

**Supplementary Materials for:**

**Theoretical Study on Surface poisoning of high-entropy Alloys  
during Hydrogen Storage Cycles: The effect of Metal Elements  
and Phases**

Ming Jiang<sup>a</sup>, Yixin Yang<sup>a</sup>, Hongjiao Li<sup>\*a</sup>, Bin Liang<sup>a,b</sup>

a. School of Chemical Engineering, Sichuan University, Chengdu 610065, PR China

b. Institute of New Energy and Low-carbon Technology, Sichuan University, Chengdu 610207, China

For all correspondence: Dr. Hongjiao Li, [hongjiao.li@scu.edu.cn](mailto:hongjiao.li@scu.edu.cn)

Table S1 – Surface energy of each surface termination of low-index surfaces in ZrCr <sub>2</sub>			
Surface termination	$\sigma$ (eV/Å <sup>2</sup> )		
	(001)	(010)	(110)
Cr1	0.161	0.162	0.157
Cr2	0.163	–	–
Zr1	0.163	0.166	–
ZrCr1	–	0.168	0.151
ZrCr2	–	0.141	–

Table S2 – High entropy alloy  $V_{35}Ti_{30}Cr_{25}Fe_{10}$ , ZrTiVNiCrFe lattice parameters of each stage of hydrogen absorption and hydrogen storage capacity (simulated values, one of the sets)

HEA	Phase	a	c
$V_{35}Ti_{30}Cr_{25}Fe_{10}$	BCC	2.97	
	BCT	2.92	3.29
	FCC	4.22	
ZrTiVNiCrFe	Laves	4.92	7.97
	Laves-H	5.24	8.41

Table S3 – The optimal adsorption sites and binding energy of  $O_2$  on surfaces V, Ti, Cr, Fe and their hydrides

Phase	Alloy	Optimal adsorption site	$E_{bind}(eV)$	note
BCC	V	para2-1	-10.97	Dissociated
	Ti	para2-1	-13.08	
	Cr	para2-1	-9.84	
	Fe	para2-1	-14.01	
BCT	$V_2H$	para2-1	-11.47	Dissociated
	$Ti_2H$	para1-1	-13.03	
	$Cr_2H$	para2-1	-9.65	
	$Fe_2H$	para2-1	-7.72	
FCC	$VH_2$	para2-1	-5.72	Dissociated
	$TiH_2$	para2-2	-7.10	
	$CrH_2$	para1-1	-4.43	
	$FeH_2$	para2-2	-2.16	

Table S4 – The optimal adsorption sites and binding energy of O<sub>2</sub> on surfaces  
AB<sub>2</sub> alloy and their hydrides

Phase	Alloy	Optimal adsorption site	E <sub>bind</sub> (eV)	note
Laves	ZrV <sub>2</sub>	para1-1	-12.58	Dissociated
	ZrNi <sub>2</sub>	para2-1	-10.09	
	ZrCr <sub>2</sub>	para1-2	-11.54	
	ZrFe <sub>2</sub>	para1-1	-11.63	
	TiV <sub>2</sub>	para1-1	-12.55	
	TiNi <sub>2</sub>	para1-1	-9.68	
	TiCr <sub>2</sub>	para1-1	-12.20	
	TiFe <sub>2</sub>	para1-1	-11.38	
Laves- H	ZrV <sub>2</sub> H <sub>3</sub>	para1-3	-11.70	Dissociated
	ZrNi <sub>2</sub> H <sub>3</sub>	para2-1	-8.30	
	ZrCr <sub>2</sub> H <sub>3</sub>	para1-2	-8.99	
	ZrFe <sub>2</sub> H <sub>3</sub>	para1-1	-8.78	
	TiV <sub>2</sub> H <sub>3</sub>	para1-2	-11.66	
	TiNi <sub>2</sub> H <sub>3</sub>	para2-1	-8.68	
	TiCr <sub>2</sub> H <sub>3</sub>	para1-3	-9.75	
	TiFe <sub>2</sub> H <sub>3</sub>	para2-1	-8.72	

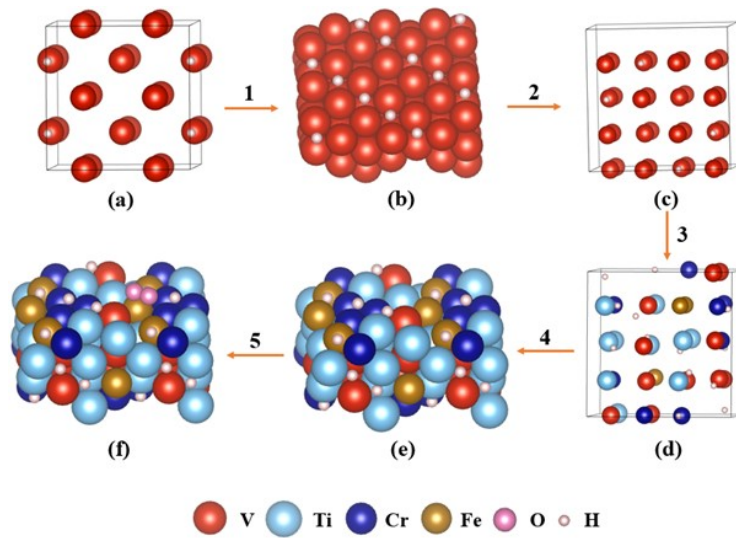


Fig. S1. Process of constructing surface models of high-entropy alloys (BCT structure as an example). (a): primitive bulk phase structure of  $V_2H$ , (b): the thermodynamically stable surface models of BCT structures, (c): new bulk BCT model derived from surface structure of (b), (d): relaxed high-entropy alloy bulk phase structure with substituted high-entropy alloy elements according to the composition, (e): surface structure of high-entropy alloys, (f) surface structure of high-entropy alloys with adsorbed oxygen molecular.

