

Electronic Supplementary Information

**DFT-based microkinetic studies on methanol synthesis from CO₂
hydrogenation over In₂O₃ and Zr-In₂O₃ catalysts[†]**

Kun Li,^{abc} Zhangqian Wei,^{ab} Qingyu Chang,^{*a} Shenggang Li^{*abc}

^a *CAS Key Laboratory of Low-Carbon Conversion Science and Engineering, Shanghai Advanced Research Institute, Chinese Academy of Sciences, 100 Haik Road, Shanghai 201210, China.*

^b *School of Physical Science and Technology, ShanghaiTech University, Shanghai 201210, China*

^c *University of Chinese Academy of Sciences, Beijing 100049, China*

* E-mail addresses: *changqy@sari.ac.cn* (Q. Chang), *lisg@sari.ac.cn* (S. Li)

Table S1 Elementary reactions considered for CO₂ conversion to methanol on In₂O₃(110) and Zr-In₂O₃(110) surface in microkinetic analysis performed with CatMAP, with further details of the adsorption sites.

R1	CO _{2_g} + * _s -> CO _{2*_s} #ln-CO2
R2	CO _{2_g} + * _s -> O _{2C_s} #bt-CO2
R3	CO _{2_s} + H _t -> CO _{2H_s} + * _t
R4	CO _{2H_s} <-> CO _{2-H_s} -> HCOO _s
R5	HCOO _s + H _t -> HHCOO _s + * _t
R6	HCOO* _s + H* _t <-> H-HCOO* _s + * _t -> H ₂ COO* _s + * _t
R7	HHCOO _s <-> HCOO-H _s -> H ₂ COO _s
R8	H ₂ COO _s <-> O-CH ₂ O -> OH ₂ CO _s
R9	OH ₂ CO _s + 2H _t -> OH ₂ COHH _s + 2* _t
R10	OH ₂ COHH _s <-> OH ₂ COH-H _s -> OH ₃ COH _s
R11	OH ₃ COH _s -> OCH ₃ OH _s
R12	OCH ₃ OH _s -> CH ₃ OH _g + O _s
R13	O ₂ C _s + H _t <-> O ₂ C-H _s + * _t -> COOH _s + * _t
R14	COOH _s <-> CO-OH _s -> COHO _s
R15	COHO _s + * _s -> CO _s + OH _s
R16	CO _s -> CO _g + * _s
R17	H _{2_g} + 2* _t <-> H-H _t + * _t -> H _t + H _t
R18	OH _s + H _t <-> H-OH _s + * _t -> H ₂ O _s + * _t
R19	H ₂ O _s -> H ₂ O _g + * _s
R20	OH _s + * _t -> O _s + H _t

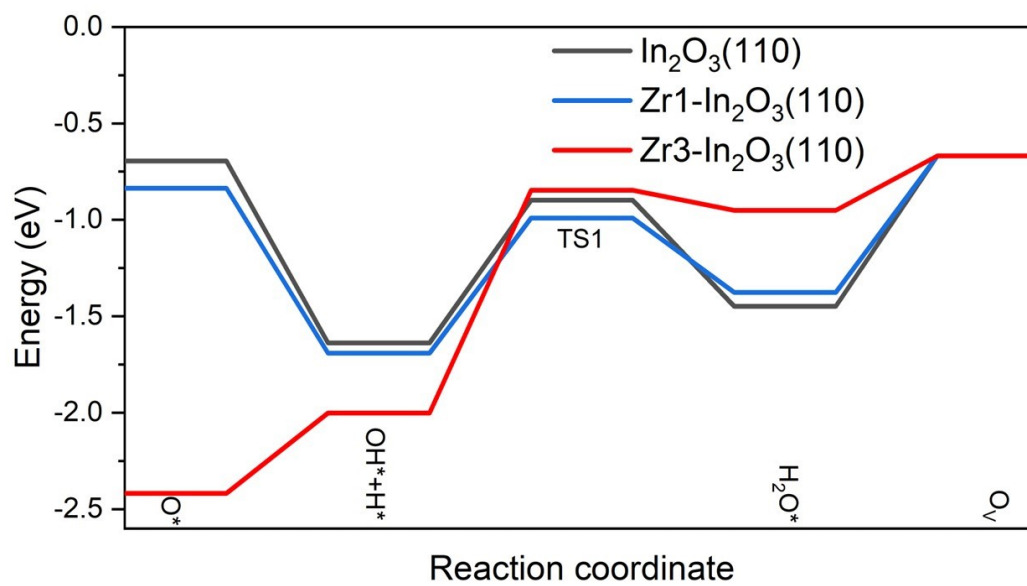


Fig. S1 Potential energy surfaces for H₂O formation on the In₂O₃(110) and Zr-In₂O₃(110) surfaces.

