
0.3926991859282840	0.3434052662390851	0.1940278527851059	T	T	T
0.2704161689254476	0.3546380545192083	0.2613675084775554	T	T	T
0.1771850586677987	0.4478267430874600	0.2981982143347665	T	T	T
0.4138185486196425	0.4486092311879827	0.3136587012836917	T	T	T
0.0689561459773643	0.6229917911181253	0.0776591439321025	T	T	T
0.0837066018721182	0.4912812560685857	0.0756846432061977	T	T	T
0.1165138063782062	0.3618485341952829	0.0600949218914184	T	T	T
0.3053950681521743	0.6277191474742461	0.1083465853521211	T	T	T
0.3228702606578435	0.4987192937677112	0.0578658114574460	T	T	T
0.2941822371600318	0.3669086517433242	0.0646681682754523	T	T	T
0.5098126333668304	0.5396896249155114	0.2936728026194151	T	T	T
0.5117910091209158	0.3618516000545992	0.2702338846375539	T	T	T
0.4397026389700689	0.7498253607390977	0.6392955403912006	T	T	T
0.1953223029504911	0.7478178232451257	0.6514303405358134	T	T	T
0.2719062023112732	0.7486035802533478	0.0532062494873163	T	T	T
0.1090527874059310	0.7477026037163442	0.0503133038255510	T	T	T
0.0669101471791105	0.2483354686203961	0.1298734278536869	T	T	T
0.3036514067710594	0.2485035129135477	0.1495604162937058	T	T	T
0.2282842587230000	0.2500653673741245	0.5517786183873055	T	T	T
0.3926222829145947	0.2508672021844996	0.5477641808732117	T	T	T
0.5574932398156935	0.2493520779263224	0.3524824831528325	T	T	T
0.8153653073455165	0.2526115995020093	0.3492169792760303	T	T	T
0.7276684971392333	0.2489851935339206	0.9425518509842191	T	T	T
0.8918244714759712	0.2505337006356488	0.9465141898444223	T	T	T
0.9449639836676560	0.7522083384106285	0.8601745646486065	T	T	T
0.6855578580656959	0.7525306227497633	0.8502263517143756	T	T	T
0.7767770284988788	0.7475127385987860	0.4419602455099139	T	T	T

Structure files (CONTCAR) involved in this work:

0.6103587470503019	0.7495903063118692	0.4498249271536018	T	T	T
0.9188020129195015	0.4810882987704211	0.5312734516008416	T	T	T
0.8245536669522139	0.3363757518897373	0.3262760668716947	T	T	T
0.7990393351892963	0.6355143827446470	0.6961401280543827	T	T	T
0.9275595380099929	0.5296991857179233	0.1950254077166557	T	T	T
0.9193520984670625	0.4344065225256370	0.4062661595021300	T	T	T
0.8629277249576882	0.5563077393198662	0.5573880262908512	T	T	T
0.0045554158638482	0.5587914535288846	0.4139898154619808	T	T	T
0.0421706051715535	0.5212998870109283	0.5228950325060407	T	T	T
0.9543348418335051	0.4705939458241739	0.5785688268680138	T	T	T
0.0866555980628324	0.5309672922537059	0.4095627319433614	T	T	T
0.0315539350155955	0.4077359493976135	0.4485373861059229	T	T	T
0.0269693691025361	0.4434622983505768	0.3232102505043356	T	T	T
0.0374201801727503	0.5185475409958019	0.4413399985197515	T	T	T
0.0166552211446742	0.4514119934333123	0.4026948515930173	T	T	T

Figure S17 ZnCu-IS

Si O Al Cu Zn H C

1.0000000000000000

20.0219999999999985 0.0000000000000000 0.0000000000000000

0.0000000000000000 19.8990000000000009 0.0000000000000000

0.0000000000000000 0.0000000000000000 13.3829999999999991

93 193 3 1 1 6 2

Selective dynamics

Direct

0.4243479482321308	0.0569721793550831	0.6474596609120674	T	T	T
0.3048015883504920	0.0264788630834405	0.7919244076539815	T	T	T
0.2828771661515828	0.0598211947631072	0.0133895084036977	T	T	T
0.1237151186277658	0.0611548586356570	0.0112456736484025	T	T	T
0.0707185252509008	0.0291301286524610	0.7998992544953951	T	T	T
0.1804838000975715	0.0548160154996445	0.6549115898898099	T	T	T
0.4209985418764333	0.8261398081323830	0.6674887185080615	T	T	T
0.3046323973603710	0.8682995060051779	0.8092821011900644	T	T	T
0.2665269518750916	0.8272431593430771	0.0271956303266931	T	T	T
0.1119340364746599	0.8255589226278881	0.0131808259813371	T	T	T
0.0660825358638867	0.8720401173972177	0.7990546092397568	T	T	T
0.1833186994615217	0.8279020123904478	0.6713088121163897	T	T	T
0.0772880131912373	0.9412179904448899	0.1479190630851650	T	T	T
0.1975732275429118	0.9716375254283260	0.2911163804143302	T	T	T
0.2197043494330645	0.9369527020579884	0.5129312418582413	T	T	T
0.3794026409640963	0.9343737947482935	0.5129752114725091	T	T	T
0.4327461358697419	0.9682470747945171	0.3005809884421068	T	T	T
0.3224968379165501	0.9427594895665611	0.1550348028811891	T	T	T
0.0821714985732686	0.1704568516607388	0.1652550869360422	T	T	T
0.1970088033616020	0.1296773695265356	0.3095744545468335	T	T	T
0.2341578539663817	0.1708537289398852	0.5262319213205660	T	T	T
0.3886311793868576	0.1729349638137600	0.5105784198757002	T	T	T
0.4369140818852262	0.1265499079835027	0.2975505241908059	T	T	T
0.3178960338050780	0.1698035579532615	0.1721835568251341	T	T	T
0.5769235458534057	0.5556085707415908	0.3557845420284570	T	T	T
0.6896725210251364	0.5253180253652201	0.1997275292598804	T	T	T
0.7152431298488504	0.5675840606973237	0.9858877547187654	T	T	T
0.8745255296093902	0.5721103014661432	0.9837137052534968	T	T	T
0.8084212968446367	0.5516919937603384	0.3400950431568310	T	T	T

Structure files (CONTCAR) involved in this work:

0.5746650283536200	0.3273327727384284	0.3299943851989345	T	T	T
0.6951495908762889	0.3714094353451452	0.1914293554342840	T	T	T
0.7315962791541767	0.3267755232657062	0.9798548276872969	T	T	T
0.8862728728437399	0.3260972313121305	0.9979409150359346	T	T	T
0.9443549273030705	0.3747214012442734	0.1948345666477653	T	T	T
0.9206056510534855	0.4437736438043798	0.8596311529923818	T	T	T
0.8021239848331457	0.4717888034504427	0.7173816892283946	T	T	T
0.7733572834079143	0.4373481778059902	0.4929493359972159	T	T	T
0.6160650943318904	0.4284197256528634	0.4890714909655914	T	T	T
0.5688143741834547	0.4680358866068793	0.7024660035179395	T	T	T
0.6776883796212873	0.4475452007539319	0.8551028815247039	T	T	T
0.9190928818389834	0.6781636616109175	0.8244610693010360	T	T	T
0.7691787058240183	0.6677898091594706	0.4631079322243295	T	T	T
0.6144358640467941	0.6729520796854015	0.4885224588483029	T	T	T
0.5621371372694824	0.6264157965731258	0.6991551566446391	T	T	T
0.6775196876823213	0.6725874302812634	0.8224175307336806	T	T	T
0.5786267568983241	0.9444295783335478	0.3579437455569988	T	T	T
0.6994979056232062	0.9726972609824288	0.2136946556806600	T	T	T
0.7218179895147142	0.9355265043391890	0.9919956822490895	T	T	T
0.8822457930331984	0.9339016982100398	0.9948891805281136	T	T	T
0.9330989384201189	0.9696722907236179	0.2058176218490100	T	T	T
0.8235439895744370	0.9456276722486771	0.3548309237896988	T	T	T
0.5796834275941724	0.1724031698604778	0.3293908054993824	T	T	T
0.6999170309390715	0.1314710569493042	0.1928196210840747	T	T	T
0.7337421603892018	0.1710795390486861	0.9720900542777705	T	T	T
0.8884236283135734	0.1734555164242975	0.9855230276779128	T	T	T
0.9369712294019381	0.1275896073082219	0.1995026031099416	T	T	T
0.8215287705077361	0.1742516242832980	0.3301699224290947	T	T	T
0.9250584858965603	0.0552152244698832	0.8568144345130693	T	T	T
0.8047327739041139	0.0270285671374636	0.7080662603390224	T	T	T
0.7824995984148603	0.0666017473247189	0.4908715344747644	T	T	T
0.6221505153231097	0.0688345479225089	0.4902731628893359	T	T	T
0.5694001544350833	0.0309220122622598	0.6995579182178771	T	T	T
0.6809585962921303	0.0527157503445223	0.8480944261375988	T	T	T
0.9241651761850787	0.8301779030837716	0.8362228429720177	T	T	T
0.8034996379153305	0.8703360451912064	0.6957889242551808	T	T	T
0.7710217748458019	0.8259189306472958	0.4799567852693880	T	T	T
0.6160403180842660	0.8263696892994261	0.4912099040327844	T	T	T
0.5649291685803444	0.8737130598535936	0.6995259188996397	T	T	T
0.6806031816305466	0.8321907120758366	0.8313639342737403	T	T	T
0.4233354604994959	0.4425639088043293	0.6453191193750268	T	T	T
0.3032524815735201	0.4713939659372710	0.7894712946489183	T	T	T
0.2785838803484974	0.4379839146547524	0.0109310804420763	T	T	T
0.1212033802097988	0.4359314855634504	0.0136718136875218	T	T	T
0.0654868524706140	0.4692861899194480	0.7996957102080661	T	T	T
0.1774882524060535	0.4440888395891477	0.6539152040429322	T	T	T
0.4185805847550725	0.6719100215915736	0.6636005260013442	T	T	T
0.3026912339610781	0.6288720982139580	0.8057669813161243	T	T	T
0.2664674217456323	0.6700053152111336	0.0240426953117067	T	T	T
0.1125663852970147	0.6719255161910348	0.0078437701681023	T	T	T
0.0622408976591175	0.6282925848337058	0.7946716181313316	T	T	T
0.1815880489908834	0.6695400518773588	0.6685577613763324	T	T	T
0.0788963785902213	0.5571209853881219	0.1470462654914706	T	T	T

Structure files (CONTCAR) involved in this work:

0.1985459018674547	0.5244763661028514	0.2886187210636523	T	T	T
0.2170667787306266	0.5606282182244962	0.5120461217044870	T	T	T
0.3760893583971349	0.5646797523048126	0.5117914438308102	T	T	T
0.4296374261043072	0.5282700868386250	0.3005156512425827	T	T	T
0.3226550454522644	0.5532402027596576	0.1511101132919148	T	T	T
0.0864914870649628	0.3229414881623498	0.1602505389722406	T	T	T
0.1977018604528348	0.3670453534099783	0.3069398124007651	T	T	T
0.2330739399340706	0.3282980194079592	0.5248354423713897	T	T	T
0.3873454911750470	0.3267784523071613	0.5062533072904376	T	T	T
0.4337479166522809	0.3705742593627650	0.2920930485547295	T	T	T
0.3156308628766248	0.3283068788148387	0.1686122531155160	T	T	T
0.3588368307735367	0.0613250797994969	0.7183614192731463	T	T	T
0.3060589251027263	0.0663240890883833	0.8977128040785491	T	T	T
0.2030630479773934	0.0458371700750416	0.0210410834859404	T	T	T
0.1014036053647946	0.0686766096334669	0.8956726203587669	T	T	T
0.1049262881502360	0.0576825164587069	0.6984613833055254	T	T	T
0.2304971241001771	0.0312191030999699	0.7439855181776790	T	T	T
0.3603192964511815	0.8267983638975244	0.7475270572838967	T	T	T
0.3053983387939628	0.8407345386132198	0.9229793883550984	T	T	T
0.1891394497029302	0.8513498160352080	0.0164365600272497	T	T	T
0.0846696762543706	0.8304848070869518	0.8997576531834025	T	T	T
0.1058980189353220	0.8394311572952950	0.7045226572854953	T	T	T
0.2310632912751242	0.8558517669312840	0.7607651891055406	T	T	T
0.3233400128410790	0.9476622608177182	0.8075933217758769	T	T	T
0.0881597150567590	0.9498130381335705	0.8133093266120203	T	T	T
0.4323053888581683	0.1270503883852569	0.5862571133366625	T	T	T
0.4187496232661743	0.9953765364936153	0.5679058829569896	T	T	T
0.3982153418148704	0.8632592643922907	0.5649289388982753	T	T	T
0.2003268577961409	0.1294164393583511	0.6168909954432863	T	T	T
0.1828038034261044	0.0013886966618708	0.5630493384140001	T	T	T
0.1983436471540681	0.8673220700713576	0.5675267187481469	T	T	T
0.9909896102509591	0.0409672489194301	0.7896508654759281	T	T	T
0.9861736653415192	0.8674390097199697	0.7790328618142710	T	T	T
0.1434596581772143	0.9367836466637306	0.2175462486447146	T	T	T
0.1969031441803591	0.9317726828848006	0.3969112088575189	T	T	T
0.2997698713667637	0.9483055509037226	0.5223838183898590	T	T	T
0.4017704914713589	0.9297144569711413	0.3971121143277596	T	T	T
0.3975870771274042	0.9392589720949045	0.2001027897455680	T	T	T
0.2717366165372166	0.9670721767910738	0.2428016425311313	T	T	T
0.1420677861769255	0.1711806670273222	0.2464417941921552	T	T	T
0.1938301113398654	0.1569580624377598	0.4233218244702076	T	T	T
0.3113452403598854	0.1471775834607519	0.5121234290099328	T	T	T
0.4173634291463690	0.1678487239754063	0.3979333277416058	T	T	T
0.3957198874035635	0.1583016250988928	0.2034765995602707	T	T	T
0.2712381519758617	0.1425506538961512	0.2635805502961003	T	T	T
0.1785242255857276	0.0502637180923457	0.3068866547285358	T	T	T
0.4171394792939445	0.0480826900217871	0.3118951354118268	T	T	T
0.0674610733028018	0.8701582897133573	0.0895852274124609	T	T	T
0.0831591102825490	0.0001434389476755	0.0641658817394724	T	T	T
0.1056045335737365	0.1314038912578392	0.0652689532141793	T	T	T
0.3021709442336099	0.8682826921343930	0.1167217475317466	T	T	T
0.3214030395287491	0.9960918655387271	0.0629760789021784	T	T	T
0.3014829946028754	0.1295462573047015	0.0696503436383202	T	T	T

Structure files (CONTCAR) involved in this work:

0.5121960134506788	0.9543565426671810	0.2900830536378308	T	T	T
0.5167569634651065	0.1332914376291987	0.2776270633698061	T	T	T
0.6380435063633750	0.5596148142116792	0.2774628787793539	T	T	T
0.6949820596872202	0.5742227059780651	0.1032430624152150	T	T	T
0.7949432778627513	0.5557324319622082	0.9715689993701329	T	T	T
0.8956445344890799	0.5803987487204062	0.0989529197208872	T	T	T
0.8856156405060892	0.5402095007127320	0.3112846320779514	T	T	T
0.7627010748493529	0.5212264651431335	0.2528088642710415	T	T	T
0.6424645787533800	0.3345533404987034	0.2662796317906608	T	T	T
0.6905181126510408	0.3331642236303941	0.0837634684437242	T	T	T
0.8087601345602863	0.3504916534727283	0.9968577289989111	T	T	T
0.9133045026954002	0.3224519842591971	0.1131083887373101	T	T	T
0.9090960774000997	0.3615346592711781	0.3049218372204450	T	T	T
0.7692088371004747	0.3686883495911621	0.2367404300411254	T	T	T
0.6687806307883143	0.4487411849894575	0.1731060518040568	T	T	T
0.9330886301352721	0.4497533119312396	0.1568605602531488	T	T	T
0.5703532402464553	0.6271335320782753	0.4129643866776797	T	T	T
0.5885164262360909	0.4972887779819159	0.4389667641543379	T	T	T
0.5808262947652091	0.3635923072519076	0.4388492963486342	T	T	T
0.7931792041291710	0.6309962546509980	0.3603450174348386	T	T	T
0.7912341936011638	0.5144495681075669	0.4499204741457651	T	T	T
0.8225817968807789	0.3863542820757409	0.4358896724727964	T	T	T
0.0125139958249155	0.5567507922892346	0.2274640421128733	T	T	T
0.0237867211854198	0.3607136868163411	0.2114304431578341	T	T	T
0.8564314971516251	0.4325468320864667	0.7859343831753124	T	T	T
0.7894844061186869	0.4336883618989983	0.6112183375855095	T	T	T
0.6960198901759916	0.4224101224670870	0.4691072121554904	T	T	T
0.6005729478799816	0.4281410716636995	0.6075087982513124	T	T	T
0.6044011979955565	0.4416682934728860	0.8038428389603420	T	T	T
0.7307029251100687	0.4760088149893494	0.7729631782931796	T	T	T
0.8614927829652170	0.6829566212538143	0.7425382625924579	T	T	T
0.8173899987152897	0.6393221433916261	0.5538684154193682	T	T	T
0.6921388141997552	0.6477449742368708	0.4888351294435425	T	T	T
0.5842141880863286	0.6677681377052733	0.6000041867147659	T	T	T
0.5984535686353867	0.6592737231640203	0.7959510760364289	T	T	T
0.7228951379595756	0.6454958772167686	0.7313543103912271	T	T	T
0.8296653735726528	0.5472191184312363	0.6899021562001404	T	T	T
0.5821050404917413	0.5477699646095343	0.6862796498246984	T	T	T
0.9300682597469137	0.3778798314369868	0.9305465506948553	T	T	T
0.9138616406684049	0.5101832254450086	0.9287174212028834	T	T	T
0.8939647557328335	0.6409627685273992	0.9257859273697143	T	T	T
0.6987245284874362	0.3734986610780679	0.8936531990220153	T	T	T
0.6749605401464731	0.5017296837249132	0.9453705832369235	T	T	T
0.6931171113245793	0.6354081093329274	0.9284119067580333	T	T	T
0.4894732717607970	0.4521373471689057	0.7135384518191571	T	T	T
0.4814061657283695	0.6320272434662009	0.7125030894646754	T	T	T
0.6432096504362372	0.9396998218319152	0.2855626420966608	T	T	T
0.7000227968603616	0.9322106594518301	0.1085219991478623	T	T	T
0.8023294732857164	0.9427750542358215	0.9802002713619012	T	T	T
0.9014344600369351	0.9284173204069899	0.1122684015282754	T	T	T
0.8988451218968401	0.9458330766266723	0.3097180199808519	T	T	T
0.7723081628453250	0.9651410362662024	0.2654252052160262	T	T	T
0.6424547487925446	0.1716221042516780	0.2535459461628811	T	T	T