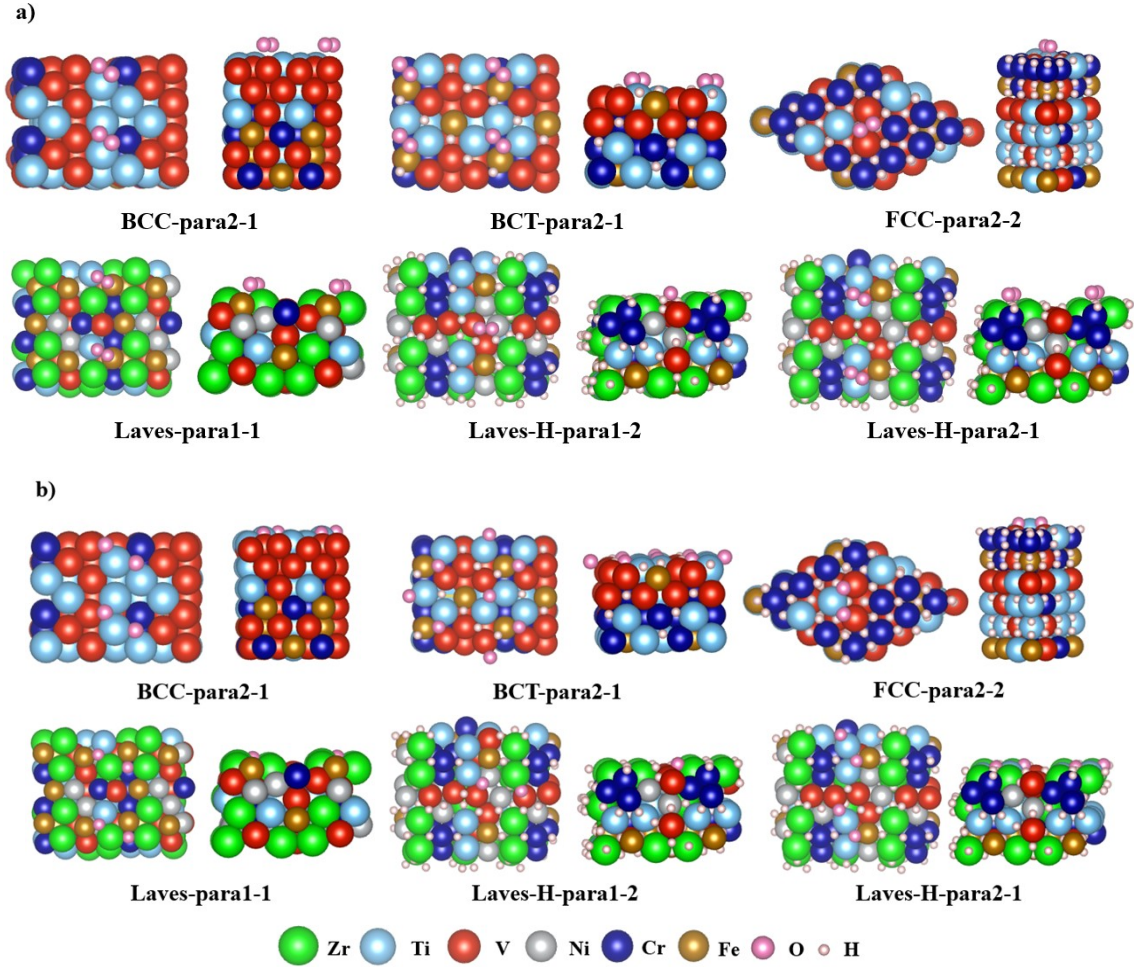


Fig. S2. Top view and side view of the initial (a) and the relaxed (b) O<sub>2</sub> adsorption geometries on the surfaces of high-entropy alloys.

As shown in Fig. 2, for pure elemental metals, there are two unequal adsorption sites on the BCC surface, i.e., top-sites of para1-1 (3-6), bridge/hollow sites of para2-1 (3-6-5-7); three unequal adsorption sites on the BCT surface, i.e., top sites of para1-1 (4-6), bridge/hollow sites of para2-1 (4-6-5-8), bridge/hollow sites of para2-2 (2-3-4-6); four unequal adsorption sites on the FCC surface, i.e., top sites of para1-1 (5-8), top sites of para1-2 (8-9), bridge/hollow sites of para2-1 (5-8-6-9), bridge/hollow sites of and bridge/hollow sites of para2-2 (5-6-8-9). For the AB<sub>2</sub> alloy, there are four unequal adsorption sites on the Laves surface, i.e., top sites of para1-1 (5-8), top sites of para1-2 (2-3), top sites of para1-3 (5-9), bridge/hollow sites of para2-1

(5-7-8-9); and five unequal adsorption sites on the Laves-H surface, i.e., top sites of para1-1 (5-8), top sites of para1-2 (2-3), top sites of para1-3 (5-9), top sites of para1-4 (3-4), and bridge/hollow sites of para2-1 (5-7-8-9). All the above-mentioned adsorption sites are considered and the most favorable adsorption sites are adopted for O<sub>2</sub> adsorption on surfaces of high-entropy alloys (Fig. S2) with each different phase structure of 20 series.

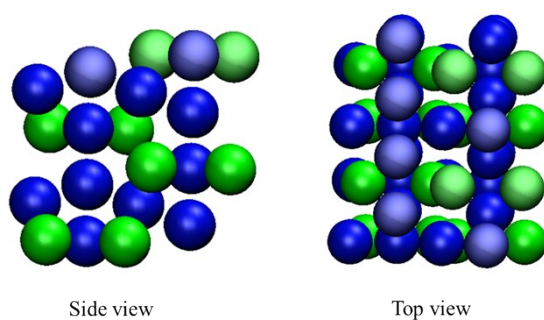


Fig. S3. Side view and top view of Laves ZrCr<sub>2</sub>(010) surface.