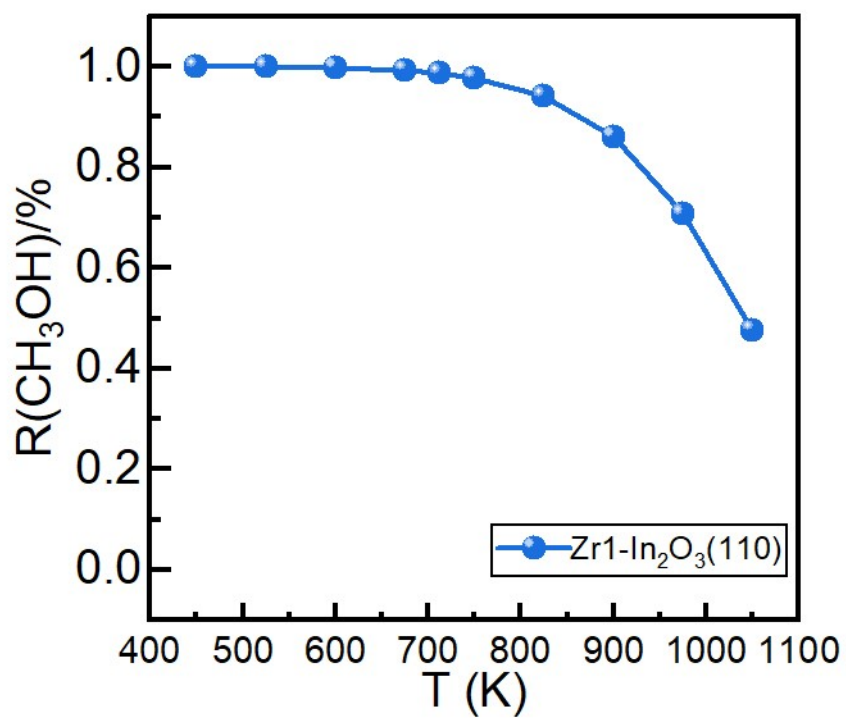


Fig. S2 CH_3OH selectivity on the $\text{Zr1-In}_2\text{O}_3(110)$ surface as a function of temperature at $P = 50$ MPa. Simulation conditions: $\text{CO}_2 : \text{H}_2 = 1 : 3$.

Table S2 Optimized fractional coordinates of $\text{In}_2\text{O}_3(110)$ surface.

O In

1.000000000000000		
10.213699999999993	0.000000000000000	0.000000000000000
0.000000000000009	14.444300000000001	0.000000000000000
0.000000000000010	0.000000000000010	15.987399999999992

O In

48 32

Direct

0.6079977758159562	0.1825443267066757	0.4362712132315722
0.1079977758159491	0.6825443267066685	0.4362712132315722
0.1088358797402761	0.9647164686301137	0.4544776404754274
0.6088358797402832	0.4647164686301211	0.4544776404754274
0.3237697993724533	0.5823222352526369	0.3458009054715419
0.8237697993724530	0.0823222352526370	0.3458009054715419
0.8249436211383252	0.5647822957564071	0.5361659930409042
0.3249436211383254	0.0647822957564142	0.5361659930409042
0.1004400036094762	0.9670707940212659	0.6664946814505766
0.6004400036094764	0.4670707940212659	0.6664946814505766
0.3276869710058980	0.8186750267869800	0.3452316937746626
0.8276869710059048	0.3186750267869800	0.3452316937746626
0.6035619394263214	0.6845843913661551	0.6839007798607878
0.1035619394263144	0.1845843913661551	0.6839007798607878
0.8347969046942195	0.3285776837991363	0.5396039931430473
0.3347969046942196	0.8285776837991363	0.5396039931430473
0.5592863488620317	0.6966328822454846	0.4602896482808987
0.0592863488620316	0.1966328822454846	0.4602896482808987