Structure files (CONTCAR) involved in this work:

0.6974287268643521	0.1577970736332697	0.0784434484978061	T	T	T
0.8114483010218919	0.1471729187620774	0.9800329988712980	T	T	T
0.9154326443164224	0.1676750346650448	0.0991349749178947	T	T	T
0.8984359424560924	0.1572549047198671	0.2962993024361644	T	T	T
0.7728483242513988	0.1454368495985527	0.2411678161593823	T	T	T
0.6829306675377013	0.0515584773862596	0.1958989245008298	T	T	T
0.9193968969159159	0.0486950838988280	0.1851534223585320	T	T	T
0.5712145051403841	0.8748020494935762	0.4206048813574277	T	T	T
0.5841212131728779	0.0062697881198207	0.4367863545737251	T	T	T
0.6001287311409657	0.1381577265758770	0.4354546911421782	T	T	T
0.8092485231638928	0.8704637779936263	0.3966831856913191	T	T	T
0.8182071864783301	0.9999676558759136	0.4447571318525389	T	T	T
0.8057409035057373	0.1341216517760101	0.4338348711427615	T	T	T
0.0125793882505951	0.9546853606841208	0.2175517709517484	T	T	T
0.0171116376811247	0.1361935815889971	0.2164426323447409	T	T	T
0.8602813250190138	0.0561100945408443	0.7845550173645039	T	T	T
0.8045856536200203	0.0726652023684357	0.6074736123396837	T	T	T
0.7020040649234894	0.0570930881552781	0.4808800922467567	T	T	T
0.5998373896695196	0.0740539662434705	0.6066824766678087	T	T	T
0.6055367576285747	0.0512895474583056	0.8036487568336160	T	T	T
0.7313992319956687	0.0301002129240906	0.7592627768546674	T	T	T
0.8583922382941983	0.8357046362509828	0.7671072620478997	T	T	T
0.8064156489968302	0.8327160594267262	0.5883921149720455	T	T	T
0.6936959988767104	0.8508842696306955	0.4873124422525489	T	T	T
0.5893053655793659	0.8281486475113449	0.6055470601915564	T	T	T
0.6039444490544157	0.8506151097865531	0.8002509714723754	T	T	T
0.7295305849214914	0.8623728446010438	0.7445870701718099	T	T	T
0.8211344203729398	0.9493101050066421	0.6800275940768108	T	T	T
0.5807735615161500	0.9518252716919927	0.6741901951332320	T	T	T
0.9335182601309315	0.1280794937971468	0.9104107499390390	T	T	T
0.9189700429031039	0.9982026318697593	0.9435924274424562	T	T	T
0.9090910477016374	0.8653001039748797	0.9434543247356968	T	T	T
0.6969275494704823	0.1285784253668154	0.8847969005555620	T	T	T
0.6867007943043401	0.0010127942221713	0.9416682214657679	T	T	T
0.6974535059483392	0.8665830506651061	0.9385599741118321	T	T	T
0.4903986809135075	0.0464907942539964	0.7155245760521136	T	T	T
0.4852100540701371	0.8632993209026594	0.7171934545871682	T	T	T
0.3581667679650800	0.4361819195627948	0.7173064987525027	T	T	T
0.3004841164961355	0.4307057733709400	0.8947775244301379	T	T	T
0.1994789083725390	0.4575889192951794	0.0213724266394514	T	T	T
0.0967794006900388	0.4344327316882995	0.8992123694996976	T	T	T
0.1029028215450169	0.4398432476960524	0.7010083949816655	T	T	T
0.2295378913251810	0.4688756000472811	0.7391890842525328	T	T	T
0.3569371091747697	0.6706857789870848	0.7420005611132410	T	T	T
0.3041158483876805	0.6582704233415404	0.9184773630983369	T	T	T
0.1892122548748971	0.6449636411889322	0.0130560385491265	T	T	T
0.0853036021763131	0.6684578692865818	0.8947917890554774	T	T	T
0.1038168315439251	0.6582285300235031	0.6997683580947726	T	T	T
0.2286880213671876	0.6385397122535804	0.7568735622084619	T	T	T
0.3228056899676609	0.5497358462034825	0.8076428811702874	T	T	T
0.0797729725841772	0.5493177303118005	0.8085670866199717	T	T	T
0.4315376139819262	0.3748963539334603	0.5783963369018311	T	T	T
0.4173241682806799	0.5061660523682062	0.5693146485024148	T	T	T

Structure files (CONTCAR) involved in this work:

0.3945495164613282	0.6372918278045197	0.5593051695440776	T	T	T
0.1978102357743265	0.3700960136853815	0.6141163522841480	T	T	T
0.1770956099425413	0.4977347234927788	0.5616867625072206	T	T	T
0.1956302252272497	0.6314278855528819	0.5628651004689814	T	T	T
0.9868774174841204	0.4518346371300205	0.7899800415112612	T	T	T
0.9831861954328207	0.6378619939085820	0.7759824577487476	T	T	T
0.1446731634659853	0.5623247964880835	0.2162485385779278	T	T	T
0.1962619799052367	0.5639576962459979	0.3945236642313073	T	T	T
0.2967943913124750	0.5484335546033658	0.5245982521899242	T	T	T
0.3960369044075322	0.5671471725445359	0.3947418720347537	T	T	T
0.3972307544471279	0.5567508835456282	0.1975230974331939	T	T	T
0.2719684469186906	0.5289002952565706	0.2395627078272699	T	T	T
0.1467480350661080	0.3225890773638069	0.2410765964136546	T	T	T
0.1924360667879520	0.3420145964041022	0.4215842362727430	T	T	T
0.3099902323267141	0.3527793223056537	0.5102571659312691	T	T	T
0.4134351251732372	0.3281978691445939	0.3915246097072973	T	T	T
0.3936765896833906	0.3425421393809525	0.1945890733540797	T	T	T
0.2728539597084864	0.3565011872284533	0.2640389663099663	T	T	T
0.1764351299748750	0.4463209248048084	0.3009342696761010	T	T	T
0.4143848148343393	0.4485874754781052	0.3123056885738910	T	T	T
0.0679976390166946	0.6239491593447775	0.0811494051004964	T	T	T
0.0771959924444731	0.4901664432459944	0.0795498957185249	T	T	T
0.1102901567233170	0.3614937704673441	0.0592125215875705	T	T	T
0.3021623860157046	0.6272695205405130	0.1119248417343379	T	T	T
0.3212427098131332	0.4990638683716562	0.0602979396437296	T	T	T
0.2932713762908566	0.3671633893805493	0.0670339883138789	T	T	T
0.5090271607560883	0.5414896458601314	0.2938707059811834	T	T	T
0.5129018622643546	0.3620110575387265	0.2690813614777980	T	T	T
0.4389890442840181	0.7489645205610646	0.6397137254061787	T	T	T
0.1971924052098876	0.7486028634262367	0.6520584923239727	T	T	T
0.2697246374849742	0.7482198213718370	0.0559269112100003	T	T	T
0.1069355374360114	0.7478523466198010	0.0499682720905112	T	T	T
0.0663967929930719	0.2469741364866933	0.1309010573244294	T	T	T
0.3029253471960597	0.2488067277459161	0.1516813730925849	T	T	T
0.2297932092490347	0.2497795058054593	0.5547987300325216	T	T	T
0.3929263730362276	0.2504330237713955	0.5476951172944926	T	T	T
0.5579251527060893	0.2492051647106943	0.3518037890779712	T	T	T
0.8124632209632423	0.2528518982248818	0.3476983397830347	T	T	T
0.7288528911363272	0.2496308045456991	0.9409334081587154	T	T	T
0.8934600871473286	0.2513431097739035	0.9501385668175758	T	T	T
0.9443004236185796	0.7528635736290287	0.8572939592154107	T	T	T
0.6897413832393838	0.7521830206442298	0.8422128368323171	T	T	T
0.7761601435586157	0.7477820418286829	0.4461931507544414	T	T	T
0.6100705239273969	0.7500109968674963	0.4497601681995970	T	T	T
0.9343472116209823	0.4809278221346861	0.5263576450475170	T	T	T
0.8228557366918957	0.3367406322510373	0.3257041530683453	T	T	T
0.8024917635082743	0.6333659367939122	0.6872674698907683	T	T	T
0.9232538756276466	0.5307670373297919	0.1946379902175966	T	T	T
0.9241643662429450	0.4214627857699433	0.4245690418055668	T	T	T
0.8733827138271686	0.5494008650253986	0.5482828269177752	T	T	T
0.9849294971537407	0.6457983600666114	0.3021359439793682	T	T	T
0.9996705241676518	0.5732733875181666	0.3804297875933176	T	T	T
0.0370033497560648	0.4374669151061632	0.5010339414372891	T	T	T

Structure files (CONTCAR) involved in this work:

0.0690241976321609	0.6176498608102996	0.3254557727848592	T	T	T
0.0397422899630601	0.4405860107380087	0.3633516602186982	T	T	T
0.0236660206400656	0.3605913167440735	0.4262767495818388	T	T	T
0.0170131452927746	0.6020703028973294	0.3156190684314429	T	T	T
0.0207043594439928	0.4156593218390460	0.4304129741311969	T	T	T

Figure S17 ZnCu-TS

Si O Al Cu Zn H C

1.0000000000000000

20.0219999999999985 0.0000000000000000 0.0000000000000000

0.0000000000000000 19.8990000000000009 0.0000000000000000

0.0000000000000000 0.0000000000000000 13.3829999999999991

93 193 3 1 1 6 2

Selective dynamics

Direct

0.4245306714235336	0.0561796539131097	0.6474713263052696	T	T	T
0.3036195959350728	0.0254364867085614	0.7904457667012670	T	T	T
0.2827047712085147	0.0599753781733224	0.0124021035766964	T	T	T
0.1234923930142578	0.0618804070296554	0.0115710442598857	T	T	T
0.0714726106630435	0.0282408881377683	0.8000703563690941	T	T	T
0.1793814386924507	0.0539175608710042	0.6514305717564277	T	T	T
0.4211306449507701	0.8264115454207602	0.6673102218634621	T	T	T
0.3040158026881173	0.8673902172148482	0.8091499845103561	T	T	T
0.2663166076833802	0.8263124917453238	0.0272398105059460	T	T	T
0.1117208553518240	0.8244165847561856	0.0130477859698256	T	T	T
0.0661065233745266	0.8711111748426956	0.7988976649632070	T	T	T
0.1828482600658086	0.8273430333712670	0.6699284930716082	T	T	T
0.0772933965018379	0.9411453774214048	0.1469544565820074	T	T	T
0.1978900684084232	0.9716437061452861	0.2895587267940714	T	T	T
0.2192962426200787	0.9364565488347911	0.5113511261690145	T	T	T
0.3787243233810079	0.9343696972201181	0.5127428970942803	T	T	T
0.4318811006206693	0.9680601674804838	0.3004851613579598	T	T	T
0.3225171417242613	0.9430172900933231	0.1527193674268831	T	T	T
0.0818188503012712	0.1715967429410152	0.1639032831400677	T	T	T
0.1976008383726250	0.1291897910699381	0.3072099963318274	T	T	T
0.2339502011097606	0.1707428468771716	0.5246054028025943	T	T	T
0.3885881086351963	0.1726076729558921	0.5116504771568131	T	T	T
0.4373994171511616	0.1262831256535977	0.2987889323810632	T	T	T
0.3193207543196026	0.1687735820017734	0.1711256771961533	T	T	T
0.5767447901746778	0.5555366676051003	0.3569970072334434	T	T	T
0.6894642285875227	0.5246590040321206	0.2003997585159663	T	T	T
0.7160573980866827	0.5673763279353901	0.9863991421541257	T	T	T
0.8748990486879428	0.5718433385265450	0.9864430170092955	T	T	T
0.8084717486571207	0.5525591564334914	0.3404496525408289	T	T	T
0.5747657916408692	0.3271008113041152	0.3308112255539340	T	T	T
0.6950727792506357	0.3706763509788246	0.1913835966259904	T	T	T
0.7307607303891992	0.3262883433993536	0.9793442620581221	T	T	T
0.8851687508039349	0.3257161729999556	0.9981713505104691	T	T	T
0.9416724851494016	0.3760930710390356	0.1922568517695503	T	T	T
0.9218687961182317	0.4438282954228494	0.8623268721312901	T	T	T
0.8034076434403368	0.4710499251520952	0.7184869886083206	T	T	T
0.7741471971064483	0.4374655169983177	0.4934428981311166	T	T	T
0.6164001436198560	0.4282479866358497	0.4903661529028320	T	T	T
0.5683933205505125	0.4686673548762235	0.7029025813064590	T	T	T

Structure files (CONTCAR) involved in this work:

0.6776964150167257	0.4473739772445838	0.8547424801819744	T	T	T
0.9194227185329995	0.6775900853004480	0.8263596802749147	T	T	T
0.7689230208848673	0.6680071564493955	0.4647362172863763	T	T	T
0.6146688214802934	0.6732545395373836	0.4902597611361055	T	T	T
0.5620925692161672	0.6269835482700661	0.7004373699993092	T	T	T
0.6784544690895070	0.6720521881356859	0.8234399659729571	T	T	T
0.5780942270863246	0.9444401581664643	0.3588192773622940	T	T	T
0.6998868531525370	0.9723124924384493	0.2152740660357112	T	T	T
0.7217535372023369	0.9342714269433077	0.9935182471628702	T	T	T
0.8822322955325140	0.9335868490125460	0.9959649452969205	T	T	T
0.9333049775063006	0.9698913590239953	0.2067427100411433	T	T	T
0.8243204215905701	0.9453568513053074	0.3570737358244721	T	T	T
0.5802128815410411	0.1720209332401692	0.3311573421926793	T	T	T
0.7005044155698843	0.1312387002450129	0.1939806312707051	T	T	T
0.7335646020008725	0.1707188042941130	0.9730262852053085	T	T	T
0.8881962401530078	0.1732626517932811	0.9865134765548372	T	T	T
0.9372066731202269	0.1281652588006439	0.2007204944923167	T	T	T
0.8217639271610747	0.1740250185574980	0.3319605850590298	T	T	T
0.9253725008085051	0.0552859781187594	0.8582311121220751	T	T	T
0.8050248882241365	0.0270140994091537	0.7097706626068947	T	T	T
0.7825700294279329	0.0660107874681394	0.4922338681045503	T	T	T
0.6224670305157577	0.0683943910120120	0.4912044737139519	T	T	T
0.5699681433926347	0.0300017096346511	0.7003611967907578	T	T	T
0.6808604729340002	0.0517059342435067	0.8500687625820968	T	T	T
0.9244968651713108	0.8298420840847596	0.8377638917547534	T	T	T
0.8034950763660424	0.8705729182688331	0.6984143769485636	T	T	T
0.7714956150066603	0.8260804884728106	0.4821367547963689	T	T	T
0.6166736468159558	0.8264724075906933	0.4918783786803902	T	T	T
0.5654656983529319	0.8729466395978761	0.7003319952609218	T	T	T
0.6805803096340044	0.8316648787139359	0.8327912766189954	T	T	T
0.4237580444760323	0.4428518378887665	0.6438694914883548	T	T	T
0.3035877876567758	0.4715329169676212	0.7882326449594170	T	T	T
0.2816482591406203	0.4365809613287523	0.0086425522766609	T	T	T
0.1243079834473655	0.4365244691330461	0.0133757311612624	T	T	T
0.0669771575008908	0.4689154639141366	0.8006810515983740	T	T	T
0.1777222835864077	0.4438197309673270	0.6535875163047938	T	T	T
0.4191463854736153	0.6722417733978647	0.6637827146576133	T	T	T
0.3021658983347553	0.6289853893405781	0.8044231124834234	T	T	T
0.2661317329799644	0.6696177302924008	0.0233291760507735	T	T	T
0.1118236052574096	0.6703296961229567	0.0111622579948316	T	T	T
0.0626166499127747	0.6279950800382909	0.7967138008129742	T	T	T
0.1805938657096836	0.6691044775250355	0.6673988750562174	T	T	T
0.0755036933211058	0.5558016329791156	0.1525614804301196	T	T	T
0.1988099670452037	0.5247171613422792	0.2869581824264201	T	T	T
0.2181685482940133	0.5603148047942200	0.5125335419861898	T	T	T
0.3765678920288691	0.5650677794233689	0.5125046423981690	T	T	T
0.4283868235791739	0.5280167946732404	0.3016462882297971	T	T	T
0.3236084879972850	0.5520566823127967	0.1483708264154459	T	T	T
0.0855442519903526	0.3249123330739654	0.1586886098882044	T	T	T
0.1968268804503134	0.3671383082894067	0.3068368534595324	T	T	T
0.2333822417641044	0.3279680690088370	0.5251313544481890	T	T	T
0.3875913263206782	0.3263704682181339	0.5071242462181662	T	T	T
0.4334994826523205	0.3701698388599126	0.2931270349584172	T	T	T

Structure files (CONTCAR) involved in this work:

0.3158405181081548	0.3272926119069233	0.1673980983370361	T	T	T
0.3593251156728338	0.0595229010207881	0.7189277617513135	T	T	T
0.3023306369527901	0.0663872323638984	0.8952824657879845	T	T	T
0.2028322076705685	0.0480742032354019	0.0261456558608710	T	T	T
0.1040494406306531	0.0676150820798054	0.8945929480034648	T	T	T
0.1044378472299342	0.0564376309445869	0.6974326828934745	T	T	T
0.2305877306906813	0.0295555627849550	0.7384249643538084	T	T	T
0.3605206237535432	0.8270784501359632	0.7473290690155510	T	T	T
0.3046631274977340	0.8389227145347287	0.9222649528039976	T	T	T
0.1889336539628096	0.8504280539276976	0.0165651084369820	T	T	T
0.0848757578407144	0.8292920760594188	0.8992054239266472	T	T	T
0.1055319195954305	0.8387975755164108	0.7037229689736846	T	T	T
0.2309021240548836	0.8547992787782537	0.7592363998046493	T	T	T
0.3218023367296103	0.9469454755361633	0.8094637806276715	T	T	T
0.0883844536064261	0.9488409090337400	0.8133352271297698	T	T	T
0.4321578328814945	0.1268720645116114	0.5877024246746069	T	T	T
0.4188017038303163	0.9954600136440893	0.5664119066711505	T	T	T
0.3982498160960690	0.8634213719115745	0.5647096609416921	T	T	T
0.1984761883626443	0.1287012427351777	0.6132855829513743	T	T	T
0.1807466983777163	0.0009245534129445	0.5588726903865182	T	T	T
0.1975423291572350	0.8670292496384787	0.5662756647036922	T	T	T
0.9916985388408935	0.0406628717697087	0.7922618358264931	T	T	T
0.9861154461303373	0.8666675077488530	0.7789566868647538	T	T	T
0.1435478318404370	0.9368030110128510	0.2164153267101968	T	T	T
0.1988000117909517	0.9305628152941117	0.3944350924249516	T	T	T
0.2991636219518516	0.9483640189791172	0.5243084189123046	T	T	T
0.3996858199879207	0.9294362505473056	0.3962141985675269	T	T	T
0.3973924176781273	0.9400366961985843	0.1988804690991510	T	T	T
0.2716107345851190	0.9685557689318723	0.2395247312874970	T	T	T
0.1435019759252546	0.1706220063657299	0.2422143073790097	T	T	T
0.1949893813479546	0.1584808982050663	0.4199973154654698	T	T	T
0.3112706229827408	0.1467608122337310	0.5128224990986802	T	T	T
0.4175666048448187	0.1675579973396811	0.3991023240583029	T	T	T
0.3969714887365186	0.1583439933569193	0.2042938210866598	T	T	T
0.2720438183705043	0.1399695692143790	0.2607869961711855	T	T	T
0.1781656343585208	0.0499432698115966	0.3079108008122161	T	T	T
0.4170660822065561	0.0479723932129271	0.3127301148467510	T	T	T
0.0673715801311263	0.8703172205229546	0.0881741759142825	T	T	T
0.0828454702208991	0.0007307936354199	0.0640459457505846	T	T	T
0.1026167221720442	0.1325186954568424	0.0624685039435148	T	T	T
0.3023674066945078	0.8682342958366411	0.1156410470587724	T	T	T
0.3215058788661790	0.9954438947280345	0.0593905309198981	T	T	T
0.3047124007893217	0.1291326181858814	0.0674714670234533	T	T	T
0.5113154582017937	0.9535090149698452	0.2915694840405413	T	T	T
0.5173750823615394	0.1326578030404163	0.2797163982559808	T	T	T
0.6363862756305801	0.5587613011044029	0.2761310481606082	T	T	T
0.6957458138492286	0.5733066237325000	0.1038075370337881	T	T	T
0.7954448745123931	0.5550261966077503	0.9709391465343052	T	T	T
0.8944901142852127	0.5807013108480671	0.1015443167521782	T	T	T
0.8855522489261300	0.5420156517534630	0.3134228111411365	T	T	T
0.7614360895913480	0.5203988865605546	0.2563738463478045	T	T	T
0.6424113882576266	0.3342219783140274	0.2667415256094423	T	T	T
0.6902088436580669	0.3323651877529639	0.0837736482896918	T	T	T

Structure files (CONTCAR) involved in this work:

0.8078425440962768	0.3505024700287590	0.9948734437450070	T	T	T
0.9107269245005447	0.3214067199341090	0.1140062506321202	T	T	T
0.9100033030213602	0.3595848329440457	0.3052338818186765	T	T	T
0.7690837219039899	0.3673000109466875	0.2370077196875751	T	T	T
0.6691495324695349	0.4480383143032907	0.1730079220788602	T	T	T
0.9229372854435770	0.4499329605570712	0.1583608994609947	T	T	T
0.5714163490234977	0.6270688094664334	0.4142397505694883	T	T	T
0.5898859036435776	0.4972204862420644	0.4398178863405529	T	T	T
0.5816158267049156	0.3634360906946579	0.4396910108757853	T	T	T
0.7911360783597575	0.6313394624147959	0.3611931395915257	T	T	T
0.7921948964202128	0.5148692335932058	0.4520353453789566	T	T	T
0.8239804710888503	0.3879842873522091	0.4341761547773310	T	T	T
0.0118084835287634	0.5496003172081464	0.2271122319411485	T	T	T
0.0219103273213453	0.3649489877254935	0.2035120844000769	T	T	T
0.8580013488120692	0.4328011115892049	0.7872132116224545	T	T	T
0.7943950616364713	0.4333261303965523	0.6106380677830094	T	T	T
0.6968435765176914	0.4218110555689203	0.4726479173237859	T	T	T
0.6003108948441953	0.4282121924815687	0.6085112839824303	T	T	T
0.6041912960156222	0.4425916192566610	0.8041795696158802	T	T	T
0.7311504254791186	0.4742037534617956	0.7713013692307505	T	T	T
0.8624411500302189	0.6823149445818825	0.7431601079915376	T	T	T
0.8180575198953294	0.6393226773587357	0.5544634814450771	T	T	T
0.6923467192422428	0.6479778944127647	0.4929926659540635	T	T	T
0.5834273323981601	0.6685717662161916	0.6011341752942589	T	T	T
0.5994262161339254	0.6591437458206096	0.7967933080896030	T	T	T
0.7239099852380935	0.6437284595825312	0.7331820105732513	T	T	T
0.8308653355797668	0.5465299710479663	0.6890545027011710	T	T	T
0.5817229907636687	0.5483120341078559	0.6860065641787012	T	T	T
0.9302122043730838	0.3774706339464117	0.9324972162113725	T	T	T
0.9149188124492555	0.5102824274942265	0.9307214480101094	T	T	T
0.8936374657922711	0.6405773011359406	0.9271463421409903	T	T	T
0.6974308595211193	0.3730480100356426	0.8934766552518941	T	T	T
0.6757321923706717	0.5019357975574991	0.9443033438008729	T	T	T
0.6934889604786088	0.6356093362396376	0.9301483261394347	T	T	T
0.4891121504385737	0.4526401158451952	0.7138478740841837	T	T	T
0.4815304214842532	0.6330225576954479	0.7153847210899273	T	T	T
0.6424724737227144	0.9402280049242906	0.2859761462004741	T	T	T
0.7010298703185343	0.9313338203577159	0.1105219761644800	T	T	T
0.8022340199742567	0.9406936505416293	0.9800094967022273	T	T	T
0.9006202599385117	0.9289779777102172	0.1136730276519085	T	T	T
0.8993232599265271	0.9461221117873457	0.3109463176680594	T	T	T
0.7721046017384025	0.9645515992611665	0.2687731624125889	T	T	T
0.6430020261627037	0.1708428340468082	0.2553817963108674	T	T	T
0.6977960470941006	0.1583503586354999	0.0800510065321826	T	T	T
0.8112795571828769	0.1467251391900413	0.9805731727819185	T	T	T
0.9149068158514282	0.1678634629154141	0.1003341799309494	T	T	T
0.8987535653955447	0.1578777312439249	0.2977014722720818	T	T	T
0.7733450504140863	0.1455981885751156	0.2424833899383662	T	T	T
0.6842375769692730	0.0511996629162958	0.1958749088023043	T	T	T
0.9200545128522500	0.0491242827670895	0.1869958801246937	T	T	T
0.5714346411424241	0.8748698807171346	0.4218345504130194	T	T	T
0.5835203811967072	0.0065087886412350	0.4373711689712486	T	T	T
0.6007242859968972	0.1382351842196312	0.4375405560427831	T	T	T

Structure files (CONTCAR) involved in this work:

0.8108642097498325	0.8701712091494873	0.3995508994110520	T	T	T
0.8192107553269653	0.9996118107479439	0.4471857612369295	T	T	T
0.8059867035383397	0.1334845240636055	0.4351662718325163	T	T	T
0.0127100261517702	0.9543691631125103	0.2171401411983409	T	T	T
0.0172785684314551	0.1376527442971322	0.2173655333164216	T	T	T
0.8610968722938137	0.0566800580743571	0.7848799029353599	T	T	T
0.8036324630328993	0.0726258229770467	0.6091691023030854	T	T	T
0.7022056181035854	0.0560304086060639	0.4804865970203935	T	T	T
0.6009607306684086	0.0732058754927777	0.6079543819292142	T	T	T
0.6055989779307177	0.0502667414673750	0.8049216358417955	T	T	T
0.7320430325268659	0.0295472446669483	0.7620309347697942	T	T	T
0.8579428242485097	0.8356625519264351	0.7701914923638656	T	T	T
0.8059580023581082	0.8325298758878511	0.5912732002974241	T	T	T
0.6942154398157608	0.8514183287231252	0.4874957354041095	T	T	T
0.5903539056837247	0.8275724905275080	0.6064626474154203	T	T	T
0.6037495164865507	0.8491309307764897	0.8013811515670203	T	T	T
0.7294074351799283	0.8635072218757487	0.7471239694378186	T	T	T
0.8218555806923765	0.9493184164193300	0.6819051428152434	T	T	T
0.5819700145675182	0.9509674952613733	0.6753937329368336	T	T	T
0.9338639767398171	0.1281421581179943	0.9118662764727222	T	T	T
0.9179296484819802	0.9986000889912483	0.9451286492043229	T	T	T
0.9108945949490881	0.8655255706950176	0.9450930469645190	T	T	T
0.6962051801481374	0.1276529069250953	0.8869744323873252	T	T	T
0.6865074127062829	-0.0001586487412457	0.9434924369151597	T	T	T
0.6963445070317215	0.8653358995219952	0.9409101199146652	T	T	T
0.4908274980498590	0.0453250741054959	0.7149582318949679	T	T	T
0.4855462717148187	0.8633647602755332	0.7168167664681512	T	T	T
0.3575937915624734	0.4374157918942066	0.7135023326165034	T	T	T
0.3031874254123468	0.4293310621344722	0.8922013210336488	T	T	T
0.2030457905857013	0.4567301596862479	0.0189635981026656	T	T	T
0.0996887300325457	0.4338062117954393	0.8984606263606174	T	T	T
0.1027371681560427	0.4402537379884950	0.6997485679818838	T	T	T
0.2293757511745963	0.4688036512489618	0.7392811784272649	T	T	T
0.3563281181425821	0.6704859864374998	0.7399181610429171	T	T	T
0.3025824925134858	0.6597445661378103	0.9161790521459503	T	T	T
0.1890747520232798	0.6443751905128293	0.0147518788300344	T	T	T
0.0856044579051792	0.6675477641407630	0.8968639731594987	T	T	T
0.1030852042945283	0.6581929564528971	0.7005366927518950	T	T	T
0.2284696338264021	0.6376449646129679	0.7541324081622062	T	T	T
0.3225716412441424	0.5498739548403990	0.8080827731146889	T	T	T
0.0806059822561564	0.5490120387452522	0.8083443963354898	T	T	T
0.4324034146036528	0.3747111676477999	0.5781409281662154	T	T	T
0.4190541984116825	0.5060645130277180	0.5668701936586678	T	T	T
0.3974333570975116	0.6373852709799774	0.5585335315216595	T	T	T
0.1976177739954487	0.3695821318695372	0.6142697290476447	T	T	T
0.1776968562216052	0.4968718520186047	0.5603140925863855	T	T	T
0.1929376722977288	0.6306457045795024	0.5613150880177873	T	T	T
0.9881330700793481	0.4511217915766482	0.7922574563833525	T	T	T
0.9834246676496188	0.6371352227286978	0.7779103233506788	T	T	T
0.1428366821933034	0.5631951250936698	0.2209297224216968	T	T	T
0.2005825826582929	0.5633008980708373	0.3942286432642378	T	T	T
0.2975462432939358	0.5500613652732139	0.5315735579143275	T	T	T
0.3925543342847848	0.5668583759229766	0.3941297535713465	T	T	T

Structure files (CONTCAR) involved in this work:

0.3973776237640513	0.5560505101374253	0.1977008523626623	T	T	T
0.2712786654904612	0.5275661197064913	0.2344018541028183	T	T	T
0.1425678940306940	0.3241303903025184	0.2448751770629487	T	T	T
0.1933448686435703	0.3416766644645517	0.4215262552488269	T	T	T
0.3103304392453827	0.3526293977485841	0.5115205115969896	T	T	T
0.4133619218267781	0.3273980131880134	0.3922540941354458	T	T	T
0.3934002149427021	0.3420101697688179	0.1959914022539210	T	T	T
0.2708180575745947	0.3552770254577603	0.2604568643147918	T	T	T
0.1768962567624457	0.4466174973211984	0.3025823514175366	T	T	T
0.4139783895268725	0.4481271093646508	0.3135617186223463	T	T	T
0.0674651323746929	0.6229347080470878	0.0839174464071325	T	T	T
0.0820354257974477	0.4910656840564316	0.0781049341354352	T	T	T
0.1136766690184678	0.3615558871488917	0.0588043206549729	T	T	T
0.3040265395282233	0.6259828210082610	0.1080778872889701	T	T	T
0.3249077513867040	0.4972514367006184	0.0582798609066773	T	T	T
0.2959040548421819	0.3654696482175943	0.0642825659469554	T	T	T
0.5077034778005404	0.5418658130742867	0.2982516048247495	T	T	T
0.5128079941558900	0.3618243328469229	0.2705074245552077	T	T	T
0.4393318680072290	0.7492793875601774	0.6397940087926662	T	T	T
0.1963822947234804	0.7480285897389004	0.6499627595992343	T	T	T
0.2699062229284392	0.7475350048165090	0.0572306081270929	T	T	T
0.1064567749550580	0.7471546592610376	0.0508369739882546	T	T	T
0.0654730698109479	0.2484567351099850	0.1316210423458723	T	T	T
0.3036820526328493	0.2476635349755731	0.1512740274275377	T	T	T
0.2299361969891116	0.2494214021135517	0.5550094051420462	T	T	T
0.3929387534495139	0.2501019098843666	0.5489570969160134	T	T	T
0.5584115473236485	0.2489222361420468	0.3528486405227680	T	T	T
0.8123744175470440	0.2525765554021803	0.3512229127760034	T	T	T
0.7283395336152201	0.2490742412326293	0.9405799478800410	T	T	T
0.8927462250512198	0.2510275741111681	0.9503678579128220	T	T	T
0.9443153811020683	0.7524665122596700	0.8586731482680371	T	T	T
0.6913027348899526	0.7517176080874526	0.8414027621115522	T	T	T
0.7762342637689125	0.7479074009625241	0.4485337828290946	T	T	T
0.6108379057173997	0.7500793694253121	0.4503627295838757	T	T	T
0.9419816628105251	0.4924039455442796	0.5024016412470069	T	T	T
0.8228819460748367	0.3359057945637159	0.3257920482756074	T	T	T
0.8033143460492376	0.6332309135616433	0.6879051329418017	T	T	T
0.9267835284804324	0.5326424602437919	0.1975293897492127	T	T	T
0.9243387862847396	0.4227449810982439	0.4166883847456552	T	T	T
0.8715254134851675	0.5479472115333285	0.5486259929770581	T	T	T
-0.0010880261935675	0.6263832006911612	0.3851154936069228	T	T	T
0.0116493200459770	0.5579863099960803	0.4826339125289076	T	T	T
0.0351300695522499	0.4225025381073932	0.5001420047313123	T	T	T
0.0755231044078593	0.5729545212269429	0.3804683426513240	T	T	T
0.0403906070360957	0.4375239880438309	0.3637509041027560	T	T	T
0.0208963840155289	0.3528444732923562	0.4104095575613503	T	T	T
0.0280117170959850	0.5849746049776559	0.4156751863287582	T	T	T
0.0204608976672886	0.4070865874437404	0.4249556816185556	T	T	T

Figure S17 ZnCu-FS

Si O Al Cu Zn H C

1.0000000000000000

20.0219999999999985 0.0000000000000000 0.0000000000000000

0.0000000000000000 19.8990000000000009 0.0000000000000000

Structure files (CONTCAR) involved in this work:

0.0000000000000000 0.0000000000000000 13.382999999999991
93 193 3 1 1 6 2

Selective dynamics

Direct

0.4240513980213980	0.0573484200287791	0.6467821878972757	T	T	T
0.3046368127768244	0.0265906368085756	0.7911514567844100	T	T	T
0.2828712621017649	0.0592714737804324	0.0131048771648852	T	T	T
0.1233143091390940	0.0617698385966132	0.0110611695530022	T	T	T
0.0700300480349071	0.0294012271383731	0.7996120844868078	T	T	T
0.1799746586650307	0.0558169199184351	0.6553435417682688	T	T	T
0.4209074246321301	0.8266025724216215	0.6674674221819055	T	T	T
0.3045520156700075	0.8677686885638098	0.8089478787503627	T	T	T
0.2676402753516588	0.8275301318138200	0.0274798465136586	T	T	T
0.1132351496082727	0.8250569065883233	0.0127464035601105	T	T	T
0.0663129578812084	0.8722732698745039	0.7992514983946816	T	T	T
0.1828511315712163	0.8271973463616517	0.6710713557837562	T	T	T
0.0780746695816562	0.9407562059436074	0.1474356509065940	T	T	T
0.1975104793051446	0.9714991237458477	0.2912330537908239	T	T	T
0.2194186482629532	0.9373519418131138	0.5133394190771069	T	T	T
0.3791368408669484	0.9347652997258473	0.5124206217226299	T	T	T
0.4333349898020200	0.9682624118651394	0.3007775638544458	T	T	T
0.3225188452905425	0.9423606173983267	0.1564998993193382	T	T	T
0.0823075697515454	0.1718359840127421	0.1644172331064399	T	T	T
0.1970128434010672	0.1297462761328914	0.3078809024251025	T	T	T
0.2332748533711073	0.1712778861451839	0.5250384775244945	T	T	T
0.3880482084761687	0.1734905622667742	0.5105782719140919	T	T	T
0.4369375042014674	0.1265876860921811	0.2981432983738869	T	T	T
0.3184228924877918	0.1693132299664390	0.1713388602893680	T	T	T
0.5771486500507697	0.5555265720486110	0.3549504375504124	T	T	T
0.6917644002155162	0.5248948657594761	0.2024711685249327	T	T	T
0.7148286954368582	0.5674758366528893	0.9864256994775162	T	T	T
0.8726868345669924	0.5722480176873577	0.9872736983600719	T	T	T
0.8117252540136213	0.5507636696101456	0.3438708955432913	T	T	T
0.5740752981413529	0.3276218096822009	0.3322609424636107	T	T	T
0.6957057619465793	0.3709421427957783	0.1945021553324717	T	T	T
0.7300738030441705	0.3261421445545277	0.9815309406150814	T	T	T
0.8846158954409430	0.3259332457511800	0.9969920253412050	T	T	T
0.9410612471987494	0.3763542445930044	0.1907932742608680	T	T	T
0.9204273576922379	0.4446539681738880	0.8624711026246211	T	T	T
0.7995145174491549	0.4709233416857384	0.7221990276374483	T	T	T
0.7743588089104925	0.4355990451537546	0.4962385862993892	T	T	T
0.6171889404137563	0.4289280925923245	0.4899066876400114	T	T	T
0.5685379953245167	0.4689137906733938	0.7028220147975590	T	T	T
0.6743748311602653	0.4466758841819208	0.8592131233828945	T	T	T
0.9205779921287763	0.6774119578663992	0.8302694253251048	T	T	T
0.7687268197608759	0.6684597342224990	0.4656792776686496	T	T	T
0.6139847159530304	0.6728195306892628	0.4881283715186608	T	T	T
0.5609439272691337	0.6270859127145205	0.6991852586945951	T	T	T
0.6732994444616871	0.6735834220055799	0.8277613936160489	T	T	T
0.5787078155281076	0.9443009749310324	0.3587417430742688	T	T	T
0.6995494563179173	0.9730252256934150	0.2156098076839942	T	T	T
0.7215917954553022	0.9371042347036862	0.9932861462320913	T	T	T
0.8819800292720009	0.9340217979600832	0.9953595820437301	T	T	T