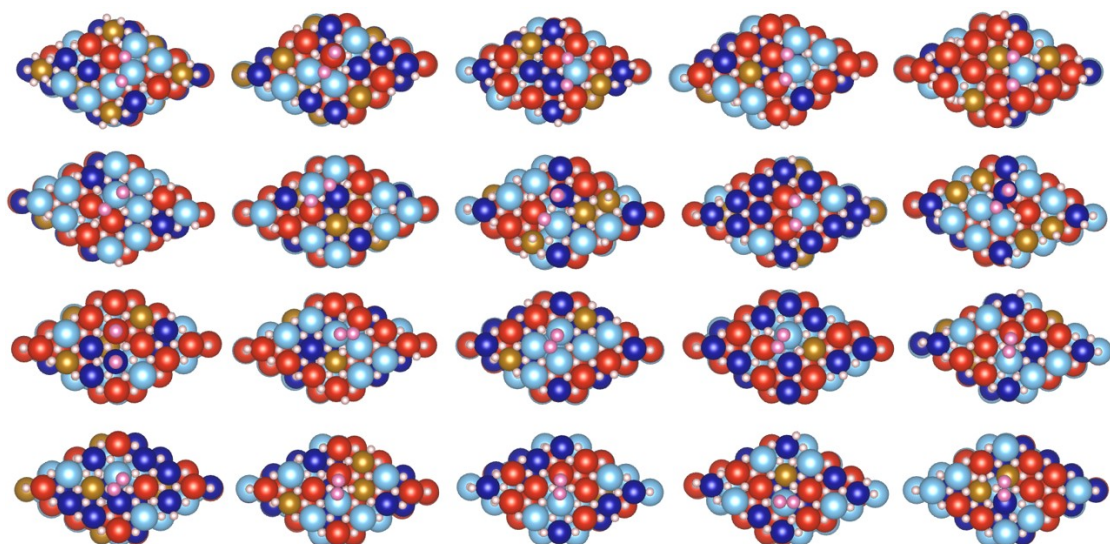


Fig. S4. Top views of the relaxed surfaces of high-entropy  $V_{35}Ti_{130}Cr_{25}Fe_{10}$  in FCC phase. (The binding energy increases from left to right.)

Below are the typical CONTCARs for the relaxed slab model for high entropy alloys in different phase states:

BCC(1110)

1.00000000000000

5.9492557918996951	-0.0159069019499387	-0.0141581668003391
-0.0225419359179620	8.3901235555575990	0.0378527693285334
-0.0301658481506720	0.0561153977788758	25.6253038500429255

V Ti Cr Fe

17 14 12 5

Selective dynamics

Direct

0.4950237255803557	0.0007669923539017	0.2462971895066035	T	T	T
0.7492554561606326	0.0038957305518537	0.1672672725120350	F	F	F
0.4885121394148868	0.2487780408902367	0.1626733774636264	F	F	F
0.7451594489351603	0.7604077310719717	0.2451480536585707	T	T	T
0.2462389656622150	0.2591702642997760	0.0846378302011885	F	F	F
0.0009444958651127	0.0021144762061949	0.2451463988434807	T	T	T
0.9949415885036278	0.5051273784341077	0.4050543266892937	T	T	T
0.7629120764058294	0.7757445573004673	0.4146285118516697	T	T	T
0.7527195600764145	0.5230461300917071	0.0061444237770303	F	F	F
0.9944550876749975	0.7501502609013525	0.3292600864341044	T	T	T
0.2456430091335093	0.9855590442035123	0.9996764973666288	F	F	F
0.4927324196776155	0.7540830754372294	0.1633110746459820	F	F	F
0.7491134201202777	0.2436589004698213	0.2407322947488640	T	T	T
0.5127020976624930	0.9972748579848895	0.4116902043342759	T	T	T
0.0056043737272589	0.9971158154681490	0.0837544994788715	F	F	F
0.9724095577863433	0.9872508749868526	0.4114900779230284	T	T	T
0.0075135252477452	0.2496184598899376	0.1623636612151884	F	F	F
0.5070454055146867	0.5039881867880796	0.4136696884477545	T	T	T
0.4909035036284187	0.4995110893924588	0.2489212144264698	T	T	T
0.5023693730517561	0.2576485546458038	0.3330976028644235	T	T	T
0.9928798627050952	0.2611431394882544	0.0034227347397007	F	F	F
0.0061987100485297	0.7534894177921956	0.1620333025759422	F	F	F
0.2387121711301381	0.2226945621279851	0.4241317629835745	T	T	T
0.7554280721408020	0.9869609449859880	0.0005643800289263	F	F	F
0.5065173526391575	0.2591774924231984	0.0035282638883558	F	F	F
0.2423520672640859	-0.0004013286915004	0.3312778275354479	T	T	T
0.9902770976145054	0.2554758612960307	0.3316747604820501	T	T	T
0.7454466895116525	0.4971676082286223	0.1613088438454895	F	F	F
0.4965393374641767	0.7457799550699169	0.3308950234557939	T	T	T
0.0140977972042441	0.5016006019260092	0.2488699538063372	T	T	T



0.5008841891868059	0.9977358897002517	0.0837116063044334	F	F	F
0.2296516790865162	0.7592195937708018	0.4071474917687842	T	T	T
0.2489418651671897	0.0037047755289947	0.1633905475619457	F	F	F
0.2543436725477690	0.5014277426725897	0.1597443889189805	F	F	F
0.4890640949250482	0.5065008256346104	0.0829100361694373	F	F	F
0.7450856884212366	0.9947655517525388	0.3276436959550609	T	T	T
0.0105822277727938	0.5061700045719633	0.0827066077913443	F	F	F
0.2518137834231737	0.7438558441756982	0.0796737203375457	F	F	F
0.2479854489650958	0.2375552140210128	0.2454685814670009	T	T	T
0.0075168639234633	0.7438898342866906	0.0023581640844128	F	F	F
0.7618058933796356	0.5144862984658312	0.3346940847258348	T	T	T
0.4933024926981062	0.7441103832420097	0.0027067120187709	F	F	F
0.2504732726367561	0.7613221735761584	0.2458801825919781	T	T	T
0.2484858846709983	0.5070149131892876	0.0021086883388151	F	F	F
0.7500051671182462	0.7529059273070260	0.0838118622993420	F	F	F
0.7519860257791819	0.2511555216056180	0.0837834618586371	F	F	F
0.2490659942933650	0.5002324574215237	0.3347908881010228	T	T	T
0.7465004218186747	0.2496596711454970	0.4066482643798515	T	T	T

BCT\(\1\1\0)