0.3876122828260632	0.0664155913604292	0.3195694488287623
0.8876122828260632	0.5664155913604222	0.3195694488287623
0.8749496178167006	0.0848903445515157	0.5594122645940717
0.3749496178166936	0.5848903445515086	0.5594122645940717
0.0591186490129696	0.4582472575521438	0.4418050676606413
0.5591186490129697	0.9582472575521440	0.4418050676606413
0.7976330763916604	0.2150198092098662	0.6903864507322498
0.2976330763916602	0.7150198092098591	0.6903864507322498
0.3115778210851878	0.4369385927663886	0.6815715884936553
0.8115778210851878	0.9369385927663886	0.6815715884936553
0.0963980041237094	0.3204479613229509	0.3135665666295812
0.5963980041237166	0.8204479613229581	0.3135665666295812
0.6084134801500255	0.8387169682347516	0.5758531430938664
0.1084134801500187	0.3387169682347519	0.5758531430938664
0.3327131938999144	0.4271886940543347	0.4593564361655760
0.8327131938999216	0.9271886940543276	0.4593564361655760
0.0906674283111391	0.0851412654712250	0.3110657182851373
0.5906674283111463	0.5851412654712179	0.3110657182851373
0.8291825599120484	0.7201845316407166	0.4358753052974278
0.3291825599120411	0.2201845316407238	0.4358753052974278
0.5968032405721470	0.0704413647463528	0.5842425191753895
0.0968032405721470	0.5704413647463528	0.5842425191753895
0.8737484761954306	0.6978499485243175	0.6700211219651597
0.3737484761954236	0.1978499485243174	0.6700211219651597
0.0302999243576119	0.8341367143849905	0.3222813343887312
0.5302999243576120	0.3341367143849976	0.3222813343887312
0.5577475925375229	0.3124571581123852	0.5632518436056515

0.0577475925375229	0.8124571581123852	0.5632518436056515
0.3697251589855949	0.9517961496304559	0.6861050408660482
0.8697251589856020	0.4517961496304629	0.6861050408660482
0.9682179951956762	0.2171449254848603	0.5833037966135592
0.4599692579064730	0.9304090492889371	0.3281802849324384
0.9599692579064730	0.4304090492889373	0.3281802849324384
0.4682179951956763	0.7171449254848604	0.5833037966135592
0.2193611289095702	0.5586595643459900	0.4601691075463029
0.2134011964617697	0.0911174480759769	0.4216006476694956
0.7134011964617700	0.5911174480759699	0.4216006476694956
0.7193611289095703	0.0586595643459899	0.4601691075463029
0.7452969211727367	0.5735795960104668	0.6668479393000794
0.1825260441747832	0.8249035604416677	0.4407489719499864
0.6825260441747972	0.3249035604416677	0.4407489719499864
0.2452969211727368	0.0735795960104668	0.6668479393000794
0.4629076550926099	0.1829749893261569	0.5479286501954356
0.9655272645636933	0.9705925897550166	0.3503764059616352
0.4655272645636933	0.4705925897550237	0.3503764059616352
0.9629076550926102	0.6829749893261498	0.5479286501954356
0.2193100812674732	0.8456208070942774	0.6565355911328576
0.2314540141486751	0.3029026133136766	0.6771607089445960
0.7314540141486752	0.8029026133136625	0.6771607089445960
0.7193100812674732	0.3456208070942847	0.6565355911328576
0.6782458658230517	0.8255794126190090	0.4428797529278882
0.2516637911520784	0.5764796956438837	0.6700539296556997
0.7516637911520783	0.0764796956438906	0.6700539296556997
0.1782458658230446	0.3255794126190090	0.4428797529278882

0.9607495810357845	0.1996548941339188	0.3383061922749663
0.4649597210201160	0.9510077479520501	0.5657591383142018
0.9666091270260179	0.6995699288742170	0.3374778360800877
0.4664404260882603	0.4478861639786720	0.5667755790775283
0.9664404260882601	0.9478861639786719	0.5667755790775283
0.4607495810357845	0.6996548941339189	0.3383061922749663
0.9649597210201158	0.4510077479520572	0.5657591383142018
0.4666091270260180	0.1995699288742170	0.3374778360800877

Table S3 Optimized fractional coordinates of defective $\text{In}_2\text{O}_3(110)$ surface.