Structure files (CONTCAR) involved in this work:

0.9340643271828317	0.9692373085014645	0.2054645563236686	T	T	T
0.8242256753844278	0.9453261917920559	0.3546670683593848	T	T	T
0.5798364402811239	0.1728621341848860	0.3299564020286357	T	T	T
0.6993731735174012	0.1317744663234279	0.1936926232508848	T	T	T
0.7331829703310858	0.1703590368144361	0.9722885800168762	T	T	T
0.8879251443634116	0.1733020900435022	0.9852828425969236	T	T	T
0.9375832180118815	0.1272945739750327	0.1985767583149219	T	T	T
0.8220691753100240	0.1732068278025999	0.3306750650888866	T	T	T
0.9246780125221257	0.0549163365657378	0.8569763328648986	T	T	T
0.8042031695796045	0.0260485833580990	0.7090398635086419	T	T	T
0.7826612469013592	0.0653401927545539	0.4914202099425908	T	T	T
0.6224379997822249	0.0686683592143178	0.4904607356453946	T	T	T
0.5691651730080109	0.0312954769967809	0.6991041703249452	T	T	T
0.6804196460369867	0.0529050166208792	0.8479982580555039	T	T	T
0.9243669837135040	0.8296850361364129	0.8367835356040618	T	T	T
0.8035673929427235	0.8688063578211201	0.6966118671970484	T	T	T
0.7709611826342108	0.8262649292115219	0.4795869465190580	T	T	T
0.6161012541882808	0.8264384249932344	0.4916188879508688	T	T	T
0.5650307331585724	0.8743798677901352	0.6992487156434579	T	T	T
0.6796926030244675	0.8326278855344348	0.8335612899718199	T	T	T
0.4239188814283892	0.4444020063235498	0.6394833335603420	T	T	T
0.3040677502684127	0.4715746944715987	0.7863325051931093	T	T	T
0.2821156119150811	0.4362993103018755	0.0049131847655652	T	T	T
0.1242635162805985	0.4354831386015754	0.0100068834913211	T	T	T
0.0655215620451812	0.4695035582741656	0.8010545563580865	T	T	T
0.1772486454764590	0.4447730983678213	0.6536609038027579	T	T	T
0.4183502380000482	0.6725885801584689	0.6595940946777784	T	T	T
0.3020073579953225	0.6293038652361457	0.8021108678017135	T	T	T
0.2685590058250853	0.6705493877991510	0.0203949108989813	T	T	T
0.1144337897050385	0.6713417344880898	0.0064723698448002	T	T	T
0.0633273874204836	0.6281914598479681	0.7959180040219319	T	T	T
0.1804606202986324	0.6683583627579371	0.6657417926564686	T	T	T
0.0755456551720228	0.5567856763116126	0.1467101779930976	T	T	T
0.1984151128898907	0.5266121629601606	0.2829826840367560	T	T	T
0.2194994271678090	0.5607561743743669	0.5097579561036347	T	T	T
0.3776685579500959	0.5661994039130931	0.5076878056115851	T	T	T
0.4292970807132603	0.5277415779325050	0.2982973791674439	T	T	T
0.3241490221708720	0.5524950084974332	0.1456876635564157	T	T	T
0.0857372320246205	0.3248914342758785	0.1582516510765483	T	T	T
0.1964910112108667	0.3686886220644253	0.3051824230256158	T	T	T
0.2318456524425126	0.3293308752085814	0.5246435362156086	T	T	T
0.3861658192458539	0.3270111613550905	0.5059703733302890	T	T	T
0.4324662574329131	0.3703316542739551	0.2924634647220418	T	T	T
0.3155020023405643	0.3278538269524086	0.1659190409423153	T	T	T
0.3585584731961868	0.0617135535875647	0.7176469460710968	T	T	T
0.3075251077472320	0.0648490909817310	0.8980440210816673	T	T	T
0.2027756885791123	0.0467261977956199	0.0188687288683197	T	T	T
0.0997684275029777	0.0689578098261737	0.8959746528501999	T	T	T
0.1043134247258459	0.0586769728965540	0.6986265303956446	T	T	T
0.2299482798768539	0.0336044827433510	0.7451796701573430	T	T	T
0.3608474026968841	0.8260919844362522	0.7484499401730169	T	T	T
0.3066766023087167	0.8430067673130092	0.9238868023214714	T	T	T
0.1902789600504831	0.8515408878930492	0.0162089282317480	T	T	T

Structure files (CONTCAR) involved in this work:

0.0857549168205414	0.8308562428571262	0.8993899718517114	T	T	T
0.1055553851294789	0.8400013544657994	0.7039233624900446	T	T	T
0.2310525141493821	0.8529309835514338	0.7615500484806781	T	T	T
0.3221189898521499	0.9473042187740459	0.8029463661294090	T	T	T
0.0881395934411513	0.9502605942350970	0.8125604485013567	T	T	T
0.4319627860100477	0.1275211696495180	0.5858282497294307	T	T	T
0.4185059158119007	0.9958573474948212	0.5671127234507878	T	T	T
0.3971361792051915	0.8638714532728857	0.5656261211080614	T	T	T
0.1992512545004891	0.1302801181568570	0.6159820528082435	T	T	T
0.1829092039016885	0.0015868318954600	0.5646744436991611	T	T	T
0.1992122430880487	0.8675905295910573	0.5685034029341985	T	T	T
0.9901850471615997	0.0407941580779188	0.7888615417731571	T	T	T
0.9862035641588344	0.8677052082321723	0.7805417108400187	T	T	T
0.1443910868356817	0.9360781420623661	0.2167282704150705	T	T	T
0.1952220826164246	0.9327667524471398	0.3979095783358544	T	T	T
0.2995527285826499	0.9491461264022630	0.5202040601612115	T	T	T
0.4027071588406282	0.9292926554649472	0.3971693849034820	T	T	T
0.3980732992173796	0.9397778165987114	0.2001298782884145	T	T	T
0.2723990932148449	0.9662084498841900	0.2454810719257264	T	T	T
0.1426416447302959	0.1722307280573948	0.2449459696952009	T	T	T
0.1935590481745115	0.1562122119934292	0.4220340052531324	T	T	T
0.3106854036528615	0.1480230968829949	0.5123476643931427	T	T	T
0.4167239752368068	0.1682969860842293	0.3978948900979160	T	T	T
0.3961282103099373	0.1577238114894298	0.2033008649977623	T	T	T
0.2714769174846690	0.1425356200154034	0.2627854836820394	T	T	T
0.1782621567111182	0.0504192942263910	0.3039875175636758	T	T	T
0.4177375888597417	0.0480450217067189	0.3132238476308912	T	T	T
0.0683569601813035	0.8701147044913660	0.0882981109924670	T	T	T
0.0835063612604977	0.0007537654266815	0.0651428990025615	T	T	T
0.1054222952892882	0.1323760917737379	0.0645223663504625	T	T	T
0.3026452698505107	0.8677841018195397	0.1184720654237512	T	T	T
0.3201633573899168	0.9954927945397063	0.0643212171837818	T	T	T
0.3020263744516173	0.1289269361321391	0.0690019445942867	T	T	T
0.5128572895868634	0.9544293853792692	0.2897899430997322	T	T	T
0.5168353051199793	0.1337116464054727	0.2787192151071232	T	T	T
0.6375397763902139	0.5601316172023358	0.2752744093431245	T	T	T
0.7011819527707709	0.5728868612158852	0.1059009617193074	T	T	T
0.7936741228991924	0.5585738345274887	0.9606841615638881	T	T	T
0.8852457632285138	0.5782458286167836	0.1047883108974371	T	T	T
0.8885553577048537	0.5369972944303850	0.3173123372258892	T	T	T
0.7623516036002973	0.5200204228156177	0.2621484109121032	T	T	T
0.6418527964385757	0.3353552457285440	0.2686310401281153	T	T	T
0.6917160051941146	0.3317256042392103	0.0877059788609258	T	T	T
0.8073377842682972	0.3511633168150272	0.9928569928393315	T	T	T
0.9095953885472607	0.3213555095054368	0.1132794435702390	T	T	T
0.9107072065389656	0.3617495097925173	0.3056234425244562	T	T	T
0.7693642351073433	0.3676962403555742	0.2414352362531647	T	T	T
0.6708376489122079	0.4485215765995328	0.1747907788143483	T	T	T
0.9222751886977709	0.4498076897095611	0.1560928323677008	T	T	T
0.5701381555472136	0.6270653692950033	0.4122673045960114	T	T	T
0.5909371682232563	0.4977742360989397	0.4384945335772210	T	T	T
0.5810912709507913	0.3641522811782274	0.4410323021832229	T	T	T
0.7971564609526652	0.6297600265433790	0.3672578878184536	T	T	T

Structure files (CONTCAR) involved in this work:

0.7953730301050463	0.5131653941139319	0.4559139063665337	T	T	T
0.8245653667914588	0.3845782730768872	0.43978444813032951	T	T	T
0.0108517214092859	0.5515267607283580	0.2158989853291939	T	T	T
0.0213257487720416	0.3646721527497784	0.2015917363860740	T	T	T
0.8565636615023370	0.4333542685794371	0.7874123674782773	T	T	T
0.7889953361745917	0.4328901190868615	0.6150491115915711	T	T	T
0.6974690843994575	0.4219961605128834	0.4693538863239496	T	T	T
0.6028744019645883	0.4298258923849332	0.6087527521280631	T	T	T
0.6016742152279484	0.4423654255389369	0.8061328467948010	T	T	T
0.7282832258770625	0.4732167621615808	0.7767730099151113	T	T	T
0.8610300381901166	0.6807244463762084	0.7508893807986557	T	T	T
0.8144816287884263	0.6421569768581615	0.5616000684848526	T	T	T
0.6917279441801736	0.6471159238328513	0.4877434733093353	T	T	T
0.5843713641299922	0.6676142686210415	0.5998887302324167	T	T	T
0.5949726497090941	0.6611145940690113	0.7969717078350054	T	T	T
0.7198466261740587	0.6473316405162356	0.7372393259095598	T	T	T
0.8249079777417774	0.5475642423843099	0.6954523009546486	T	T	T
0.5823856111084875	0.5486899531233915	0.6883621104556352	T	T	T
0.9299207968650354	0.3776201759023404	0.9309519587175583	T	T	T
0.9131328638255271	0.5102305742822660	0.9323878774379429	T	T	T
0.8978525814170191	0.6409846955216859	0.9332457803441507	T	T	T
0.6936711226057097	0.3722574268408008	0.8978042587484057	T	T	T
0.6736314133332615	0.5011164867340105	0.9490976478144190	T	T	T
0.6870561171206895	0.6347660629917800	0.9328827167349095	T	T	T
0.4891964757551842	0.4527428931504057	0.7099667793080352	T	T	T
0.4801132420034512	0.6317913726025433	0.7100172738163968	T	T	T
0.6439719062658236	0.9390207863980535	0.2876809601845188	T	T	T
0.6994775449421191	0.9335533381741500	0.1096311362616323	T	T	T
0.8020946055659449	0.9443739696530644	0.9819868712496614	T	T	T
0.9018274102304646	0.9278831090365028	0.1124292010918914	T	T	T
0.8994801620663585	0.9462827433353310	0.3096527429322414	T	T	T
0.7729179965630343	0.9654668828821903	0.2656529572228951	T	T	T
0.6420588401417069	0.1732315851654473	0.2528597095540985	T	T	T
0.6967676842367903	0.1556436237114311	0.0781304302584581	T	T	T
0.8109914380083423	0.1469422771916419	0.9804268010011277	T	T	T
0.9152511761785408	0.1676910256353053	0.0987489596003475	T	T	T
0.8984863280807013	0.1555826776342423	0.2958193514326389	T	T	T
0.7723653880234213	0.1468040115674654	0.2413883986101281	T	T	T
0.6822925069797924	0.0520134727731538	0.2004729719117521	T	T	T
0.9210838734216681	0.0482769890516296	0.1834343810935766	T	T	T
0.5707953082429778	0.8747709331454604	0.4216313546768283	T	T	T
0.5838373996570861	0.0063316992893843	0.4373544184798948	T	T	T
0.6015255043477199	0.1380721891633808	0.4350130630552423	T	T	T
0.8096531954132796	0.8700247516854768	0.3959779908718546	T	T	T
0.8185980861463278	0.9987630892637246	0.4457535515143341	T	T	T
0.8058990526549633	0.1327087657358472	0.4338390219099798	T	T	T
0.0133753844256534	0.9538336299582488	0.2175104195374686	T	T	T
0.0174198722684303	0.1373592029736799	0.2160303408026615	T	T	T
0.8593608949593563	0.0555644610597163	0.7857332025941811	T	T	T
0.8045518686771083	0.0713993681412380	0.6081048936783156	T	T	T
0.7022078918340581	0.0559386289289070	0.4813986378778422	T	T	T
0.5999693972211730	0.0747240442846884	0.6067427131502279	T	T	T
0.6049770706542289	0.0512415778775912	0.8037143174470256	T	T	T

Structure files (CONTCAR) involved in this work:

0.7306135335702432	0.0291804654706720	0.7594286361083684	T	T	T
0.8592928162656280	0.8334972434367615	0.7656732288926225	T	T	T
0.8061920972999873	0.8325328245081269	0.5881077162793783	T	T	T
0.6936865356647838	0.8512270828806239	0.4866283725332068	T	T	T
0.5901827306640918	0.8280756202610553	0.6063963828134852	T	T	T
0.6037180840414847	0.8522436166343752	0.8007196562565038	T	T	T
0.7299201499824534	0.8590019146841903	0.7457263720811550	T	T	T
0.8205191781421149	0.9480666420361054	0.6825782173224355	T	T	T
0.5808993192176350	0.9523389776057041	0.6728531667034223	T	T	T
0.9329765943150617	0.1280386797400761	0.9100068026081612	T	T	T
0.9193182416559509	0.9979963319575742	0.9439843167302804	T	T	T
0.9069936874112673	0.8651466612924974	0.9429117025179495	T	T	T
0.6969038779967972	0.1289778314765076	0.8833397668862717	T	T	T
0.6863400613552719	0.0025307501901863	0.9430888516997179	T	T	T
0.6972988423813905	0.8684490029406384	0.9392462471321865	T	T	T
0.4901702609944722	0.0467538934613611	0.7147493610870230	T	T	T
0.4852943152558196	0.8640329381847380	0.7162789314436850	T	T	T
0.3572734851153000	0.4396980131596605	0.7082733881703380	T	T	T
0.3069732252287416	0.4287926589528015	0.8897533968518955	T	T	T
0.2031153416205166	0.4552256690338756	0.0090422253894379	T	T	T
0.0962422288620525	0.4301551899919250	0.8963809705303132	T	T	T
0.1011485210558754	0.4439463617411273	0.6977706111143497	T	T	T
0.2286652975616122	0.4670140062225618	0.7412442861814043	T	T	T
0.3550913334412287	0.6700599461782202	0.7345915475848044	T	T	T
0.3051995625983279	0.6609285837773077	0.9132231430108111	T	T	T
0.1916230354223981	0.6453579225115206	0.0105806722579515	T	T	T
0.0889825784331055	0.6711641892518124	0.8912963471187674	T	T	T
0.1028628249648783	0.6540440819309793	0.6961838236957915	T	T	T
0.2275799607132129	0.6380207971808156	0.7544814634830064	T	T	T
0.3217530452350195	0.5501022914620641	0.8063952094895250	T	T	T
0.0795053927496937	0.5491346795451958	0.8147765626446506	T	T	T
0.4320613713969625	0.3759358862685931	0.5743972914950386	T	T	T
0.4209614819119438	0.5078495632307247	0.5626424324830884	T	T	T
0.3971679831623610	0.6390978597884943	0.5532130224828073	T	T	T
0.1950190189141903	0.3698763302434943	0.6142255188686718	T	T	T
0.1799797736488777	0.4977624208516988	0.5607986277034511	T	T	T
0.1961676106954398	0.6311974831348283	0.5598559202421848	T	T	T
0.9857999217692097	0.4534033918548803	0.7891700612927131	T	T	T
0.9837831484376416	0.6373398729027703	0.7786078147449812	T	T	T
0.1432448466517624	0.5643816480856186	0.2151806366170120	T	T	T
0.2005455037541873	0.5631271378687371	0.3919566951015653	T	T	T
0.2990524235958893	0.5495147683141006	0.5262131250128633	T	T	T
0.3943928069965359	0.5685500692315366	0.3895744660818476	T	T	T
0.3986259463736694	0.5545521619753011	0.1934393773229491	T	T	T
0.2717925513417353	0.5298865875891648	0.2326172075249761	T	T	T
0.1417993451335185	0.3245300349337645	0.2456705387931552	T	T	T
0.1928083874636616	0.3453852546273913	0.4209913804656143	T	T	T
0.3090983343682933	0.3534654339711989	0.5132277524989783	T	T	T
0.4104433683861298	0.3272637727545066	0.3903602462100465	T	T	T
0.3931128400284917	0.3429195737317699	0.1941578895683715	T	T	T
0.2703886512359115	0.3553195529274961	0.2592134599459612	T	T	T
0.1770067546333942	0.4479902864153896	0.2972473862866867	T	T	T
0.4135228819311564	0.4483619711773127	0.3134831973285476	T	T	T

Structure files (CONTCAR) involved in this work:

0.0691059469133897	0.6226282869116158	0.0747303372523966	T	T	T
0.0836477305576000	0.4910171373236136	0.0737179733285160	T	T	T
0.1149181787488581	0.3612890684570079	0.0589441957508897	T	T	T
0.3064788616487222	0.6268513270983249	0.1050633095886848	T	T	T
0.3235673222432286	0.4976367002660461	0.0557462682779753	T	T	T
0.2955540570138326	0.3658049482795230	0.0627095727759483	T	T	T
0.5090168909149090	0.5401191701879194	0.2946945565829544	T	T	T
0.5119677907762838	0.3617714111668219	0.2717129239072439	T	T	T
0.4396208201079524	0.7497531062748202	0.6386998684536536	T	T	T
0.1945325901818410	0.7477799507120531	0.6500891715265678	T	T	T
0.2722289527549447	0.7484014969926436	0.0544178069439927	T	T	T
0.1092256236650467	0.7475105377854296	0.0489976743398305	T	T	T
0.0656222325533893	0.2483978295682046	0.1309177185584665	T	T	T
0.3038712131883545	0.2481555749271954	0.1497378960737965	T	T	T
0.2279655063978065	0.2504142389530409	0.5520633651826706	T	T	T
0.3923220924925511	0.2509198882499405	0.5482672425706209	T	T	T
0.5578459479912362	0.2494166571147148	0.3541999231816187	T	T	T
0.8149100834108665	0.2518763562972738	0.3507067982714347	T	T	T
0.7277116460123418	0.2491108701121762	0.9426700433572817	T	T	T
0.8922414040632585	0.2512005044132147	0.9492342620654722	T	T	T
0.9456502838695744	0.7528213269479822	0.8591866184044149	T	T	T
0.6859960143195344	0.7527094596386841	0.8496116810734776	T	T	T
0.7755212973302048	0.7478859130962618	0.4462531779959333	T	T	T
0.6102820686878159	0.7500153393246137	0.4500795150029037	T	T	T
0.9221130266742879	0.4774097550446557	0.5354432600191884	T	T	T
0.8242236549403847	0.3354878535374992	0.3277826241353683	T	T	T
0.7995069860222266	0.6350081802619064	0.6960574486412116	T	T	T
0.9268411152366922	0.5326537408516732	0.1960323010988475	T	T	T
0.9220556395192027	0.4223713170929289	0.4202191753530467	T	T	T
0.8637049110916990	0.5536960604088318	0.5564961738984621	T	T	T
0.0045986095797394	0.5545664149949550	0.4070721654907314	T	T	T
0.0419530155487242	0.5216344687165506	0.5208222873265643	T	T	T
0.9514614836621301	0.4637309460329718	0.5900382966896297	T	T	T
0.0868117415053364	0.5267158522990113	0.4068706340301226	T	T	T
0.0220707420037150	0.4398545663032289	0.3248486204914476	T	T	T
0.0387762006263111	0.4048620113011709	0.4494140835609296	T	T	T
0.0371708437812696	0.5159381641962257	0.4398320715174462	T	T	T
0.0196340823566868	0.4476793105733433	0.4057589489156540	T	T	T

Figure S17 ZnPd-IS

Si O Al Pd Zn H C

1.0000000000000000

20.0219999999999985 0.0000000000000000 0.0000000000000000

0.0000000000000000 19.8990000000000009 0.0000000000000000

0.0000000000000000 0.0000000000000000 13.3829999999999991

93 193 3 1 1 6 2

Selective dynamics

Direct

0.4240221635106289	0.0571787760333591	0.6473991697090935	T	T	T
0.3046886196234119	0.0265666335498725	0.7919920492182539	T	T	T
0.2826332140771163	0.0600649760155477	0.0133869084722019	T	T	T
0.1233267290872297	0.0614100272651859	0.0111304553368132	T	T	T
0.0706877645285091	0.0291074817378118	0.7995894406946313	T	T	T
0.1804983488389093	0.0549343796833597	0.6550309807576976	T	T	T

Structure files (CONTCAR) involved in this work:

0.4205986442550527	0.8261678544461604	0.6676036489784001	T	T	T
0.3042280277598668	0.8684150420667820	0.8091940452016276	T	T	T
0.2663375501990216	0.8275004918133100	0.0273774954485099	T	T	T
0.1117152707729650	0.8259618715302214	0.0140964840197217	T	T	T
0.0660681475457063	0.8722472915578645	0.7996976285374796	T	T	T
0.1828591048322562	0.8279197839512965	0.6716205003073027	T	T	T
0.0767218426752060	0.9417327767497888	0.1483806521578373	T	T	T
0.1972646777339709	0.9717987650818689	0.2915762539992483	T	T	T
0.2194971892472637	0.9368682894487020	0.5131669640893850	T	T	T
0.3792574102965777	0.9344174036368875	0.5130285331593416	T	T	T
0.4325509476845423	0.9687017483545934	0.3006569027117235	T	T	T
0.3222119900279959	0.9429198705561941	0.1551851747745460	T	T	T
0.0814000342919569	0.1706897764079399	0.1654132051870058	T	T	T
0.1965590481431082	0.1300573703289588	0.3098187294291681	T	T	T
0.2340217382959820	0.1711191010181526	0.5263675799291611	T	T	T
0.3884959530521151	0.1732968336704992	0.5105877557734827	T	T	T
0.4368152084240076	0.1270464360482757	0.2976340247488763	T	T	T
0.3176238054516863	0.1701989227756701	0.1720895571218607	T	T	T
0.5759602068738788	0.5565532907559576	0.3550499733321520	T	T	T
0.6905496585492761	0.5249966269652607	0.2028776405602427	T	T	T
0.7161405531784211	0.5661746370357182	0.9867160087319414	T	T	T
0.8756900880333826	0.5712714452736740	0.9842450071106835	T	T	T
0.8105180266099433	0.5529536350841672	0.3419880171173186	T	T	T
0.5755938760500787	0.3273574850382787	0.3297538285304333	T	T	T
0.6947012842902340	0.3712788005216293	0.1893171909278087	T	T	T
0.7323347078719660	0.3270134337866027	0.9773839117698008	T	T	T
0.8873006852009581	0.3252316943435281	0.9921228602107466	T	T	T
0.9433091824335788	0.3707628787298100	0.1942320927309789	T	T	T
0.9204969940316965	0.4441672529716798	0.8567772726634970	T	T	T
0.8007862072266977	0.4724626661987580	0.7162817251385705	T	T	T
0.7754368715577076	0.4377955393501767	0.4916837869112201	T	T	T
0.6163849609271309	0.4305760329919394	0.4889253546883312	T	T	T
0.5682939758897912	0.4683813424740490	0.7025911118304665	T	T	T
0.6774121059951305	0.4466225088804328	0.8536455696983039	T	T	T
0.9194701923782310	0.6780502447911450	0.8260229170229482	T	T	T
0.7666665238821131	0.6690008528574817	0.4644765750650261	T	T	T
0.6125232130285158	0.6733368089638360	0.4891724171068182	T	T	T
0.5606340573337939	0.6264833390983591	0.6999261368047912	T	T	T
0.6746554531827089	0.6726226952608294	0.8261114625482326	T	T	T
0.5780308548951666	0.9441607337816045	0.3582966275465396	T	T	T
0.6981536480332163	0.9720988833656492	0.2141039916049271	T	T	T
0.7215535865479674	0.9362763486387558	0.9926632500155572	T	T	T
0.8818099588787445	0.9339058194415759	0.9947280443870711	T	T	T
0.9322967045340154	0.9706330385640592	0.2057560555025752	T	T	T
0.8225114472329299	0.9456456412147888	0.3545166294075904	T	T	T
0.5797650017176691	0.1726213696142564	0.3297498838798356	T	T	T
0.6985722393263344	0.1295945116208400	0.1925846762791898	T	T	T
0.7334398161566421	0.1706731602424212	0.9721385673495468	T	T	T
0.8879673447724969	0.1729340360518895	0.9830881961661172	T	T	T
0.9356851433628834	0.1288950505668340	0.1984352451792437	T	T	T
0.8192144206665090	0.1724659512426417	0.3295863048464961	T	T	T
0.9251195824494581	0.0541685197802455	0.8558658146064662	T	T	T
0.8036999901026842	0.0259707129168278	0.7090060085263821	T	T	T

Structure files (CONTCAR) involved in this work:

0.7823483793042577	0.0654101050526696	0.4916725964454842	T	T	T
0.6220010013617376	0.0687544223190785	0.4903795273737900	T	T	T
0.5689713601682381	0.0310122320152507	0.6996888513021080	T	T	T
0.6800904102047545	0.0527626802390894	0.8491985182347476	T	T	T
0.9238927453426353	0.8300438448679989	0.8362761744537812	T	T	T
0.8028940795103329	0.8687404838146002	0.6953545470819629	T	T	T
0.7693911158323496	0.8266585511109491	0.4789963906222592	T	T	T
0.6148700233414570	0.8268305442080293	0.4919778473099800	T	T	T
0.5642439056084060	0.8739521457983169	0.7000818975353829	T	T	T
0.6795646829221053	0.8317232646868467	0.8327866534291732	T	T	T
0.4230198360329914	0.4430664165747512	0.6445083802048389	T	T	T
0.3030927404434043	0.4715023181097295	0.7890035518007298	T	T	T
0.2778281956326110	0.4379678869124067	0.0098512368844209	T	T	T
0.1200768440566265	0.4354950611267260	0.0125777890922488	T	T	T
0.0649244563087644	0.4701087518060640	0.7993573577837509	T	T	T
0.1772585011777195	0.4445406220883154	0.6534826887332087	T	T	T
0.4176340228670988	0.6720115091043535	0.6631419779818263	T	T	T
0.3021778498679153	0.6288959555906294	0.8056382131092564	T	T	T
0.2661402715472342	0.6702302222294066	0.0237201019525718	T	T	T
0.1121726626632234	0.6724479856199170	0.0080941769700511	T	T	T
0.0620564671307683	0.6288179734147593	0.7952366147746074	T	T	T
0.1813045819622052	0.6695225901867139	0.6686495177339228	T	T	T
0.0789541834803333	0.5567890398406825	0.1462393676839064	T	T	T
0.1982904283168582	0.5243786352213068	0.2883647865396713	T	T	T
0.2167627375150856	0.5610425881286928	0.5110948268944512	T	T	T
0.3758848118174913	0.5651148468440008	0.5105433261954671	T	T	T
0.4295070292309294	0.5287727335805316	0.2992651315343041	T	T	T
0.3218516299122571	0.5533435888758044	0.1508182131943060	T	T	T
0.0860645591665466	0.3232592571642531	0.1607079503612894	T	T	T
0.1976320743781406	0.3670771590534804	0.3070076335660064	T	T	T
0.2327397665969018	0.3283856531950262	0.5254222735466784	T	T	T
0.3869228394635867	0.3270822689756619	0.5065733304339824	T	T	T
0.4336128835954793	0.3708903468448852	0.2924871594421086	T	T	T
0.3156023064569623	0.3287556349351475	0.1684288344716716	T	T	T
0.3584771571569076	0.0615776985403034	0.7182031435555561	T	T	T
0.3062168724514880	0.0662841420418639	0.8978491317056178	T	T	T
0.2027454414994163	0.0463783924834901	0.0203776694406425	T	T	T
0.1006365566376089	0.0688816342615238	0.8956716890063048	T	T	T
0.1049146566324993	0.0579628166548115	0.6983985745035999	T	T	T
0.2303119296025764	0.0313337269444521	0.7443396627787812	T	T	T
0.3596485317714123	0.8266708221194746	0.7471950319176697	T	T	T
0.3049590331878044	0.8410113388104515	0.9229657780431626	T	T	T
0.1889143827238592	0.8517472023739552	0.0175167404766791	T	T	T
0.0846726690678116	0.8308700133747903	0.9005297619752759	T	T	T
0.1053801028310245	0.8391059669407042	0.7050276422833357	T	T	T
0.2305353782099195	0.8560562087552507	0.7609755661933095	T	T	T
0.3232395268841417	0.9476950806243702	0.8072082913810066	T	T	T
0.0887698666783452	0.9498935357350068	0.8130804847026629	T	T	T
0.4320584007599846	0.1272243905220378	0.5861521502219684	T	T	T
0.4184894164913249	0.9954546974476116	0.5680582351194021	T	T	T
0.3982360632777723	0.8632717607327236	0.5648472332699628	T	T	T
0.2005105208802100	0.1294413951413962	0.6170083632950992	T	T	T
0.1828247380711644	0.0014170053517420	0.5632929742405502	T	T	T

Structure files (CONTCAR) involved in this work:

0.1978581822859531	0.8672939454833217	0.5678386860654089	T	T	T
0.9908941999865365	0.0401190886871168	0.7883368974529192	T	T	T
0.9860065759658455	0.8681490399187841	0.7806748463346580	T	T	T
0.1426681638307498	0.9373445036513683	0.2183999614106328	T	T	T
0.1966548144790236	0.9316803487134009	0.3971871135204278	T	T	T
0.2995802113632978	0.9480049211590782	0.5225640418177502	T	T	T
0.4016371585101416	0.9300536490655720	0.3971574293561380	T	T	T
0.3973030630029626	0.9398167664998534	0.2002122859773628	T	T	T
0.2712952014507012	0.9668796200332721	0.2429373065326803	T	T	T
0.1409834528998391	0.1708791399783595	0.2471206580093321	T	T	T
0.1935869114263085	0.1575055893886432	0.4235088809925469	T	T	T
0.3112089273119672	0.1476078546382846	0.5117352824116639	T	T	T
0.4173836359092722	0.1683802090796303	0.3980393746283076	T	T	T
0.3953672912590827	0.1586027822737938	0.2037106207557688	T	T	T
0.2705636738337563	0.1433535143352762	0.2632410239816930	T	T	T
0.1787495062244781	0.0504680576930349	0.3077695265647608	T	T	T
0.4171256496514674	0.0485591390862824	0.3122382002311457	T	T	T
0.0670281690269680	0.8704497674037249	0.0904453699781892	T	T	T
0.0830855728679915	0.0001389658450859	0.0639851479829261	T	T	T
0.1050668286829071	0.1313934862622812	0.0656659195632032	T	T	T
0.3023755370541514	0.8683220665797747	0.1167464264365085	T	T	T
0.3208692816575955	0.9962491938173691	0.0631811292119933	T	T	T
0.3013510774867519	0.1297514127692938	0.0696596369653300	T	T	T
0.5119774293624185	0.9546615773664807	0.2898777740642635	T	T	T
0.5166066388063918	0.1340907138231403	0.2776018920185606	T	T	T
0.6381973633859855	0.5605815929341325	0.2784684805252025	T	T	T
0.6979546980976561	0.5724030935529343	0.1049247556377182	T	T	T
0.7959033954764794	0.5565981385937292	0.9696548952254797	T	T	T
0.8967637078441404	0.5777328250029721	0.0993670570424324	T	T	T
0.8873382002406456	0.5452586191882884	0.3116987388670855	T	T	T
0.7625010870135808	0.5199615378154874	0.2594672633490610	T	T	T
0.6418731957801631	0.3330526508577545	0.2623268718669369	T	T	T
0.6899991763545261	0.3359672353842403	0.0795524594150055	T	T	T
0.8097590467326979	0.3502732280495367	0.9940524967045924	T	T	T
0.9175782221854929	0.3213757741013071	0.1045342029233295	T	T	T
0.9073922146859251	0.3474600920085974	0.2985915945339011	T	T	T
0.7688738322391465	0.3672606304073605	0.2333368468255343	T	T	T
0.6682091529745062	0.4490187821632886	0.1761170579541230	T	T	T
0.9284948436166002	0.4468044060766144	0.1635819670424553	T	T	T
0.5688017187031411	0.6279065228821037	0.4126844137613491	T	T	T
0.5856084916379144	0.4979670270726253	0.4385430858779999	T	T	T
0.5850765941470950	0.3640941590605594	0.4377454899458311	T	T	T
0.7920825745437805	0.6313555031678371	0.3634658139954733	T	T	T
0.7993840504464749	0.5148033641185138	0.4535016487378944	T	T	T
0.8197567164621784	0.3841443518287629	0.4323244345265160	T	T	T
0.0132228460907379	0.5557011448980297	0.2271379948169869	T	T	T
0.0236272451262059	0.3613798356828508	0.2115630791553716	T	T	T
0.8554900485550497	0.4341538785782951	0.7847704997732995	T	T	T
0.7940615064015581	0.4337445966806115	0.6094487173420379	T	T	T
0.6967626814405591	0.4302522940677058	0.4705482383400121	T	T	T
0.5999604195849019	0.4288112908488057	0.6071648049734194	T	T	T
0.6033991893618282	0.4419236759199214	0.8045343936030883	T	T	T
0.7284111151999786	0.4751359681617270	0.7684467247902120	T	T	T

Structure files (CONTCAR) involved in this work:

0.8605515036911070	0.6826323192250270	0.7461542323361602	T	T	T
0.8145008075016547	0.6430200443889551	0.5574254675534676	T	T	T
0.6900856248699047	0.6475893733686743	0.4899693655472119	T	T	T
0.5823208162044567	0.6679841637121403	0.6006447315632722	T	T	T
0.5960046096479401	0.6593134235725523	0.7975780878183392	T	T	T
0.7203398294392387	0.6478531854838764	0.7338974318141851	T	T	T
0.8265208934812707	0.5489851507360445	0.6914321224734450	T	T	T
0.5817962405616810	0.5481602904641933	0.6870361630139724	T	T	T
0.9306704000896502	0.3765058320967768	0.9228107506982234	T	T	T
0.9145509458821587	0.5091896761307544	0.9285523983513607	T	T	T
0.8963168714377058	0.6404835766502889	0.9279944615199743	T	T	T
0.6998863188134622	0.3723330738584336	0.8889085731955123	T	T	T
0.6772297701668238	0.4995334821661391	0.9457574066512022	T	T	T
0.6909221242358883	0.6333247474718824	0.9301780347972758	T	T	T
0.4889283595576861	0.4527235902308757	0.7132187425091436	T	T	T
0.4798247864250495	0.6313696039647860	0.7125807834199832	T	T	T
0.6427472115588262	0.9377645566499451	0.2862289761134041	T	T	T
0.7002310411574070	0.9312588654098075	0.1092462455685293	T	T	T
0.8019998938314103	0.9441508475607877	0.9803534679393047	T	T	T
0.9012089154802505	0.9289858412275798	0.1120568557917373	T	T	T
0.8977516916553859	0.9460667997023778	0.3091664072206338	T	T	T
0.7711294688337740	0.9670948977024634	0.2662171993752755	T	T	T
0.6424419341588165	0.1714092538492323	0.2536629422972330	T	T	T
0.6974446825726723	0.1569644121188674	0.0786458109251084	T	T	T
0.8110361257834943	0.1463277046018280	0.9789437794300759	T	T	T
0.9149799758546070	0.1680615880664156	0.0967928739111859	T	T	T
0.8966715244934772	0.1600774799985863	0.2937812921412337	T	T	T
0.7718576751349184	0.1397539961276496	0.2417594557623035	T	T	T
0.6788211305040938	0.0502247637055275	0.1947517177834234	T	T	T
0.9180288115322275	0.0496823213165365	0.1859466150279515	T	T	T
0.5694430603509839	0.8749693206499132	0.4218025016018615	T	T	T
0.5841188718019930	0.0062154546595620	0.4365880922672523	T	T	T
0.5998433851657158	0.1380364030740073	0.4356924580718983	T	T	T
0.8075465100565478	0.8700715116713192	0.3943606604373293	T	T	T
0.8175082797673985	0.9980157451643621	0.4469712891670528	T	T	T
0.8072882701284027	0.1319009245015133	0.4340557244939728	T	T	T
0.0118523765979743	0.9558609291602376	0.2175112835824183	T	T	T
0.0158206614744936	0.1370016155824496	0.2160281870000589	T	T	T
0.8599697560595040	0.0545924961102963	0.7845390765740038	T	T	T
0.8035018627815639	0.0716774784831738	0.6085924362609447	T	T	T
0.7018086530161184	0.0570490062669927	0.4806343975561541	T	T	T
0.5997694797108114	0.0739499533134311	0.6068779244833076	T	T	T
0.6048736623545627	0.0509556374680651	0.8041570510585033	T	T	T
0.7307230796790081	0.0292991507031310	0.7611695470266977	T	T	T
0.8590382093333367	0.8345914001484612	0.7650428707353316	T	T	T
0.8058173117903454	0.8325326305304059	0.5867972598837476	T	T	T
0.6922977363481502	0.8522040935751029	0.4876863151886640	T	T	T
0.5886196172954989	0.8280055010042459	0.6065356479028435	T	T	T
0.6034175402335539	0.8513700669098500	0.8008609532778891	T	T	T
0.7293292224222955	0.8580429319502914	0.7443217491714140	T	T	T
0.8190534252816996	0.9480682814480511	0.6811030936428419	T	T	T
0.5800627528989797	0.9519159973929430	0.6739343875002498	T	T	T
0.9333696858668086	0.1270867015140068	0.9090828490154674	T	T	T