1.00000000000000

6.5998902412711553	0.0134794419517220	0.0068709953729304
0.0159807924434084	8.2673510421460641	0.0098607952333174
0.0086245674725776	0.0100100274621219	21.4447687187555047

V	Ti	Cr	Fe	H
11	10	8	3	16

Selective dynamics

Direct

0.8453961456735417	0.1158573824550913	0.0947547516325891	T	T	T
0.8668154586424350	0.3661665360232575	0.0027388995825248	F	F	F
0.1142131539768684	0.8717974350911638	0.2862939384617063	T	T	T
0.3595759515824919	0.1238928308575284	0.2867074573995659	T	T	T
0.6417235440025166	0.1149386384617230	0.0035888733159055	F	F	F
0.4077298095160700	0.1158393981785534	0.0946718233115694	T	T	T
0.1360509840992272	0.8736497757357203	0.0950937478267155	T	T	T
0.9042179310824494	0.8793888221687212	0.0050219603511934	F	F	F
0.8886214281907856	0.3589959173868278	0.1950469093679265	T	T	T
0.1419398371195863	0.1151297341162270	0.1898915296687150	T	T	T
0.0944506771985710	0.6256589042856291	0.1956892541524902	T	T	T
0.6270920947542322	0.6375868048642062	0.0037912841601155	F	F	F
0.3618702008701908	0.6235756964149807	0.0962034333762457	T	T	T

0.6450825453757197	0.3755888947477179	0.2933004793005214	T	T	T
0.6487189385098721	0.8631969099360731	0.2940042481483670	T	T	T
0.4066958756316852	0.8708885085419320	0.1943759593067068	T	T	T
0.8986189793422513	0.1164820259149109	0.2899120097008309	T	T	T
0.0930728950654620	0.3750741668169814	0.0935279197858474	T	T	T
0.3699747284555288	0.3672333075105675	0.1953969150185592	T	T	T
0.3867294403673114	0.3668059373625283	0.0018776116782462	F	F	F
0.3526748501950733	0.6267458791340824	0.2921265393611668	T	T	T
0.8561319464241325	0.8659666332769000	0.1920332928064064	T	T	T
0.3471229391439792	0.8698150521495407	0.0024704892216434	F	F	F
0.6580866266384436	0.6256149728801533	0.1949287786670354	T	T	T
0.1029874381051741	0.1150281222441123	0.0028511757485816	F	F	F
0.1113095068888419	0.3558197088229264	0.2831393491104593	T	T	T
0.8971693755686408	0.6212650530853480	0.2827948762191055	T	T	T
0.1409865083191235	0.6397475380120383	0.0015549091968197	F	F	F
0.6532851244346563	0.3700098559870922	0.0926416948351319	T	T	T
0.9115163032771462	0.6323212259610368	0.0987095942897526	T	T	T
0.5954491569946405	0.1206091132332785	0.1930168655524787	T	T	T
0.5856891739401121	0.8716156423005493	0.0996495086864723	T	T	T
0.3860456589235466	0.3694605333649161	0.0957812365343519	T	T	T
0.3620567914910471	0.8856360270395801	0.3286526211388263	T	T	T
0.1247816115181877	0.4266424937710696	0.9822999548253293	F	F	F
0.1200994014191351	0.8843845947793173	0.1881444795346191	T	T	T
0.1266063774854347	0.1126045307229698	0.0952825926732683	T	T	T
0.0873387133583096	0.6899619905384099	0.3365658105908276	T	T	T
0.8894549901560609	0.5910566516052498	0.9793164165976407	F	F	F
0.8565810251043772	0.1112456452928847	0.1932994481823199	T	T	T
0.8496571102445434	0.8717781493676978	0.0983210909807115	T	T	T
0.9049720022192020	0.4412557880155606	0.3319575685217973	T	T	T
0.6217884389735104	0.8819867935920627	0.9917507148251445	F	F	F
0.6384953886241601	0.4211721770209407	0.1742492282080035	T	T	T
0.6586093828482671	0.6027832253980272	0.0989834863271417	T	T	T
0.6204784573602597	0.1342681220436178	0.3312154669074893	T	T	T
0.3663716713311800	0.1150032298067600	0.9923320986947743	F	F	F
0.3816946202084919	0.6170057533000355	0.1983045298162144	T	T	T

FCC(1\1\1)

1.00000000000000

8.9483324509993221	-0.0092465813515133	-0.0023294746002584
-4.4821769530994304	7.7394498746981855	0.0008493825952624
-0.0038057225612677	-0.0005936344296927	28.3871039922196928