O In

1.0000000000000000		
10.2136999999999993	0.0000000000000000	0.0000000000000000
0.0000000000000009	14.4443000000000001	0.0000000000000000
0.0000000000000010	0.0000000000000010	15.9873999999999992

O In

47 32

Direct

0.6079304306729710	0.1825690215715158	0.4368002770924072
0.1077085674083970	0.6835891347653099	0.4371468220022620
0.1100480918313145	0.9633439022381499	0.4553092194490885
0.6077253005124805	0.4661751638983551	0.4553921428562343
0.3237124704458665	0.5840065164061800	0.3487404656572097
0.8241468588000934	0.0821072274832828	0.3453147846174471
0.8241227375003781	0.5649687914808678	0.5355691360838742
0.3268854739590573	0.0620937287386814	0.5357844922084158
0.0984780605025536	0.9713631139336384	0.6650067682517364
0.6004802351847963	0.4681976078818302	0.6674738275809342
0.3304425657164959	0.8190602812738225	0.3488488857939541
0.8269792518189398	0.3184267961972426	0.3458629052755592
0.5974900948387206	0.6873539464590392	0.6837149025575708
0.1033444385326377	0.1854841090061509	0.6838518813614721
0.8346515694965811	0.3292829040744734	0.5390688790005360
0.3341159384508046	0.8203128109655429	0.5460974891796149
0.5644195933562155	0.6958761821581845	0.4543376655933901
0.0598527968167493	0.1952141829568810	0.4606225176410749

0.3874214964378343	0.0670870879797024	0.3199669742895427
0.8884523512670672	0.5660829758312650	0.3195937585155770
0.8734078586249732	0.0854749803648107	0.5586596772107414
0.3714820135440350	0.5896106914100475	0.5662293537973380
0.0598778175509802	0.4588971357099526	0.4413756320873790
0.5594752245616545	0.9573426159928082	0.4411161338596047
0.7975955963560550	0.2155033927532374	0.6896138580944809
0.3112948481602416	0.4340634312167818	0.6764807594143428
0.8106182611231411	0.9373086741816931	0.6807203383760182
0.0965799062839993	0.3193089031172244	0.3144034443756113
0.5959681253277086	0.8214345714748595	0.3102518517591656
0.6123664047864682	0.8379121633542027	0.5717297093354891
0.1072337655653284	0.3379081612069428	0.5750318070410076
0.3324472462534441	0.4287908027453287	0.4612040273618646
0.8340787551045923	0.9276507090835280	0.4578727472570610
0.0916507471849532	0.0845702549981880	0.3115310722236380
0.5902304220608053	0.5835707030308743	0.3086238491082409
0.8309704378604588	0.7200353252756559	0.4348064170010208
0.3293881233756207	0.2200145002068597	0.4373622066178390
0.5963986355486008	0.0685731294441945	0.5845115122679980
0.0986509815324042	0.5709100272980906	0.5839517924289470
0.8699293695454243	0.6974976268767483	0.6695950515764795
0.3743549725308298	0.1956172678515657	0.6693640077880189
0.0315738792764035	0.8340621355862500	0.3221982291338083
0.5290401108347905	0.3346681723110753	0.3239527557737026
0.5572894227413215	0.3130876971873919	0.5637893317637325
0.0564702221374198	0.8124596368857852	0.5662283789511928