Structure files (CONTCAR) involved in this work:

0.9198120772261081	0.9971344535933686	0.9427595822442874	T	T	T
0.9069031165460548	0.8645349951503751	0.9433719015581395	T	T	T
0.6959376344234791	0.1288995599882425	0.8846563271796787	T	T	T
0.6857579320392994	0.0020035899184895	0.9440484395726602	T	T	T
0.6975532474310383	0.8677804462094587	0.9380701232520786	T	T	T
0.4900434181586357	0.0468053964462034	0.7155413484692885	T	T	T
0.4845746009747681	0.8633979165254189	0.7178698548889131	T	T	T
0.3577261558104051	0.4365280332486438	0.7162010360065735	T	T	T
0.3007521543456472	0.4305439709384649	0.8940816562823826	T	T	T
0.1984468270286634	0.4571080421633670	0.0176083555763529	T	T	T
0.0936892503515735	0.4333344261139605	0.8987165935915201	T	T	T
0.1024044739903490	0.4416431336463088	0.7002121336820707	T	T	T
0.2291757094134856	0.4689844654183929	0.7391266679962847	T	T	T
0.3556329353737673	0.6710497555066862	0.7408883770185568	T	T	T
0.3040635404521566	0.6582455034325730	0.9183564422339412	T	T	T
0.1888441552375179	0.6455396706493313	0.0119002885802062	T	T	T
0.0844019010413069	0.6695374588623673	0.8950785649505262	T	T	T
0.1034901231456628	0.6580160091764473	0.6997617421909341	T	T	T
0.2279582395431224	0.6382016157830365	0.7572147901298342	T	T	T
0.3226343890284418	0.5498461637527307	0.8072488388574991	T	T	T
0.0797139827815383	0.5498915716254693	0.8107289225369814	T	T	T
0.4316698022464373	0.3753169782139489	0.5778627895952236	T	T	T
0.4169528958166362	0.5065927271320355	0.5683435290899203	T	T	T
0.3940336618260011	0.6377409561089514	0.5583875282916654	T	T	T
0.1967556019588422	0.3702813270360620	0.6141154186845563	T	T	T
0.1771769556341473	0.4979726374635346	0.5610368320697229	T	T	T
0.1954128143799993	0.6315975495714204	0.5628239604767793	T	T	T
0.9857705420882801	0.4545199939187407	0.7844133468711503	T	T	T
0.9829411059927591	0.6378142986481108	0.7751962162936819	T	T	T
0.1453625188461477	0.5616924671798710	0.2140364565981277	T	T	T
0.1952790615557611	0.5644772066364258	0.3938830770391518	T	T	T
0.2965269766857362	0.5488817629793296	0.5227736523284408	T	T	T
0.3962085925350759	0.5678087401274575	0.3936416172576201	T	T	T
0.3967307790277119	0.5565322090380749	0.1961283538133163	T	T	T
0.2720709739866277	0.5288841917161420	0.2403166794936527	T	T	T
0.1467259375001563	0.3227019005357875	0.2410293079012367	T	T	T
0.1928850388159200	0.3416285179395018	0.4215175993705605	T	T	T
0.3096624564606453	0.3532057132210569	0.5119699941430700	T	T	T
0.4123021273250039	0.3285922530714546	0.3915059950443683	T	T	T
0.3936891654982916	0.3432586068705086	0.1945067054347265	T	T	T
0.2728152359792118	0.3567183124008786	0.2639121185985828	T	T	T
0.1764984934849120	0.4463422386527576	0.3016467787006207	T	T	T
0.4148096428675543	0.4490968232810338	0.3123843829997039	T	T	T
0.0679774655121564	0.6239858641137973	0.0810388369016249	T	T	T
0.0764240860238274	0.4902294681219059	0.0778976123162341	T	T	T
0.1100482667325836	0.3614036429260065	0.0592179873560481	T	T	T
0.3012641887089143	0.6274539736239529	0.1120465347745119	T	T	T
0.3195471390120823	0.4995569273058237	0.0595744865341000	T	T	T
0.2928184229324875	0.3676165571687162	0.0669676020002346	T	T	T
0.5087740710706739	0.5428152023302198	0.2913194440380469	T	T	T
0.5129268272701869	0.3621498789518716	0.2711164556805586	T	T	T
0.4387649719048871	0.7489691310157276	0.6399474439768661	T	T	T
0.1968816435973486	0.7485955263259032	0.6525257087028532	T	T	T

Structure files (CONTCAR) involved in this work:

0.2695907985219133	0.7484086986184180	0.0556220967072313	T	T	T
0.1066616903350128	0.7482292227758534	0.0508214739100868	T	T	T
0.0662971412911553	0.2472442945796624	0.1309541415438977	T	T	T
0.3031996907538708	0.2492453449119015	0.1511177154095349	T	T	T
0.2296659281662994	0.2499380911597986	0.5557118538525579	T	T	T
0.3928350324044345	0.2507579109242535	0.5480095301706822	T	T	T
0.5586793407528740	0.2494896172270361	0.3531281744998690	T	T	T
0.8037972326795993	0.2500376082312703	0.3470372445963052	T	T	T
0.7289526117054649	0.2492860855232869	0.9416350750329827	T	T	T
0.8924900374112137	0.2501962650734782	0.9445882417269711	T	T	T
0.9449507228353413	0.7528975063466580	0.8574578014714457	T	T	T
0.6860795314481603	0.7518461096090593	0.8491313693005921	T	T	T
0.7729349879087991	0.7485680356740453	0.4448056337439850	T	T	T
0.6091055077464892	0.7504244466200588	0.4505728712008069	T	T	T
0.9450808347634045	0.5006695694284109	0.5251733886997613	T	T	T
0.8205920689472718	0.3329601425963136	0.3232862720731310	T	T	T
0.7997748241893330	0.6355400427757525	0.6909092417878541	T	T	T
0.9240944184713588	0.5290020910233368	0.1966674815483234	T	T	T
0.9331634546882169	0.4075320939253566	0.4339841932881414	T	T	T
0.8713365948556029	0.5563450690086421	0.5537522953748567	T	T	T
0.9849111491135761	0.6438918212938372	0.3031574382636911	T	T	T
0.0028178247742361	0.5717729090035938	0.3807441424985862	T	T	T
0.9687281802677784	0.4865707464385873	0.5856031828456257	T	T	T
0.0700273330852291	0.6178956782912938	0.3229080644150315	T	T	T
0.0589378746363960	0.4373794501550614	0.4691015365588826	T	T	T
0.0489201066892945	0.3522709692248120	0.4117072800768554	T	T	T
0.0182599285452527	0.6009876092425647	0.3153300911405009	T	T	T
0.0257553201637155	0.3952131025013746	0.4500282564736074	T	T	T

Figure S17 ZnPd-TS

Si O Al Pd Zn H C

1.0000000000000000

20.0219999999999985 0.0000000000000000 0.0000000000000000

0.0000000000000000 19.8990000000000009 0.0000000000000000

0.0000000000000000 0.0000000000000000 13.3829999999999991

93 193 3 1 1 6 2

Selective dynamics

Direct

0.4241333936805568	0.0566965949388104	0.6466758775319218	T	T	T
0.3037771150239818	0.0255906681801306	0.7900012024125296	T	T	T
0.2828799416683996	0.0590281006368185	0.0120980007639117	T	T	T
0.1234942596338956	0.0610129655917610	0.0110119305634804	T	T	T
0.0710011265174686	0.0284556044742638	0.7995410247543885	T	T	T
0.1793352753010015	0.0547430760562468	0.6527406949949836	T	T	T
0.4208653727084360	0.8263849475249138	0.6664901319666615	T	T	T
0.3039835280636011	0.8670697184880921	0.8083120455933249	T	T	T
0.2670847899511237	0.8263676236027495	0.0270179148985513	T	T	T
0.1125308827967803	0.8242802887339713	0.0135173944389328	T	T	T
0.0664007329891144	0.8715781305021810	0.7995261595911104	T	T	T
0.1823431516424361	0.8270208345689679	0.6698225980099484	T	T	T
0.0773618150838536	0.9406093409717592	0.1470949599188876	T	T	T
0.1978511784370783	0.9716589293220044	0.2896941617267916	T	T	T
0.2191199574982971	0.9370140065791918	0.5119921734353657	T	T	T
0.3786413663731347	0.9346915997396387	0.5122453492404749	T	T	T

Structure files (CONTCAR) involved in this work:

0.4322935301536418	0.9683394772273483	0.3003344616354213	T	T	T
0.3227482555223472	0.9422885597883458	0.1535644547770832	T	T	T
0.0816761513311768	0.1713075265606998	0.1637571317328967	T	T	T
0.1971262884247768	0.1298196371121089	0.3072610643536883	T	T	T
0.2334433100520690	0.1709576965005919	0.5247672736562650	T	T	T
0.3880849327903884	0.1730949009312407	0.5110378393999113	T	T	T
0.4370054285825123	0.1267359262243289	0.2982614615229116	T	T	T
0.3188382781986858	0.1691561124995566	0.1703100237404555	T	T	T
0.5770979494054718	0.5561256406345987	0.3541491367725146	T	T	T
0.6917914532980447	0.5248369555253121	0.2021547634487029	T	T	T
0.7164779017078871	0.5667463034144649	0.9856633983218399	T	T	T
0.8747987263706319	0.5715388076236165	0.9868870033014301	T	T	T
0.8113597302974073	0.5525787803773420	0.3436563300839438	T	T	T
0.5748320237346338	0.3276379163861780	0.3311695076027233	T	T	T
0.6958273151675829	0.3708292624200398	0.1923247081445102	T	T	T
0.7303780052095137	0.3261614336118368	0.9788989845249519	T	T	T
0.8848384384383654	0.3252335788059905	0.9934341220932443	T	T	T
0.9403371782769848	0.3735433898261504	0.1903308285028211	T	T	T
0.9210769029047817	0.4443512177810825	0.8609607517825655	T	T	T
0.8003634913314260	0.4714163874983614	0.7206042405570277	T	T	T
0.7759980024864340	0.4366762504770905	0.4950052575358153	T	T	T
0.6177472892071808	0.4297361207633322	0.4894336061301380	T	T	T
0.5679185222856877	0.4691483688883334	0.7022131883649754	T	T	T
0.6750291957798545	0.4463064611845747	0.8563678702798930	T	T	T
0.9203523715658429	0.6775690554230289	0.8295230313183661	T	T	T
0.7679778139194759	0.6688979181650729	0.4668005932501374	T	T	T
0.6136491369191311	0.6731826997140271	0.4889816812801682	T	T	T
0.5604493252131882	0.6271880064669126	0.6994343718831193	T	T	T
0.6737028595929433	0.6731844640632877	0.8271686709153254	T	T	T
0.5779755065303499	0.9443315004024923	0.3594103487119920	T	T	T
0.6990495909844718	0.9726234326150694	0.2161568517689879	T	T	T
0.7213718239785415	0.9363453981999234	0.9941651897097812	T	T	T
0.8816324876049866	0.9336971357041545	0.9959678225868780	T	T	T
0.9332710654109296	0.9701282041091769	0.2059084964883642	T	T	T
0.8239804577079821	0.9455813585360333	0.3561766042641986	T	T	T
0.5800483461903246	0.1727531622664504	0.3306916764872824	T	T	T
0.6991831311090653	0.1308823165459842	0.1936742741719778	T	T	T
0.7330673305273082	0.1702427134589193	0.9724714591623754	T	T	T
0.8876661586216210	0.1729483643463237	0.9844906383300343	T	T	T
0.9365790553707942	0.1283824151770642	0.1988459577274091	T	T	T
0.8207021130273700	0.1726252066812863	0.3314031206574598	T	T	T
0.9252208053051140	0.0542293022306873	0.8575562026661209	T	T	T
0.8041582837565311	0.0258138601255868	0.7103624414726629	T	T	T
0.7824079399393125	0.0650326910362900	0.4927971131268399	T	T	T
0.6223119463409970	0.0685781930858053	0.4909953267798881	T	T	T
0.5692953657502630	0.0307518347397121	0.6995237515012714	T	T	T
0.6800709792352996	0.0521869760619640	0.8497739976489594	T	T	T
0.9243582234932177	0.8297483878233627	0.8376652749306844	T	T	T
0.8033392067374121	0.8688542918928480	0.6975828046624195	T	T	T
0.7708155965121315	0.8266066665294857	0.4804268240179292	T	T	T
0.6161914079405313	0.8266288724294367	0.4919546635231908	T	T	T
0.5650131788438705	0.8739320696029123	0.6994422004449277	T	T	T
0.6793841334204226	0.8322742724907127	0.8341288465391419	T	T	T

Structure files (CONTCAR) involved in this work:

0.4234604193924323	0.4438831486760739	0.6395715768927750	T	T	T
0.3032094236621409	0.4715235299100733	0.7847865658140820	T	T	T
0.2815441068758853	0.4361771486279034	0.0042424434675567	T	T	T
0.1239234413653702	0.4350809089963668	0.0085496207960393	T	T	T
0.0655650234689875	0.4694383705667451	0.7985559905721301	T	T	T
0.1766843829604357	0.4445169170565494	0.6510304774692897	T	T	T
0.4178121614103599	0.6724015662444787	0.6602068555191355	T	T	T
0.3015687142975498	0.6290671551593355	0.8020752558197137	T	T	T
0.2671685915514818	0.6694700806152375	0.0211232014307396	T	T	T
0.1128151416324101	0.6703688935960970	0.0080041422929638	T	T	T
0.0625546306139824	0.6283083138863977	0.7951834948530326	T	T	T
0.1801847631905555	0.6686658064022880	0.6652219097677524	T	T	T
0.0760877438690199	0.5548727718973810	0.1471932139097017	T	T	T
0.1988106740680340	0.5248297817795681	0.2834270768834017	T	T	T
0.2182277486320148	0.5604727348729689	0.5088450253134834	T	T	T
0.3763954380524542	0.5656433197457166	0.5081719316615302	T	T	T
0.4287112881854455	0.5276199187036612	0.2987866544684413	T	T	T
0.3237965336704277	0.5514123074365475	0.1455595590659078	T	T	T
0.0854881571032952	0.3243862195025011	0.1556005800217622	T	T	T
0.1966533213184461	0.3671784408093773	0.3044152598177870	T	T	T
0.2321604048750180	0.3282728491157010	0.5236838795791321	T	T	T
0.3863323455958955	0.3266054206885676	0.5055698066308268	T	T	T
0.4326447210909075	0.3700647711563338	0.2922099339180505	T	T	T
0.3158164050160576	0.3275295811176819	0.1645219087880840	T	T	T
0.3586120180400599	0.0601550098700321	0.7174916190996794	T	T	T
0.3045732285630496	0.0653828057979484	0.8958118966824116	T	T	T
0.2029293129138504	0.0466274653279834	0.0224521189677917	T	T	T
0.1021644314350240	0.0680511941056335	0.8949100094127296	T	T	T
0.1041015853745361	0.0575396332165535	0.6975619452111458	T	T	T
0.2299075517454213	0.0310415057670576	0.7409680591924618	T	T	T
0.3605382064599398	0.8263295268166861	0.7470297179140760	T	T	T
0.3053605642375091	0.8403893185127973	0.9223533128671022	T	T	T
0.1896727399785884	0.8505300731085494	0.0172396526862439	T	T	T
0.0856017044671880	0.8301203530042252	0.8998449704027673	T	T	T
0.1051164931184916	0.8386924064949901	0.7040868874103697	T	T	T
0.2307211719694048	0.8531429088208945	0.7597318625154255	T	T	T
0.3215294491519846	0.9466731923234568	0.8055368147614063	T	T	T
0.0891804148716791	0.9493011608258641	0.8123630749539107	T	T	T
0.4318903054260427	0.1272810557055131	0.5866596105563442	T	T	T
0.4187724072957582	0.9956913481950582	0.5660469292634125	T	T	T
0.3976651384438919	0.8636927453351064	0.5643524427316898	T	T	T
0.1987283270843212	0.1294162321257506	0.6145478933702986	T	T	T
0.1812659332373386	0.0014436524474128	0.5606849181414243	T	T	T
0.1975963712475116	0.8675864744377352	0.5670438763979516	T	T	T
0.9911070321704523	0.0398386507668646	0.7905035900572858	T	T	T
0.9861765853497728	0.8678640734464932	0.7813986273667177	T	T	T
0.1435281199853257	0.9366431388188998	0.2167683424375241	T	T	T
0.1976625130875738	0.9316608106173292	0.3954509660646737	T	T	T
0.2991100953114104	0.9488095076823532	0.5231857844039950	T	T	T
0.4002277085240806	0.9297138896334727	0.3960360447352602	T	T	T
0.3978520333902972	0.9399609318473882	0.1989443720823939	T	T	T
0.2718716923278170	0.9672401450717401	0.2408070856104430	T	T	T
0.1422675480490950	0.1713627082739619	0.2439077631483171	T	T	T

Structure files (CONTCAR) involved in this work:

0.1941940243842860	0.1574354357793791	0.4208682934383687	T	T	T
0.3108128237272029	0.1473389026205277	0.5125356826007474	T	T	T
0.4168621432575936	0.1679882913830094	0.3984157243914974	T	T	T
0.3964114540145127	0.1583360438468188	0.2035701997758321	T	T	T
0.2713529637450277	0.1424942683425608	0.2611264020203570	T	T	T
0.1787546036552184	0.0503394913698498	0.3054954744955218	T	T	T
0.4172983267851575	0.0482487101551013	0.3123093826791053	T	T	T
0.0678003961308732	0.8694009571565533	0.0892384761360434	T	T	T
0.0831311704897733	0.9996430649565843	0.0633541594377701	T	T	T
0.1039555106251434	0.1312613457584860	0.0640008827625202	T	T	T
0.3031037194285914	0.8674038186526054	0.1164066653795371	T	T	T
0.3212303646754576	0.9947671175918787	0.0603970659692995	T	T	T
0.3035242705423971	0.1282571922338985	0.0680437112939157	T	T	T
0.5117659912380258	0.9539957684526473	0.2911367383251948	T	T	T
0.5169431625518238	0.1337762747305626	0.2793794428574359	T	T	T
0.6366345653041563	0.5606128176987006	0.2729704338600593	T	T	T
0.7021413767101539	0.5722045674573399	0.1049866272090870	T	T	T
0.7955723789394619	0.5577443660554633	0.9618966108184098	T	T	T
0.8895973709654976	0.5774332446591380	0.1036925784553498	T	T	T
0.8881868305331371	0.5435940193660795	0.3155336517949957	T	T	T
0.7616317842253432	0.5196561961652191	0.2639276639321002	T	T	T
0.6418539870077312	0.3346747284261465	0.2656901026922489	T	T	T
0.6916685140997673	0.3327309969030309	0.0846340181511115	T	T	T
0.8077127571943238	0.3511123629771392	0.9896861496696089	T	T	T
0.9104423723966434	0.3204095368155028	0.1088123034092274	T	T	T
0.9107039528449800	0.3519690749178135	0.3021811240883903	T	T	T
0.7694991167282187	0.3669460673882388	0.2388471999874487	T	T	T
0.6707887233314239	0.4485292549372979	0.1743779898998511	T	T	T
0.9193605671281844	0.4477348953898175	0.1615771725453496	T	T	T
0.5706026062421750	0.6275001498143418	0.4119805057695575	T	T	T
0.5914327439754793	0.4982237649984991	0.4372583382251853	T	T	T
0.5831970713011255	0.3645620181260538	0.4393769939167178	T	T	T
0.7938751918328996	0.6309303365686683	0.3665686208830239	T	T	T
0.7983779149549867	0.5139657521643001	0.4560177373991532	T	T	T
0.8240261300488307	0.3847351916684632	0.4364706011621877	T	T	T
0.0121574010613542	0.5479737901569741	0.2194350310061104	T	T	T
0.0211997420057139	0.3644949500935850	0.1980875274112337	T	T	T
0.8563560506323655	0.4340033672934502	0.7877158946044601	T	T	T
0.7942071583643587	0.4331313644698226	0.6128015263068322	T	T	T
0.6984180662731702	0.4243540685635851	0.4719250545714005	T	T	T
0.6014712584387664	0.4299706834843560	0.6077071902635139	T	T	T
0.6015770528258263	0.4429141981887909	0.8053415399011860	T	T	T
0.7278692352583523	0.4721984208440232	0.7716819663316631	T	T	T
0.8603381256968969	0.6814927449646542	0.7511197707200346	T	T	T
0.8152203211761390	0.6424798795004752	0.5608816160706003	T	T	T
0.6913129436195597	0.6475023965934052	0.4912928564431689	T	T	T
0.5828188314675693	0.6681911014957719	0.6000674079267377	T	T	T
0.5951974325514127	0.6604006131497002	0.7973131284718938	T	T	T
0.7197054367189457	0.6476632760928005	0.7356501237948607	T	T	T
0.8251504082281994	0.5482205089459394	0.6950856626202627	T	T	T
0.5817550775747423	0.5488520582794537	0.6872541968078805	T	T	T
0.9306487705652923	0.3766587824949057	0.9277155662593377	T	T	T
0.9151532259051384	0.5095408393223433	0.9319013035282797	T	T	T

Structure files (CONTCAR) involved in this work:

0.8987135116264552	0.6405291277872217	0.9324338288052587	T	T	T
0.6941703682263577	0.3716490100582692	0.8940940753663390	T	T	T
0.6759674328179754	0.5003778491071554	0.9467798999825772	T	T	T
0.6888584560279736	0.6339785156635597	0.9316461635412470	T	T	T
0.4885827683668392	0.4529285531082614	0.7102094577943747	T	T	T
0.4796296769471863	0.6318916856673170	0.7110077279249805	T	T	T
0.6428538697601430	0.9390375130823433	0.2876086208335323	T	T	T
0.7003889442830994	0.9321757405757622	0.1109474721981012	T	T	T
0.8017864058495786	0.9436268361126965	0.9811373899970561	T	T	T
0.9007234140437014	0.9284681797166121	0.1133794562723054	T	T	T
0.8990067505405679	0.9470869547526891	0.3103017244747898	T	T	T
0.7718572032272292	0.9659917294593600	0.2682981836359516	T	T	T
0.6422856390473956	0.1722801072883408	0.2537767372408857	T	T	T
0.6971350510277864	0.1566198232570272	0.0790001659283770	T	T	T
0.8107699706314119	0.1462792940840608	0.9797486296747810	T	T	T
0.9145522267973132	0.1682203188642423	0.0983114134171561	T	T	T
0.8975790210212589	0.1576660808043989	0.2956037855294362	T	T	T
0.7722171388770734	0.1437916402727143	0.2422704180057291	T	T	T
0.6812621350818400	0.0511996205111889	0.1979635738432265	T	T	T
0.9200663524618888	0.0492056186789584	0.1845708010861113	T	T	T
0.5703592637199139	0.8749030750049456	0.4226243807210937	T	T	T
0.5833757644426012	0.0064936969009007	0.4377450966209015	T	T	T
0.6011993926798790	0.1381517606312939	0.4361554469427526	T	T	T
0.8101132391828220	0.8699843578608031	0.3969450663874983	T	T	T
0.8185967827144379	0.9982198023986956	0.4483033340358206	T	T	T
0.8065318757270302	0.1318287563320597	0.4349078897775343	T	T	T
0.0126331626010818	0.9544354047031052	0.2167663587534821	T	T	T
0.0165215744513403	0.1380128600168218	0.2162337380389455	T	T	T
0.8602617712741640	0.0550667340921920	0.7856289497030371	T	T	T
0.8032492799442345	0.0715525751876712	0.6098403339145789	T	T	T
0.7019929927831348	0.0557558797529575	0.4811458984559701	T	T	T
0.6003480116586856	0.0743464583488207	0.6075456907055018	T	T	T
0.6049212033465521	0.0503117837761766	0.8043849303454411	T	T	T
0.7310841025256087	0.0284072003832656	0.7624008322537318	T	T	T
0.8591281708920905	0.8339129323601953	0.7669641365499379	T	T	T
0.8058010903086716	0.8324465855884047	0.5892051092741627	T	T	T
0.6935922607733898	0.8519952315350416	0.4866332381648770	T	T	T
0.5905727679549539	0.8276325145041397	0.6069059200196103	T	T	T
0.6033996138398556	0.8518411483099976	0.8011700036443692	T	T	T
0.7297102548939148	0.8591597139289007	0.7467746437763152	T	T	T
0.8203386417317490	0.9480080765830065	0.6828242983039972	T	T	T
0.5809444615474975	0.9518558847390088	0.6729408661846182	T	T	T
0.9333688189419101	0.1273152023023936	0.9106167343757242	T	T	T
0.9192167874100545	0.9974364817005179	0.9445819533234486	T	T	T
0.9073673449200926	0.8647198617598113	0.9443795536834769	T	T	T
0.6958774601572596	0.1284151959921909	0.8848339789615642	T	T	T
0.6855723110653180	0.0019297055331366	0.9451275212895247	T	T	T
0.6966328388345249	0.8678424041590483	0.9401287860549010	T	T	T
0.4902299695805557	0.0461471281804738	0.7146918636966351	T	T	T
0.4852193747011908	0.8635365146175700	0.7158269091669933	T	T	T
0.3568614557829899	0.4386746751306955	0.7083488481680522	T	T	T
0.3046147905413409	0.4288404532708487	0.8883285879969455	T	T	T
0.2026092372283161	0.4554953177632291	0.0104555209613306	T	T	T

Structure files (CONTCAR) involved in this work:

0.0966231791427733	0.4309882438321485	0.8945719291093736	T	T	T
0.1010102583321385	0.4428003014465973	0.6960401101955879	T	T	T
0.2283399897083917	0.4681042214065450	0.7375667190064678	T	T	T
0.3549602362805580	0.6706208283688575	0.7361687815464761	T	T	T
0.3036852910144197	0.6595080820127888	0.9139767510690929	T	T	T
0.1900822289618558	0.6445246622872520	0.0114309921701517	T	T	T
0.0867229382130068	0.6693553149177508	0.8933440323079934	T	T	T
0.1026509888416916	0.6562433937865704	0.6973174404839538	T	T	T
0.2274543829874979	0.6380433283555211	0.7534745421459526	T	T	T
0.3215959096027664	0.5498850663500920	0.8050018659243627	T	T	T
0.0794630240681060	0.5491441227906869	0.8109615703007961	T	T	T
0.4320625309821330	0.3755597579099045	0.5742740718997360	T	T	T
0.4197335813917110	0.5072451002754829	0.5627568535690137	T	T	T
0.3958726887810503	0.6383174961113005	0.5545132322000629	T	T	T
0.1951339594528136	0.3698552947106895	0.6118853650662822	T	T	T
0.1776662125269940	0.4972677671680075	0.5575170909224301	T	T	T
0.1943799094585524	0.6306474262114712	0.5593908245817857	T	T	T
0.9858753370447997	0.4533211250155684	0.7865712647695903	T	T	T
0.9831740954303799	0.6375366598220013	0.7766016706228915	T	T	T
0.1441072717875134	0.5623758466904168	0.2142117814432399	T	T	T
0.2003720167268214	0.5637769521456367	0.3905927693375262	T	T	T
0.2976503215666637	0.5490450730467906	0.5266903155249691	T	T	T
0.3930422565711292	0.5679823020780631	0.3899819898057745	T	T	T
0.3981453073717695	0.5541518331507992	0.1936055648542363	T	T	T
0.2719661447956642	0.5272227325664125	0.2323608219997954	T	T	T
0.1414266565077972	0.3246625608799953	0.2433912457907047	T	T	T
0.1933037747766550	0.3417692991818027	0.4191398538673005	T	T	T
0.3092258338532754	0.3530636963293837	0.5120055549900233	T	T	T
0.4107815319443751	0.3267723573391136	0.3900071749384781	T	T	T
0.3932458843320665	0.3428618667796734	0.1937052000301369	T	T	T
0.2703616999972565	0.3547208169610694	0.2575488154726728	T	T	T
0.1773404896374953	0.4466845696934588	0.3001928807942796	T	T	T
0.4136461908594681	0.4480459676072548	0.3135655136396717	T	T	T
0.0680494292974325	0.6219199953941599	0.0781789091318207	T	T	T
0.0823965515103482	0.4900950579300867	0.0725406120674987	T	T	T
0.1147367076786345	0.3605062553041253	0.0560077044239999	T	T	T
0.3048706696858427	0.6257477565901856	0.1060664574449920	T	T	T
0.3236953499044827	0.4972780565979359	0.0545898547244700	T	T	T
0.2957497240963577	0.3655903132265169	0.0613696050422693	T	T	T
0.5082320326274804	0.5409052957064507	0.2956763542334071	T	T	T
0.5121743896804597	0.3616548768286205	0.2716463599568751	T	T	T
0.4391239047109339	0.7493946548334154	0.6379041526414578	T	T	T
0.1950948178842306	0.7478027250667431	0.6481663156972278	T	T	T
0.2712054572623983	0.7473431581972559	0.0551919075965664	T	T	T
0.1077784067051229	0.7467123847097792	0.0498631544932804	T	T	T
0.0659080017788615	0.2477600513154766	0.1289245786666310	T	T	T
0.3041963561222851	0.2478831540766878	0.1477527387455173	T	T	T
0.2287984494333630	0.2498085044647780	0.5538486033207491	T	T	T
0.3923268876589046	0.2506184604030904	0.5483366557647279	T	T	T
0.5587324435216403	0.2495633815395684	0.3543691218052885	T	T	T
0.8092753337124156	0.2507240526790716	0.3515511659927985	T	T	T
0.7278389066361214	0.2487805230076592	0.9415629967567285	T	T	T
0.8916081268657082	0.2503441744461010	0.9459661176997393	T	T	T

Structure files (CONTCAR) involved in this work:

0.9456962906578225	0.7527786734030041	0.8591272597124961	T	T	T
0.6859020440104163	0.7523297155157691	0.8496245393655889	T	T	T
0.7748752840384437	0.7482973540376132	0.4471948871674604	T	T	T
0.6104968094939655	0.7502647072979037	0.4502045019724035	T	T	T
0.9376193430565393	0.4897767363703142	0.5402385840893933	T	T	T
0.8231729430152813	0.3334843133352268	0.3260792122772512	T	T	T
0.7995475379522720	0.6353260117814802	0.6949563149157615	T	T	T
0.9268022288027461	0.5307657594101218	0.1978988772011559	T	T	T
0.9300344555086968	0.4172730700002019	0.4258079498248025	T	T	T
0.8673315090570709	0.5546860278788325	0.5569899711084287	T	T	T
0.9952557119906468	0.6186764920821480	0.3642634678220126	T	T	T
0.0105476242070124	0.5500346278054532	0.4571688859689093	T	T	T
0.9537351804437328	0.4706166548273507	0.6031290131188244	T	T	T
0.0824670953930334	0.5876696042475834	0.3849905874308478	T	T	T
0.0526209549009529	0.4474753501387304	0.4722486641187478	T	T	T
0.0462521877193930	0.4055569947226435	0.3450629614456486	T	T	T
0.0291869336078069	0.5829830033917642	0.3986669682494273	T	T	T
0.0222321351650371	0.4275818008971199	0.4108600678419829	T	T	T

Figure S17 ZnPd-FS

Si O Al Pd Zn H C

1.0000000000000000						
20.0219999999999985	0.0000000000000000	0.0000000000000000				
0.0000000000000000	19.8990000000000009	0.0000000000000000				
0.0000000000000000	0.0000000000000000	13.3829999999999991				
93	193	3	1	1	6	2

Selective dynamics

Direct

0.4238459265996131	0.0575645296919481	0.6466780836718798	T	T	T
0.3049899830556511	0.0267609149308747	0.7916131357069971	T	T	T
0.2829035484374978	0.0590465944143720	0.0133202090739601	T	T	T
0.1233776226079829	0.0614005205834960	0.0107069448797361	T	T	T
0.0697081713970722	0.0292012390677860	0.7993881447477627	T	T	T
0.1803752446690632	0.0560196438753118	0.6565193974925423	T	T	T
0.4208456583464164	0.8267066179663095	0.6677275475611621	T	T	T
0.3046604906798430	0.8679396028853166	0.8090877569008093	T	T	T
0.2675456930057464	0.8277628686325786	0.0276042914356831	T	T	T
0.1132215349588973	0.8251000250215511	0.0131525406825612	T	T	T
0.0662520694760252	0.8720253984235190	0.7995447954726841	T	T	T
0.1829201892705461	0.8271797261463296	0.6715181481673447	T	T	T
0.0780121551018140	0.9406413554811650	0.1477113428742628	T	T	T
0.1971443115760000	0.9713198525221169	0.2918191561800068	T	T	T
0.2192811422128180	0.9374149792241143	0.5137363356567506	T	T	T
0.3791183543705197	0.9347741703327750	0.5123670154986837	T	T	T
0.4336464735389697	0.9681350541275064	0.3008842319875470	T	T	T
0.3222787229539470	0.9420795366134995	0.1576549118584626	T	T	T
0.0826905691953277	0.1717498928522777	0.1641145308748007	T	T	T
0.1967979786868250	0.1297511960567352	0.3084173689076068	T	T	T
0.2334072086009616	0.1711766338316306	0.5254712684482524	T	T	T
0.3881769188966671	0.1736498694622884	0.5103729709354179	T	T	T
0.4368586682873530	0.1265661222209462	0.2978613170952345	T	T	T
0.3179959480522349	0.1694282273476642	0.1715287457630801	T	T	T
0.5764921327252123	0.5553967774685410	0.3557014796786818	T	T	T
0.6918500282658212	0.5248670703595156	0.2035236569732930	T	T	T

Structure files (CONTCAR) involved in this work:

0.7145485114758482	0.5670390744073865	0.9873107319576648	T	T	T
0.8725769062774779	0.5715732462193025	0.9887602100332502	T	T	T
0.8121440352231520	0.5484648850867274	0.3463969163441021	T	T	T
0.5738452053730904	0.3277090729234292	0.3317891337574818	T	T	T
0.6951710836956153	0.3709801494078876	0.1932991279755011	T	T	T
0.7295773724806979	0.3258509739886232	0.9803403303911106	T	T	T
0.8841237238139643	0.3249479100182878	0.9928261416750445	T	T	T
0.9403820631842971	0.3737320644223021	0.1875844894869377	T	T	T
0.9200945284700290	0.4449289583872051	0.8618350403708154	T	T	T
0.7985327290466880	0.4710721393459356	0.7220673930756670	T	T	T
0.7732185094296542	0.4343791061773562	0.4973159278409939	T	T	T
0.6152175292474495	0.4290851086699327	0.4912484502692561	T	T	T
0.5671039464285086	0.4687496135682835	0.7043873423658487	T	T	T
0.6737034946173094	0.4462982182108348	0.8592044536686522	T	T	T
0.9206063804592073	0.6767130720072646	0.8317131565854460	T	T	T
0.7694452799705948	0.6682373505443163	0.4647331420891970	T	T	T
0.6144836875560382	0.6724403559554901	0.4873272393138888	T	T	T
0.5612577265335160	0.6268600225096825	0.6990133818017277	T	T	T
0.6722458864806463	0.6737004517630641	0.8291245642443763	T	T	T
0.5788747377011666	0.9439261215343849	0.3584882434866063	T	T	T
0.6990833173537967	0.9723250889805636	0.2149386958250576	T	T	T
0.7217805699535527	0.9373932266502191	0.9928269624204424	T	T	T
0.8820258712596492	0.9337668975065535	0.9950694273069738	T	T	T
0.9340091835235388	0.9695189102768198	0.2047872145854765	T	T	T
0.8238813607110763	0.9451888538992704	0.3538448124741230	T	T	T
0.5797980199774356	0.1727705895090124	0.3293948917143107	T	T	T
0.6986697206433994	0.1305227183451874	0.1927261310144070	T	T	T
0.7328135983472368	0.1698170864721189	0.9717578922648682	T	T	T
0.8874431978356122	0.1727519519217743	0.9834325661255064	T	T	T
0.9373993020502862	0.1275583017731483	0.1967324213312911	T	T	T
0.8212639398852072	0.1717792736885888	0.3289769491161499	T	T	T
0.9245667008763887	0.0539246685767158	0.8560181299454210	T	T	T
0.8037350840566003	0.0248966855791571	0.7085220029960054	T	T	T
0.7825917577362025	0.0647533752718339	0.4913216917542392	T	T	T
0.6222360289472372	0.0687098061939563	0.4901580198802936	T	T	T
0.5688355284693317	0.0312891739254558	0.6987290894262679	T	T	T
0.6802089115911567	0.0526666430408602	0.8474106973477481	T	T	T
0.9240874478629748	0.8290497510201105	0.8366537791961520	T	T	T
0.8035202598181465	0.8673926483165760	0.6952734087079384	T	T	T
0.7712589235442985	0.8256773346931298	0.4779674304750513	T	T	T
0.6163377675977517	0.8262450717971781	0.4915668114668387	T	T	T
0.5650906318720923	0.8744589456742180	0.6988735345124689	T	T	T
0.6796260486948046	0.8322999129206231	0.8333071290732500	T	T	T
0.4233209095219782	0.4445632899330773	0.6400626823495698	T	T	T
0.3037236558729619	0.4715324541916954	0.7865027020728371	T	T	T
0.2820208096027198	0.4367055302093127	0.0049543173828502	T	T	T
0.1242806517652733	0.4357225581833665	0.0099238974038331	T	T	T
0.0653320404468492	0.4698756129428779	0.8011511310345031	T	T	T
0.1771450956186199	0.4446244848247717	0.6543646625066900	T	T	T
0.4183751695786717	0.6727986867052285	0.6592855229659099	T	T	T
0.3023360336042867	0.6292661636146668	0.8023698817658648	T	T	T
0.2685079034119174	0.6706047512612561	0.0204731998828549	T	T	T
0.1144297326112188	0.6714238134164935	0.0072294565547943	T	T	T