V	Ti	Cr	Fe	H
19	16	14	5	108

Selective dynamics

Direct

0.8843239644080354	0.4411337218775820	0.3657558031476323	T	T	T
0.2178683144323369	0.4350602346284690	0.3652068282242247	T	T	T
0.1125952583545313	0.2274789374331405	0.0170235540513204	F	F	F
0.5580393247354181	0.1126877524356544	0.1041572612678578	F	F	F
0.5557833206225100	0.4483899377508732	0.3658196868202137	T	T	T
0.4430850721438446	0.2168491953883560	0.0193568782892015	F	F	F
0.1120564286374300	0.8882630313322850	0.2819058302532673	T	T	T
0.6679139562706636	0.6674744901196226	0.4464980808994282	T	T	T
0.3355936343272248	0.9965467724502020	0.1937975702142722	F	F	F
0.6592642495179462	0.6611609062807702	0.1938614408790542	F	F	F
0.3299896089376352	0.3223169536142037	0.4466199581275240	T	T	T
0.8870266568996499	0.4397456634941008	0.1064562365436217	F	F	F
0.5558298182265151	0.1096161743265602	0.3662494086498578	T	T	T
0.4435094800919606	0.8883973176531661	0.2794896712725706	T	T	T
0.1096809223246356	0.2241967131586847	0.2819397309364393	T	T	T
0.6711650767813353	0.3356322379675518	0.1937991037505640	F	F	F
0.2224243592848824	0.7850767773361853	0.3649014980345068	T	T	T
0.5555587376023892	0.7781318387140884	0.3654329136388983	T	T	T
0.5578986048933388	0.4470230603808645	0.1061683873240540	F	F	F
0.4507562441474604	0.2274813103140867	0.2806370720372874	T	T	T
0.2312977874639017	0.7818410618591187	0.1040357145675586	F	F	F
0.7746816489119689	0.8843590178515631	0.2828413405547808	T	T	T
0.2263849853674600	0.1112527824854865	0.1037024391445485	F	F	F
0.3360427362856271	0.3436634797105071	0.1949227545357886	F	F	F
0.3382183367521044	0.6704588049561402	0.4494571398589056	T	T	T
0.6581734517869364	0.9983294294381722	0.1932384756029606	F	F	F
0.8842617686759979	0.1150186038791290	0.1057022967114705	F	F	F
0.7766513830200168	0.5488497968873034	0.0199332960875509	F	F	F
-0.0037269012262500	0.6696261895500426	0.4499145047320514	T	T	T
0.0026442484645770	0.0032663534139417	0.1952541489477539	F	F	F
0.8846474700181446	0.7754791471153055	0.1056823085746643	F	F	F
0.7707209562542374	0.8893905003435378	0.0177217978026931	F	F	F
0.0006738611627810	0.6623427246228957	0.1947943221633253	F	F	F
0.2260540553606063	0.4514813539912623	0.1061472503175978	F	F	F
0.1100381518885410	0.5509182826853797	0.2794469432968649	T	T	T
0.7788384406333458	0.2237647285679344	0.2796061780556287	T	T	T
0.7798979469454039	0.2251136837606040	0.0190880165186513	F	F	F
0.6653757855926152	0.3259177246567363	0.4455935690238718	T	T	T
0.8925449135022061	0.7759484656321265	0.3661582387539971	T	T	T

0.5529498369544683	0.7755425310896769	0.1061564728459459	F	F	F
0.1094180054217659	0.5477550468061665	0.0194756581480107	F	F	F
0.0011297985168866	0.0050191566399724	0.4440708843356075	T	T	T
0.4460170763066075	0.5567472459022941	0.2796430955568080	T	T	T
0.9935208441728981	0.3243827567333578	0.4451451318086237	T	T	T
0.9978451101064465	0.3373951426180213	0.1945745055593449	F	F	F
0.2213886495615235	0.1081003291304185	0.3659721846046033	T	T	T
0.3386931650006280	0.0087363851123023	0.4460488489834032	T	T	T
0.6713349105091033	0.0080611120924314	0.4451551616351577	T	T	T
0.4401549341447151	0.5505188105651015	0.0207554478784289	F	F	F
0.1093087178601095	0.8913305255765351	0.0180084621007310	F	F	F
0.8878114892637686	0.1133054994677430	0.3658337429137365	T	T	T
0.4463208568879793	0.8891470343423080	0.0196848199848745	F	F	F
0.3344978195308101	0.6683212092622455	0.1933797194381555	F	F	F
0.7766987403875648	0.5540202395766221	0.2795636998744808	T	T	T
0.5560451983988273	0.1034519826749118	0.0390175176812519	F	F	F
0.3404462989581347	0.3391187470055712	0.1283020225608169	F	F	F
0.1219342842370708	0.5523836082166795	0.2136600671796529	F	F	F
0.5639160007492724	0.1106485466493025	0.3021572315774045	T	T	T
0.3313114219477923	0.3263703719709379	0.3850044440971245	T	T	T
0.1006316666523841	0.5351212537477785	0.4768026976841372	T	T	T
0.3371149028248368	0.3341191715834384	0.9991215157422673	F	F	F
0.1052433473989183	0.5539948052128807	0.0817743817282164	F	F	F
0.5531753205004364	0.1169703250444272	0.1693486531934028	F	F	F
0.3330471975235781	0.3409999428309598	0.2607908919703999	T	T	T
0.1093270869256081	0.5544638187329833	0.3461858958840151	T	T	T
0.5557831885664342	0.1098192027971066	0.4298034136762724	T	T	T
0.5464200056827551	0.4392454431968389	0.0412527877904196	F	F	F
0.3435407824269063	0.0041505009147116	0.1289876741333558	F	F	F
0.1073327651126377	0.2332947342685046	0.2178108218522254	F	F	F
0.5667368156609663	0.4606815687592543	0.3013820140827218	T	T	T
0.3336326462017475	0.0057056722871008	0.3861786771234221	T	T	T
0.1035051484015125	0.2170491291794838	0.4742008415650744	T	T	T
0.3275984952946231	0.9873748872058457	0.9991409097324038	F	F	F
0.1114223112865815	0.2254624173584716	0.0811102810126840	F	F	F
0.5610617408531553	0.4453528206735839	0.1707255146701456	F	F	F
0.3320687132801719	0.9972393414034206	0.2583346808423459	T	T	T
0.1028116864105962	0.2102218369730228	0.3462408005209940	T	T	T
0.5568050130803068	0.4383552836822295	0.4297783242855010	T	T	T
0.2237250260165666	0.4474987655888967	0.0394557490706902	F	F	F
0.0003933730293681	0.0032497746752327	0.1283596121374941	F	F	F
0.4491716789346967	0.2228932185606212	0.2144633705782439	F	F	F
0.2303772698861009	0.4450161822660549	0.3015266134024273	T	T	T