0.3686526544532605	0.9492010850853387	0.6864338558918153
0.8698344140413419	0.4521567319971163	0.6855585160410870
0.9675189864106216	0.2178452079166702	0.5830350654726754
0.4598586596943248	0.9312785992289118	0.3274643328884503
0.9601019777880750	0.4293166614818133	0.3287817416581935
0.4811463952202831	0.7139124370851010	0.5739090872649887
0.2196793630738668	0.5598246955379115	0.4641527010011173
0.2138724193119459	0.0908825637450463	0.4222246859180634
0.7168712740127819	0.5890757792855817	0.4185556299930151
0.7192480870643766	0.0588684797593408	0.4595714863703799
0.7442270052733285	0.5736010689004185	0.6664604300533979
0.1822014573664816	0.8239414870759709	0.4414419367547601
0.6810347471891793	0.3261640843475209	0.4415160209609933
0.2453771768528208	0.0749635582971302	0.6657460311966732
0.4644969882140590	0.1825067568865118	0.5479538388074916
0.9671235161326845	0.9706865201750098	0.3497222358375572
0.4641785311812667	0.4713181310009989	0.3522851694199939
0.9628603044959312	0.6815998838166549	0.5481411920090332
0.2140930781652488	0.8491110250649558	0.6574941179119635
0.2320455781729497	0.3021627899985138	0.6765504792171636
0.7302673527834967	0.8037806641437882	0.6765875731530203
0.7194551412829500	0.3467230316121135	0.6557044964604436
0.6820557090221204	0.8261878324325261	0.4382637803024193
0.2458806932649837	0.5791393267272685	0.6816772041096553
0.7514993533179353	0.0773223247024540	0.6698899674189539
0.1785237309962821	0.3259752960020086	0.4436088015334787
0.9607839461139976	0.1994263219471198	0.3391466434515312

0.4662088688332464	0.9489103517959434	0.5656198490101498
0.9688095605917886	0.6991472543110302	0.3369609086349577
0.4609572182108231	0.4480790719232645	0.5709655405364465
0.9644488321498866	0.9488861957917152	0.5658986214715223
0.4615970514296781	0.6991018305054362	0.3348068197688859
0.9664206796342327	0.4516153205498062	0.5657800972797521
0.4661977768321241	0.2001894360048248	0.3381434025873608

Table S4 Optimized fractional coordinates of Zr1-In₂O₃(110) surface.

O In Zr In

1.000000000000000			
10.213699999999993	0.000000000000000	0.000000000000000	
0.000000000000009	14.444300000000001	0.000000000000000	
0.000000000000010	0.000000000000010	15.987399999999992	

O	In	Zr	In
48	8	1	23

Direct

0.6081751382365200	0.1836668020697766	0.4373394366065556
0.1082280470806027	0.6830188910621765	0.4369151423874010
0.1080881261708425	0.9652439084825356	0.4544998070909977
0.6077204946199337	0.4657334709641098	0.4533294302570063
0.3225665016399233	0.5825513995963343	0.3446163458945188
0.8230516735635108	0.0820444223500023	0.3465618023662485
0.8158318674861913	0.5638700378264527	0.5418050551955425
0.3246953870536911	0.0646711749718297	0.5362389265323095
0.1012638505963335	0.9678554632957733	0.6669179910639184
0.6076251641681081	0.4741882567591653	0.6579690648975784
0.3282199555656653	0.8189270970937395	0.3444147342377131
0.8286008597498070	0.3182214128782598	0.3464132556388707
0.6100938955672673	0.6763109337991308	0.6788036514994874
0.1046943916869544	0.1851336770903588	0.6851962628530718
0.8353784353573821	0.3313668522461583	0.5415245203507024
0.3348925461873569	0.8288737979666682	0.5391957688329508
0.5589391196780891	0.6956075261617580	0.4598078147150156
0.0590645224776527	0.1967947653224527	0.4607495510438274