Structure files (CONTCAR) involved in this work:

0.0634453214904373	0.6283686603680031	0.7965229564085929	T	T	T
0.1806663241651459	0.6684789307155106	0.6663472130030345	T	T	T
0.0756599958078825	0.5567707449655863	0.1473843443978257	T	T	T
0.1985189870652092	0.5266478220403351	0.2838454466231765	T	T	T
0.2198933123370803	0.5606287313538137	0.5105779126751782	T	T	T
0.3779024854952430	0.5662953916282653	0.5079882357971995	T	T	T
0.4293051337443624	0.5279690704793575	0.2980469640932282	T	T	T
0.3238978090262410	0.5528535220332401	0.1458937876239653	T	T	T
0.0859076381640201	0.3247544515608707	0.1579118604687106	T	T	T
0.1962483146724061	0.3686356610193474	0.3058830846952267	T	T	T
0.2318138432934900	0.3293452626588209	0.5251634418375896	T	T	T
0.3861929435951434	0.3272552526383550	0.5061793509713860	T	T	T
0.4322731924933439	0.3704771372896382	0.2923155441225398	T	T	T
0.3150924968596513	0.3279093520992127	0.1661016714474091	T	T	T
0.3582898600351793	0.0621755747418345	0.7173692933207837	T	T	T
0.3090235474610519	0.0644221920427534	0.8989123159472299	T	T	T
0.2028508424276386	0.0460639672732226	0.0163774736659763	T	T	T
0.0984884208043142	0.0688308632809331	0.8962933693712781	T	T	T
0.1045415350580980	0.0587862096687811	0.6990618035422277	T	T	T
0.2299316593427286	0.0340924217805088	0.7471127003491694	T	T	T
0.3609772554194829	0.8259539118268697	0.7490535144502162	T	T	T
0.3066947820007020	0.8436434307803129	0.9242531045264388	T	T	T
0.1901880711711947	0.8518269124028024	0.0164577746094451	T	T	T
0.0857568343430934	0.8307569567304636	0.8997926838575898	T	T	T
0.1055554318105921	0.8396164423309802	0.7043671131669829	T	T	T
0.2310959433125414	0.8530316873721659	0.7619754745038959	T	T	T
0.3224908689024788	0.9473821170685631	0.8021198895136854	T	T	T
0.0879388729057788	0.9500694160796455	0.8124114084134111	T	T	T
0.4320710196298637	0.1276633125519366	0.5856714035813445	T	T	T
0.4181355357289694	0.9960198002364118	0.5671811643695334	T	T	T
0.3967505777316016	0.8640294160306322	0.5661628714596585	T	T	T
0.1998835510359128	0.1303707961847658	0.6170279645562294	T	T	T
0.1835912090230336	0.0017017198904509	0.5660438973636240	T	T	T
0.1992154457300429	0.8677014676010099	0.5690891040846029	T	T	T
0.9898794144020814	0.0402457432761931	0.7873014696866351	T	T	T
0.9861359091787855	0.8671207171460316	0.7810609574840012	T	T	T
0.1442653932514644	0.9357710616400867	0.2170873142163163	T	T	T
0.1939777940378177	0.9330829672785500	0.3988173137130074	T	T	T
0.2994847929484715	0.9489380803625145	0.5188234554536689	T	T	T
0.4035248412168324	0.9291081666922050	0.3975346217337137	T	T	T
0.3979765918539763	0.9394909146369711	0.2006891364267716	T	T	T
0.2722822723457508	0.9653509920362461	0.2470940125774234	T	T	T
0.1422182364285934	0.1723028898207475	0.2460300097184843	T	T	T
0.1933351016384336	0.1554674978650415	0.4229458607556687	T	T	T
0.3108496635876448	0.1481357263060690	0.5121129675043276	T	T	T
0.4168635066820484	0.1683111469192049	0.3976716586750105	T	T	T
0.3957266235296918	0.1575162286013007	0.2031956783349812	T	T	T
0.2712413046953441	0.1430892435739477	0.2634568989462029	T	T	T
0.1782411162277792	0.0503822384503053	0.3033459174079149	T	T	T
0.4179870273422793	0.0479348094128994	0.3131864603203281	T	T	T
0.0681299383945007	0.8699886470492186	0.0886529319442436	T	T	T
0.0838276326941289	0.0004521431628292	0.0653017448652564	T	T	T
0.1066292389070967	0.1319345440649953	0.0650151891816255	T	T	T

Structure files (CONTCAR) involved in this work:

0.3025239652568422	0.8676289497847171	0.1189961569390328	T	T	T
0.3196933975922962	0.9955463527259863	0.0659845676407815	T	T	T
0.3011185223630783	0.1288121221031410	0.0695672946650216	T	T	T
0.5131255324344437	0.9542070803604401	0.2893436374470368	T	T	T
0.5167110154149210	0.1338738703166430	0.2779806999665262	T	T	T
0.6381228259808776	0.5593389493033009	0.2779121341317918	T	T	T
0.7008606164539767	0.5729373158707839	0.1068750680348633	T	T	T
0.7935083419304619	0.5587903114553016	0.9618191359396102	T	T	T
0.8847994483837175	0.5771014986397676	0.1067416442993296	T	T	T
0.8893991116848220	0.5314289706321147	0.3195792376704290	T	T	T
0.7629624914423393	0.5201894067518085	0.2626155140485268	T	T	T
0.6415383084778853	0.3355577150886245	0.2679532890110864	T	T	T
0.6908695080845415	0.3321880638029767	0.0861893172991637	T	T	T
0.8069565757771036	0.3508034117637467	0.9907515709508483	T	T	T
0.9101978398109981	0.3196204667706061	0.1081964119947045	T	T	T
0.9087710471174045	0.3569729978389540	0.3005123314241163	T	T	T
0.7690521070651172	0.3674443012559740	0.2388996880699782	T	T	T
0.6707245001070756	0.4488131947053090	0.1748358262172653	T	T	T
0.9213567023563629	0.4477917613578455	0.1553622984996834	T	T	T
0.5694415033876065	0.6272174232157471	0.4123039746899113	T	T	T
0.5882542361029270	0.4978501246566872	0.4402578984535239	T	T	T
0.5805269306866739	0.3641093738120750	0.4406610545923221	T	T	T
0.8012250484382911	0.6281568031517368	0.3692260552879057	T	T	T
0.7957038455576297	0.5119816402068101	0.4578954813475920	T	T	T
0.8202504480369033	0.3819408065810240	0.4388197484583062	T	T	T
0.0105099097751317	0.5509152054188218	0.2156973133526728	T	T	T
0.0206044167806463	0.3634994521510918	0.1999217457460297	T	T	T
0.8557163352963100	0.4345163471424078	0.7879570052449884	T	T	T
0.7893895170600671	0.4319628690629884	0.6155981713512644	T	T	T
0.6955937230079741	0.4238450997059025	0.4720844771994837	T	T	T
0.5999209781225575	0.4288960860466393	0.6098411100402719	T	T	T
0.6004615858306456	0.4424464955660755	0.8076322862806424	T	T	T
0.7268920774524305	0.4726716441136654	0.7757673528963890	T	T	T
0.8606527579403062	0.6798321483102702	0.7530651533730764	T	T	T
0.8134709768127343	0.6436954441397985	0.5632565174852548	T	T	T
0.6921794128030653	0.6463638754054686	0.4831479512461306	T	T	T
0.5865381991567322	0.6666872407135183	0.6000408304082754	T	T	T
0.5941023318970545	0.6610187294279976	0.7976607122169634	T	T	T
0.7186669266117224	0.6486822016300614	0.7378361277445245	T	T	T
0.8221626136418524	0.5482240308123384	0.6963793190816723	T	T	T
0.5820647730829531	0.5482533077590946	0.6892268066817744	T	T	T
0.9296758951683967	0.3766111169626125	0.9273503125685831	T	T	T
0.9129090084588275	0.5092383422863082	0.9345881034643865	T	T	T
0.8986129140315008	0.6401667929148767	0.9350949424714229	T	T	T
0.6929748368020010	0.3715564376746952	0.8963757019868830	T	T	T
0.6740900231740492	0.5002742003000703	0.9498740334271527	T	T	T
0.6863422285699834	0.6340150778404060	0.9334437420815220	T	T	T
0.4876354277579070	0.4532808357960968	0.7124939543411725	T	T	T
0.4804621574015586	0.6319567418979722	0.7083969417204452	T	T	T
0.6440979156645731	0.9377707481072406	0.2874464178446315	T	T	T
0.6994107985545817	0.9328508161388149	0.1089822288246013	T	T	T
0.8022466955983790	0.9452062510674378	0.9821832567959791	T	T	T
0.9021351696977441	0.9275420079757417	0.1120395874837560	T	T	T

Structure files (CONTCAR) involved in this work:

0.8991471245390235	0.9470964151979917	0.3090410378609482	T	T	T
0.7725499595488046	0.9656779736731859	0.2649838868340899	T	T	T
0.6421925915731003	0.1727380989361778	0.2525374569087458	T	T	T
0.6960940066649979	0.1547985410721982	0.0773354861202852	T	T	T
0.8105234546043749	0.1461894888189450	0.9802527245460566	T	T	T
0.9153186807233717	0.1679529450174080	0.0967330745260968	T	T	T
0.8979841601963421	0.1558535158505159	0.2937494696636297	T	T	T
0.7720791523098685	0.1437313108229122	0.2401566980052898	T	T	T
0.6804724079095267	0.0509794604845523	0.1993111852415761	T	T	T
0.9210579943446884	0.0484489232596446	0.1816800141059479	T	T	T
0.5708344796636085	0.8746095509327102	0.4218760184885758	T	T	T
0.5841987895940096	0.0061766793267982	0.4366645601707179	T	T	T
0.6011672411764249	0.1379942471598837	0.4345948479552204	T	T	T
0.8097191296748290	0.8695363716801997	0.3941925754773428	T	T	T
0.8177074565381495	0.9976403011705814	0.4460533680375827	T	T	T
0.8065039658588955	0.1314810075696246	0.4328084959843085	T	T	T
0.0132691416244015	0.9540899469229935	0.2175634285372268	T	T	T
0.0171734882335063	0.1376493589530565	0.2145662633275177	T	T	T
0.8588417803028660	0.0537614066563732	0.7857110635681206	T	T	T
0.8046880697672729	0.0706951156150182	0.6079593548378887	T	T	T
0.7020422770748904	0.0562968462668609	0.4817671100149288	T	T	T
0.5993810658076808	0.0748061923375304	0.6062649537093894	T	T	T
0.6047313119703228	0.0510515466614715	0.8033378642137640	T	T	T
0.7301000530378106	0.0283346345009283	0.7588036179391877	T	T	T
0.8595956970942313	0.8325917781073007	0.7642846679253656	T	T	T
0.8066800957478725	0.8313849396189062	0.5864933082375908	T	T	T
0.6940281874783489	0.8507412883907371	0.4860579167864434	T	T	T
0.5905099212803743	0.8279685722851868	0.6063941930271852	T	T	T
0.6038641724449468	0.8526119678752572	0.8004103596612124	T	T	T
0.7299788827730938	0.8563921551829192	0.7441954252292861	T	T	T
0.8194943579065123	0.9468808990752686	0.6815722834394182	T	T	T
0.5806980243540980	0.9524099789206807	0.6720702623253506	T	T	T
0.9324764235178566	0.1271896687985170	0.9086222807266235	T	T	T
0.9201903767599149	0.9970506698653615	0.9432655142338571	T	T	T
0.9057882577935988	0.8645182360505618	0.9424325872716413	T	T	T
0.6968682661186750	0.1288182248671083	0.8820744996333277	T	T	T
0.6861729873224429	0.0027797089573109	0.9430902965801429	T	T	T
0.6981630603489486	0.8689561671117191	0.9378463591474588	T	T	T
0.4898729391548508	0.0467061172288711	0.7147832719928072	T	T	T
0.4853926276892675	0.8640865911559344	0.7161218356358744	T	T	T
0.3560266334223476	0.4394455594925900	0.7072915311272673	T	T	T
0.3074512103020517	0.4289526020973819	0.8900700058085664	T	T	T
0.2030317869832270	0.4558427717024988	0.0078768736250504	T	T	T
0.0954037972260473	0.4302759347631502	0.8967435062948617	T	T	T
0.1008841723530300	0.4440088177216210	0.6979571818574842	T	T	T
0.2279804522437419	0.4669686601775565	0.7427444320950064	T	T	T
0.3555506639064948	0.6700643908860259	0.7351079826656044	T	T	T
0.3055296332428309	0.6605340516616578	0.9137128150901963	T	T	T
0.1915858313552479	0.6453221777579373	0.0105775649832548	T	T	T
0.0885196007793111	0.6712588995661798	0.8923227593325433	T	T	T
0.1030205744456664	0.6546777093092221	0.6971051666799689	T	T	T
0.2278411776646044	0.6382614307130646	0.7550743292582340	T	T	T
0.3219278459803853	0.5500216923157167	0.8059992260789780	T	T	T

Structure files (CONTCAR) involved in this work:

0.0801511942952100	0.5493846232001209	0.8148941513014006	T	T	T
0.4320422022382567	0.3762262882844900	0.5747362032705320	T	T	T
0.4212144992847436	0.5081575338994839	0.5634263450411180	T	T	T
0.3968648462059869	0.6394688921705475	0.5530021092869517	T	T	T
0.1952261544695725	0.3697327673947048	0.6151854689847409	T	T	T
0.1805683897095615	0.4975067289699667	0.5614469162401983	T	T	T
0.1961935768619363	0.6309669439119062	0.5606900290516021	T	T	T
0.9854259733291468	0.4549899640748777	0.7889096137372290	T	T	T
0.9837845869624315	0.6370482463870335	0.7792644202075659	T	T	T
0.1429036315014314	0.5643886180909758	0.2166809085039109	T	T	T
0.2015751169325263	0.5633598276148640	0.3925781014271381	T	T	T
0.2994129760366258	0.5494510730850461	0.5269771060065467	T	T	T
0.3948366786848790	0.5684966361682696	0.3899562269797389	T	T	T
0.3983671297176096	0.5549921642074475	0.1935625057992363	T	T	T
0.2716074783667294	0.5300017471409113	0.2326256378182629	T	T	T
0.1412396644955694	0.3248782710905553	0.2463681203935422	T	T	T
0.1926279928432637	0.3454514388301175	0.4217044997249882	T	T	T
0.3090757792333633	0.3534599910269680	0.5134989650043674	T	T	T
0.4104188728748321	0.3276824913102502	0.3905365313191732	T	T	T
0.3927227653719476	0.3429971016926027	0.1942674512341053	T	T	T
0.2700435026030706	0.3547336660067759	0.2597964663035134	T	T	T
0.1773929754922553	0.4480478709279688	0.2979223887101293	T	T	T
0.4135933184730265	0.4485766985463965	0.3130627121289465	T	T	T
0.0692418269661811	0.6228821031397039	0.0760187499444313	T	T	T
0.0838299992903688	0.4912233270226180	0.0740669529211436	T	T	T
0.1155542579224376	0.3616193882173225	0.0592508142931049	T	T	T
0.3061861980130037	0.6273098229541821	0.1058041121094606	T	T	T
0.3233072107218777	0.4981552911487276	0.0557679999992803	T	T	T
0.2949842817105878	0.3663339486948100	0.0633302191163845	T	T	T
0.5090322682791850	0.5405264521229916	0.2934761725379275	T	T	T
0.5117187432856397	0.3617058230793423	0.2711234465528717	T	T	T
0.4396280189711137	0.7499683404649059	0.6385894698851284	T	T	T
0.1949103242012021	0.7478421608747264	0.6503008670080119	T	T	T
0.2720420613448767	0.7485606761560760	0.0538481441159269	T	T	T
0.1094712946824660	0.7476078207058605	0.0497143926363388	T	T	T
0.0668161138281598	0.2481898911297103	0.1295082405965800	T	T	T
0.3036920380307979	0.2482169787865932	0.1492198344861624	T	T	T
0.2280502693197122	0.2503508229605582	0.5521034168358491	T	T	T
0.3925743503999860	0.2510638325472768	0.5480880839049317	T	T	T
0.5581448103552514	0.2493871849910412	0.3535709199367313	T	T	T
0.8116339507013136	0.2502350174177088	0.3480988735980954	T	T	T
0.7272750380092058	0.2486011543065970	0.9425575061934114	T	T	T
0.8909301640352808	0.2501984077359579	0.9449687350876428	T	T	T
0.9453676036200334	0.7523142322452430	0.8600653184964372	T	T	T
0.6846904948911009	0.7526193758711053	0.8524862735260904	T	T	T
0.7757735659655371	0.7474541762395668	0.4432661471140907	T	T	T
0.6104546011404687	0.7498028997781715	0.4502270341356772	T	T	T
0.9246946453721004	0.4851420301725979	0.5442185031320222	T	T	T
0.8221437268485660	0.3338345265485434	0.3266551157030776	T	T	T
0.7982410426688082	0.6356773131946346	0.6976572016255218	T	T	T
0.9272791293690903	0.5302264584824414	0.1955361565865636	T	T	T
0.9257434943267071	0.4278191150325856	0.4156633512043056	T	T	T
0.8634321022949409	0.5567262597011023	0.5594904110741357	T	T	T

Structure files (CONTCAR) involved in this work:

0.0068071525676454	0.5587807044350815	0.4100350759054046	T	T	T
0.0450632050099404	0.5252145083866955	0.5219979826960294	T	T	T
0.9593199970101035	0.4766567660618454	0.5938594305587921	T	T	T
0.0904113696017939	0.5356566574611100	0.4099562909636538	T	T	T
0.0465098467457738	0.4103128887501348	0.4474711853693292	T	T	T
0.0323695487547439	0.4459205336088979	0.3230833392044918	T	T	T
0.0413680133019466	0.5210771076003173	0.4406069153523278	T	T	T
0.0257382994116286	0.4524194778510792	0.4037716779516793	T	T	T