0.9970075780194846	0.0022983158390226	0.3836101584584171	T	T	T
0.4494464962081051	0.2192595312651341	0.4752189623672806	T	T	T
0.0062507642030383	0.0004242400669128	0.9968774313725461	F	F	F
0.4544509298768631	0.2275176010941991	0.0826829025200269	F	F	F
0.2183110881282317	0.4565913852733061	0.1734483003821836	F	F	F
0.0034771736999993	0.0018316781903529	0.2617687659080891	T	T	T
0.4420536783170243	0.2217338750859211	0.3471270321912974	T	T	T
0.2142421625662990	0.4336104519009609	0.4296304657188427	T	T	T
0.2175258414293708	0.1047781685906344	0.0369686075822315	F	F	F
0.0004439056470176	0.3395452946953412	0.1309115249294237	F	F	F
0.4423214259500483	0.5698986438595171	0.2173225415797333	F	F	F
0.2198847269492260	0.1114431564724607	0.3036983935370945	T	T	T
0.9930769420502152	0.3240035997033240	0.3850968355674122	T	T	T
0.4484059779012636	0.5458675570519155	0.4761677939545200	T	T	T
0.9962452248163913	0.3346080423444207	0.9979897538296996	F	F	F
0.4529488553878167	0.5628947473446644	0.0832131471061075	F	F	F
0.2313266245513717	0.1135536736057929	0.1715576779831238	F	F	F
0.9916020142697907	0.3240365179087454	0.2573262956009404	T	T	T
0.4428684689638409	0.5548721095373833	0.3432459793690859	T	T	T
0.2179192334986464	0.1028251554584718	0.4281987588486875	T	T	T
0.5413727866523672	0.7730062276828065	0.0419245363781826	F	F	F
0.5450750978105930	0.7696610350743841	0.3016430685857827	T	T	T
0.5441492949153286	0.7675560721950205	0.1700502741983030	F	F	F
0.5678987922198786	0.7902562239516030	0.4293085999988501	T	T	T
0.3460293551635658	0.6751910612477090	0.1313747422343283	F	F	F
0.1177570010378233	0.8893541276391304	0.2180674144645565	F	F	F
0.3299418677662420	0.6649066509999952	0.3841473431789158	T	T	T
0.1188656855395303	0.9107404874123597	0.4756377233263875	T	T	T
0.3356272755324952	0.6706429841308363	0.0036169091175466	F	F	F
0.1101501616642793	0.8851143716786822	0.0791961677800472	F	F	F
0.3396766148434908	0.6650810324444604	0.2562448880872990	T	T	T
0.1078456997957821	0.8918580091320012	0.3458489808359212	T	T	T
0.0022232211371005	0.6613354709527712	0.1276924865578550	F	F	F
0.4326681596510653	0.8750145377886511	0.2157205865183656	F	F	F
0.9986354883798056	0.6669002666086572	0.3848588363632441	T	T	T
0.4570631312182150	0.9106068553420792	0.4760908090260941	T	T	T
0.0138648390319034	0.6731913517053272	0.0021830152366391	F	F	F
0.4580442508966485	0.8919500023524733	0.0805654663890110	F	F	F
0.9907433557839058	0.6651971409602322	0.2609260225923993	T	T	T
0.4452331260769906	0.8895351000359564	0.3441763491334822	T	T	T
0.2276719438764943	0.7840574587385376	0.0356638363233515	F	F	F
0.2241067010025342	0.7798574253113513	0.3014164230431266	T	T	T
0.2326555921895022	0.7757568657080611	0.1716741807934312	F	F	F

0.2270151348352594	0.7908057089361964	0.4295363489544492	T	T	T
0.7717230184188750	0.5536923351356577	0.2183971458292078	F	F	F
0.7609544700131450	0.5399069825868351	0.4760032550855027	T	T	T
0.7756404547368163	0.5471510508530741	0.0852425997204236	F	F	F
0.7803463368944239	0.5597027539345480	0.3425119521319843	T	T	T
0.7824225311676685	0.2278712386161317	0.2167731972307934	F	F	F
0.7780375166075401	0.2221998318957673	0.4744604894712196	T	T	T
0.7733196697625786	0.2257424352453654	0.0812797450434033	F	F	F
0.7798364406329981	0.2175194664173675	0.3435307113567741	T	T	T
0.8949014896455196	0.4380944515184382	0.0415114700493717	F	F	F
0.6542410775438228	0.9918064742394321	0.1267357037614119	F	F	F
0.8759775301525027	0.4408567384735375	0.3007576466759243	T	T	T
0.6754639400087707	0.0039955770606831	0.3849180465235888	T	T	T
0.6553611280530944	0.0067246985245291	0.9975447844396967	F	F	F
0.8872524102570978	0.4368612672381431	0.1710573028229803	F	F	F
0.6663773956275063	0.0049532082221350	0.2601170555956573	T	T	T
0.8845248740225433	0.4354982008267700	0.4297543054028666	T	T	T
0.8902961656579009	0.1203201790189823	0.0388031496653127	F	F	F
0.6652658447628355	0.3318051669020363	0.1285750760336484	F	F	F
0.8861274539302278	0.1176973934200755	0.3043158527814570	T	T	T
0.6635987545699498	0.3323607219008990	0.3856756942925740	T	T	T
0.6632552590660694	0.3208258311467773	0.9974987638255968	F	F	F
0.8898426683828689	0.1212171288248030	0.1729534961883132	F	F	F
0.6811087128628518	0.3432533742335784	0.2584300638762941	T	T	T
0.8873956946942873	0.1086683635686482	0.4274558223571591	T	T	T
0.7699269635521375	0.8809202997125354	0.2163342903607059	F	F	F
0.7830633002176036	0.8988289472965845	0.4736039257317618	T	T	T
0.7649845271328388	0.8850017757965176	0.0836540511870680	F	F	F
0.7860710362445006	0.8936759725576794	0.3492034150627643	T	T	T
0.6553371434867614	0.6650329745756665	0.1293230574441822	F	F	F
0.6730465723795114	0.6717285879778262	0.3845274665150140	T	T	T
0.6544429823958637	0.6576367200036302	0.9979496722118526	F	F	F
0.6629251390385105	0.6541530617412666	0.2590807141757162	T	T	T
0.8966969167983052	0.7836816861599800	0.0389223260737808	F	F	F
0.8881026794805246	0.7646253404015789	0.3036073854402951	T	T	T
0.8804670855725547	0.7716791030427430	0.1728801418305608	F	F	F
0.8891698704626881	0.7882942647756542	0.4282995024275634	T	T	T

Laves\0\1\0)

1.00000000000000

7.9738475510405022      0.0005032370251708      -0.0112980912980975

0.0009804805802823    9.8496029270137075    -0.0719412224975174  
 -0.0120975736811735    -0.0623398780022642    22.0972872239984000