0.3885893878994097	0.0660203957851848	0.3207649736194471
0.8849917678350618	0.5661638187560231	0.3225799362114343
0.8743586955454971	0.0853105475711573	0.5604969823907774
0.3704405489689614	0.5848806132393782	0.5583547664729525
0.0570912446598973	0.4590913737895065	0.4428619948520192
0.5597638103084877	0.9572318027726373	0.4427445914653429
0.7976772978029185	0.2159349453233784	0.6906700139843019
0.3001605523539919	0.7152148718473338	0.6894646859274771
0.3141835597002695	0.4373195551950051	0.6804210213932387
0.8116894412806330	0.9365478818456442	0.6821822702653770
0.0970371550367970	0.3210257754536378	0.3138697397765333
0.5984927326904298	0.8198305278608885	0.3146811944265934
0.6061096905790786	0.8363468630370335	0.5777110337028800
0.1104819496020358	0.3380858945981394	0.5767839222012620
0.3312619085533887	0.4270652782562528	0.4578053965608655
0.8324645157930290	0.9262291190812177	0.4607944572845751
0.0900676947137505	0.0852291033473583	0.3109739274503345
0.5884904532197660	0.5854301330139655	0.3085478871396178
0.8303917839921514	0.7171191994290576	0.4394017040002641
0.3298625940956357	0.2200853448615069	0.4358258423619532
0.5968707416154463	0.0705470694284030	0.5843206800484261
0.0908191327151766	0.5705640408677323	0.5867600334244064
0.8710266649688277	0.6959762326227932	0.6687475688164292
0.3759106253288291	0.1975361863282616	0.6701198243186480
0.0293655304893394	0.8341272432524662	0.3236179920550251
0.5310230554284340	0.3344714923002514	0.3228085392081093
0.5563983016101108	0.3140066380040432	0.5645293829250274

0.0594177208507446	0.8137480993033617	0.5643241228804139
0.3710371064992727	0.9518255858291355	0.6865876872447175
0.8657588735910402	0.4558644907705776	0.6888652900892822
0.9695088335136360	0.2163180440658462	0.5842432762106328
0.4619128703267296	0.9301786474185190	0.3281007139295537
0.9597252048473386	0.4300990132961821	0.3280914101994045
0.4661952271089457	0.7161978438284099	0.5826272008861269
0.2186794735537982	0.5586699515932375	0.4584809581938857
0.2143800172788712	0.0906774137876923	0.4209407190629167
0.7111547624998757	0.5910499803953674	0.4186898969280803
0.7190991994568940	0.0585701533623428	0.4608733321768382
0.7540263652778508	0.5716617892398173	0.6615778886991834
0.1836643188998238	0.8262009250330223	0.4400870563689782
0.6816577575962136	0.3259520692991601	0.4397542308538714
0.2464421700326436	0.0737680341433121	0.6673404599073980
0.4625990054755051	0.1827597482225865	0.5472827783834283
0.9645331020967661	0.9706884905514167	0.3503614417809621
0.4639992751707245	0.4707271042782106	0.3478867933136154
0.9667555415726097	0.6856919682064442	0.5468624148439833
0.2207533910950263	0.8466704259310547	0.6569891120715314
0.2340720424361232	0.3023749321932661	0.6783423854204201
0.7305688441935074	0.8034157883667202	0.6777123252519012
0.7159637547638780	0.3435815951434624	0.6550339588562482
0.6785907206960718	0.8248097120749667	0.4439089969846653
0.2502354522345033	0.5768066364833474	0.6705395028128075
0.7504757454572119	0.0763757883823033	0.6711852086650646
0.1784552773122194	0.3247530586234607	0.4422522001667673

0.9606031490838437	0.1992446777223590	0.3384443254648393
0.4646447733381387	0.9510804523968324	0.5657792576529838
0.9660874603119951	0.6996204166978089	0.3373513846698640
0.4619344669524018	0.4480875770086936	0.5649444948680042
0.9673063835560426	0.9489126746184676	0.5671415219728689
0.4599667130984318	0.7000963974065889	0.3371231094935748
0.9691603861089049	0.4483552062513810	0.5667803938376730
0.4676238000392227	0.1994134702697347	0.3368152261104792

Table S5 Optimized fractional coordinates of defective Zr1-In₂O₃(110) surface.

O In Zr In

1.0000000000000000			
10.2136999999999993	0.0000000000000000	0.0000000000000000	
0.0000000000000009	14.4443000000000001	0.0000000000000000	
0.0000000000000010	0.0000000000000010	15.987399999999992	