Zr    Ti    V    Ni    Cr    Fe  
 8    8    8    8    8    8

Selective dynamics

Direct

0.0596359875449721	0.9993732562020554	0.0003532716837782	F	F	F
0.9488488997156078	0.7711886836855797	0.3190630997279980	T	T	T
0.0626208475898901	0.7391550388470831	0.1921027578910780	T	T	T
0.4419810656057611	0.7576343364292047	0.1932130341229442	T	T	T
0.9324617783489590	-0.0049761013213289	0.1329564395928923	T	T	T
0.5687198566593298	0.5013426616667211	0.1276799360586334	T	T	T
0.5575813500045359	0.7422050458612852	0.3246429438437941	T	T	T
0.4320182758065911	0.5039778826679111	0.9995270166303456	F	F	F
0.5598547453654998	0.2599352017651955	0.3134600857903481	T	T	T
0.4354795503785889	0.2452373072501858	0.1931660492978378	T	T	T
0.9437014014715459	0.4919778607225037	0.1251561122529217	T	T	T
0.0539523116435490	0.5015501640981768	0.0019298020696468	F	F	F
0.0664253383947474	0.2525900831494345	0.1921103100219444	T	T	T
0.5634343239945012	0.9991930039371167	0.1256749815002175	T	T	T
0.9299893419868779	0.2377638496734145	0.3108830280493058	T	T	T
0.4416619377077851	0.0066809947824424	0.0016330729688150	F	F	F
0.2541719212241577	0.1193798769799114	0.0953811400444962	T	T	T
0.2494174748658651	0.2566737402913404	0.9987658002032944	F	F	F
0.7478845236272499	0.3611294405963680	0.2187056536457584	T	T	T
0.5177058530687828	0.0049813079969200	0.2680746127726221	T	T	T
0.5057084753709375	0.2448835428643932	0.0667191614754827	F	F	F
0.7461705582625413	0.8798046511562276	0.0340300263653361	F	F	F
0.2389356404868022	0.1262129357164579	0.2928379598988139	T	T	T
0.4827702675049387	0.4948368755656163	0.2552442980521735	T	T	T
0.7513151307707782	0.1237722942485594	0.2222349193347380	T	T	T
0.2563266744228596	0.8663482838560862	0.2863540839213510	T	T	T
0.7541179153212667	0.3771242894664439	0.0306417224559610	F	F	F
0.7556120083015734	0.8704021155658798	0.2265820111457356	T	T	T
0.2444300432959267	0.6192937205795122	0.2875770257384263	T	T	T
0.0005955816912149	0.2543010122010685	0.0659134150686498	F	F	F
0.2478142921490445	0.7479374052029328	0.9985730867824643	F	F	F
0.2588727466244771	0.0061335164353559	0.1918656689415840	T	T	T
0.7483356801584122	0.1244073195591682	0.0332748057236287	F	F	F
0.7197920881309434	0.0081589549756967	0.3194146401583740	T	T	T
0.2568964640672785	0.8720343990465730	0.0921215132257159	T	T	T
0.4991883439144118	0.7553730774533278	0.0668295060092348	F	F	F
0.9929024431797111	0.4892302809587071	0.2603983389483742	T	T	T

0.2502771106538385	0.3815152235867413	0.0953343907995863	T	T	T
0.7827454010218049	0.4901611112968826	0.3120029677286166	T	T	T
0.7575873275339688	0.6239907281911741	0.0312201223513426	F	F	F
0.7491239960440084	0.2494071125507892	0.1276943063642441	T	T	T
0.2427874740336327	0.3441477219910610	0.2781114505039214	T	T	T
0.7417646951108908	0.6258819700598189	0.2250553634115724	T	T	T
0.7529989235797517	0.7417327569599438	0.1319208012511406	T	T	T
0.2484227097744922	0.4886061540027571	0.1869214918634853	T	T	T
0.0094468575497068	0.0193570487694646	0.2600266366970582	T	T	T
0.9988511881177544	0.7400261563627737	0.0654238291747191	F	F	F
0.2472742671152350	0.6223014197633306	0.0935237612213042	T	T	T

Laves-H(0\1\0)

1.00000000000000

8.4084160025020847	-0.0929687286761127	-0.0352733371081418
-0.0303398055683045	10.4861394173438516	-0.0964817561321420
-0.0382289009216598	-0.0826987722580370	23.9573516419523358

Zr	Ti	V	Ni	Cr	Fe	H	
8	8	8	8	8	8	8	48

Selective dynamics

Direct

0.9232445160718796	0.9972101615850685	0.1467869106874252	T	T	T
0.5712337780835774	0.2872350985436042	0.3360312041809346	T	T	T
0.4359727172859696	0.2428343816504135	0.2102005385818479	T	T	T
0.4340712579746082	0.9985626671542676	0.0287319728063551	F	F	F
0.0551939994612949	0.7553156577911231	0.2100347709295390	T	T	T
0.5506735824872832	0.5019033523210463	0.1524068038981032	T	T	T
0.9188398570269866	0.5042216614534288	0.1456953704579042	T	T	T
0.0584316017413223	0.2562619850020300	0.2097305288626242	T	T	T
0.9398169038745733	0.7381488309125155	0.3255581670025558	T	T	T
0.5478722494784740	0.9947195020737941	0.1579389043809739	T	T	T
0.5685040226911084	0.7208123808067256	0.3252472202837657	T	T	T
0.4282777059278616	0.7417109068551085	0.2115097996663283	T	T	T
0.9429096122397213	0.2603344944007400	0.3257473106259900	T	T	T
0.0497235209570519	0.5101072665305963	0.0187634715200531	F	F	F
0.0570015903617431	0.0017886003341729	0.0209754469981291	F	F	F
0.4299143579923381	0.5048495033283018	0.0231320291733113	F	F	F
0.4754379623365987	-0.0030084115321709	0.2852742982881433	T	T	T
0.7437564897743053	0.8893116128460581	0.2537261510570203	T	T	T
0.2502897742049228	0.2612095761201161	0.0301559324271850	F	F	F
0.5147515868965868	0.7517971506270911	0.0875492474186501	F	F	F



0.7857294665267190	0.0300209934893302	0.3290623348975018	T	T	T
0.2266536392592960	0.1245467033594308	0.3141376116521497	T	T	T
0.2479948729706710	0.3831974524551816	0.3136221283191581	T	T	T
0.9821463263908186	0.2590515065811232	0.0888404414936588	F	F	F
0.7444301227427000	0.5234335863026869	0.3336249688681578	T	T	T
0.7420345908739989	0.3834931132647981	0.0560254298374971	F	F	F
0.7351794776122648	0.3887773818929482	0.2487002246662333	T	T	T
0.7346814493711236	0.1311501579340657	0.0585768483866147	F	F	F
0.9813192969427863	0.5089762466774517	0.2751876313533769	T	T	T
0.2347330709744255	0.1199873051674798	0.1184314002336199	T	T	T
0.2633900013655435	0.7542232046067099	0.0248443277492854	F	F	F
0.4946166057224965	0.5039701510040897	0.2749854123058398	T	T	T
0.2365626176974502	0.6072526370284644	0.2987124848460360	T	T	T
0.2421473579414701	0.5159725076067305	0.2188561660630664	T	T	T
0.2308303054892967	0.3647152559168529	0.1078824646749762	T	T	T
0.0031829601047093	0.7396687098467538	0.0882547905340303	F	F	F
0.2310311068493967	0.8715903521970005	0.3079488024575121	T	T	T
0.2703604596518617	-0.0010578738379131	0.2174293747965356	T	T	T
0.0182918410630182	0.0026490580334948	0.2796100396281138	T	T	T
0.2237085351861223	0.6293979679752767	0.1124972714945847	T	T	T
0.7493925173855449	0.1287143384906815	0.2516804054870196	T	T	T
0.7710611056389851	0.2555003903820018	0.1441812493735679	T	T	T
0.4912825038300426	0.2546570004100701	0.0822487118815971	F	F	F
0.7254994590713935	0.6423333292157878	0.0573120286322961	F	F	F
0.7476044945399352	0.8752342506905819	0.0590364090906235	F	F	F
0.2415092234248324	0.8677800737174256	0.1187706057831638	T	T	T
0.7642984952280304	0.7582314559951692	0.1456166999311699	T	T	T
0.7312073745837050	0.6263819040890741	0.2457379430856036	T	T	T
0.0489597053141893	0.1872676359538090	0.0222649297113904	F	F	F
0.0518289342080864	0.4527361738211639	0.2123607695753914	T	T	T
0.4247545232458018	0.3386808102199563	0.1374660134397634	T	T	T
0.4432641437201291	0.1078381428056192	0.3454363679020632	T	T	T
0.4435095029647660	0.1517544633227821	0.1307864988806956	T	T	T
0.3787547680324024	0.3668481438925076	0.3706991170285980	T	T	T
0.3579785011321274	0.4999331054349430	0.0984781718154852	T	T	T
0.3704236554828018	0.2512275392891866	0.2925169379679654	T	T	T
0.6405349640418765	0.1497636079461226	0.1871426611321076	T	T	T
0.6284529408069091	0.4301247401377140	0.0016394448196664	F	F	F
0.6345959701504285	0.9978381850580931	0.0809559133862052	F	F	F
0.6290399499611472	0.2546276600705537	0.2587612631634434	T	T	T
0.8663495860815971	0.4024756331519228	0.9968767392648203	F	F	F
0.8579162768138757	0.1574949834437786	0.1898395472579773	T	T	T
0.8665587709421771	0.0134052878329669	0.0656559732090045	F	F	F

0.8618500020055627	0.2698247610670757	0.2561451940715290	T	T	T
0.7394411582626431	0.3899408202196990	0.1798118174535212	T	T	T
0.7723376257020196	0.2019470718819795	0.3752062843656949	T	T	T
0.2353123661617929	0.4195440980691316	0.0043028714487221	F	F	F
0.2380853614603046	0.1428026674210199	0.1869068482069323	T	T	T
0.1068486140867080	0.4924252169747945	0.0969477908743741	F	F	F
0.1502205642595742	0.2623327844427362	0.3594927267110997	T	T	T
0.2378192761406908	0.0955699968877610	0.0436549062625318	F	F	F
0.2555043921596963	0.3581703638767279	0.2374937291248176	T	T	T
0.0592824833993788	0.6961405496234434	0.0201381042294528	F	F	F
0.0633078108823277	0.9537007229732820	0.2114877463992400	T	T	T
0.4227385135935262	0.8430300874999327	0.1472764470587490	T	T	T
0.1956355668345512	0.5139819234945753	0.3565945879647673	T	T	T
0.4219014566132544	0.6584052605806551	0.1403044610841803	T	T	T
0.4269748978328952	0.8852945794230672	0.3428120739870821	T	T	T
0.3617011234864666	0.9900174191515825	0.1091578860463268	T	T	T
0.3673450581589900	0.7359066757538840	0.2913940635411067	T	T	T
0.6321244673697216	0.6714969528854868	0.1869559924129747	T	T	T
0.6326927248589200	0.8993740786933486	0.0044965353592019	F	F	F
0.6119108922854082	0.5178659545180366	0.0710527602454789	F	F	F
0.6118925994809704	0.7555841721474381	0.2547269319672815	T	T	T
0.8787315664833173	0.8908052021191040	0.0065533246107634	F	F	F
0.8514070540061465	0.6577532003561252	0.1894448239997510	T	T	T
0.8629874952413843	0.5264813275655200	0.0655796323905236	F	F	F
0.8589179031046467	0.7489452972938977	0.2566695570656881	T	T	T
0.7316115052354331	0.8985736300128927	0.1781818665406603	T	T	T
0.7545770675492650	0.6594404468775459	0.3719373732541196	T	T	T
0.2305870631014812	0.8991558699734128	0.0035976998260239	F	F	F
0.2391011844790711	0.6560509134634167	0.1838055221714915	T	T	T
0.1210634076762602	0.9781063368465723	0.0995584748241853	F	F	F
0.1639192862843424	0.7395378504372543	0.3486708904277535	T	T	T
0.2495962009108652	0.6049244621752123	0.0403813878998349	F	F	F
0.2603137055699538	0.8425543322259645	0.2380582846225635	T	T	T