O	In	Zr	In
47	11	1	20

Direct

0.6085413404815252	0.1835291752756111	0.4373118694140167
0.1081015213609581	0.6838297450136619	0.4374488862271114
0.1096916136801709	0.9647130747628530	0.4529545394222271
0.6070687948659901	0.4672635083178537	0.4555776918846583
0.3231967946500799	0.5832546241073059	0.3495005066065773
0.8227676688918406	0.0824283818464371	0.3440114044746452
0.8236518527915861	0.5653386630702877	0.5355948941189144
0.3178934230782695	0.0618362402403157	0.5405828143313167
0.1073620491708970	0.9756404999280534	0.6558901394679668
0.6010578771433425	0.4690556935238095	0.6685408660594858
0.3307036632302112	0.8182323265242523	0.3505300625640442
0.8279003536962783	0.3193031449729125	0.3451491456834082
0.5984520122429623	0.6881227456299478	0.6840727917262133
0.1108856775031225	0.1764079211472495	0.6785740030244075
0.8345680765749093	0.3297133887629016	0.5390943191725041
0.3356271702568655	0.8234935439282532	0.5495533982152158
0.5641315291030410	0.6962256720419906	0.4543491478718840
0.0589771522728553	0.1948048128286315	0.4600226997653858

0.3848789493468351	0.0670826540730108	0.3226343243611118
0.8902745880565278	0.5658391824001550	0.3197515200966398
0.8700501444707807	0.0846249437751347	0.5579454072714859
0.3705044933026446	0.5906221634265072	0.5675463392589749
0.0601922852260282	0.4577860298140982	0.4426653336868792
0.5565591540965040	0.9578761116795643	0.4422566123083752
0.7996193255366733	0.2153447105377388	0.6886686413464760
0.3102187887517601	0.4342114927126203	0.6779525709601085
0.8132571181838667	0.9374880077125834	0.6803749435562361
0.0989706544075131	0.3192606498972024	0.3154091439988300
0.5957361819404543	0.8219697293434263	0.3099731826191230
0.6151693852629037	0.8376787551574219	0.5720003025629056
0.1045736194456830	0.3355743357592576	0.5773307140386413
0.3319623546603336	0.4282931620917264	0.4634802661127205
0.8330511407774139	0.9276571610897082	0.4558354373606121
0.0891927525747463	0.0854721709877795	0.3087234390073254
0.5894342571680470	0.5837116940273199	0.3082882021742115
0.8311230119984314	0.7197064888139849	0.4335804138263287
0.3303265663285877	0.2176630993019835	0.4404136516721081
0.5913631157838058	0.0689417412592727	0.5856904840592462
0.0976656795001817	0.5710677253748734	0.5840922102682443
0.8712628782762221	0.6974122805463885	0.6695903547069442
0.3718474726034157	0.1941551878566274	0.6678853058751235
0.0326151041907458	0.8341925600678227	0.3213824303716051
0.5284117598441396	0.3351953101469455	0.3252608184154724
0.5584583636543500	0.3150016596572264	0.5650118626644897
0.0552830338990327	0.8136627185664264	0.5645325482546041

0.3685133878993194	0.9565705254397151	0.6897476972888034
0.8703075545407496	0.4525801090615665	0.6862327085510468
0.9660132038787158	0.2161729813266663	0.5827721078126703
0.4587328971497971	0.9309401628577509	0.3274849617178777
0.9626428544636445	0.4295273367306988	0.3285222512527472
0.4820989263354945	0.7141890877075950	0.5742354998644618
0.2190648426031808	0.5597095748379360	0.4647579051177239
0.2116651587615292	0.0911601039943152	0.4191881013573772
0.7175100574604383	0.5890652023491801	0.4175081006670481
0.7183602508374527	0.0586378602843423	0.4579444381737412
0.7448540139520311	0.5742160817824260	0.6667501773355483
0.1820227771017848	0.8248607613088510	0.4423434744819795
0.6822956445482992	0.3278620911130383	0.4409842952382097
0.2542690845857022	0.0702188739735560	0.6607520033446174
0.4680466473962889	0.1855470497783566	0.5473693690253157
0.9659251311741417	0.9706262593123092	0.3470906198337312
0.4632799529731437	0.4714197002853512	0.3525889680715016
0.9619011349325256	0.6822111087166793	0.5471690536665696
0.2111590394238863	0.8399325338143065	0.6634028046823616
0.2312172021249671	0.3019989779316941	0.6770997670321536
0.7323481250473147	0.8036918530989415	0.6773380670970934
0.7206668908380882	0.3474756411594672	0.6564052547486252
0.6821982440941212	0.8257965594604926	0.4371350463411143
0.2432030646211824	0.5800342034725153	0.6821887958072648
0.7496276835345775	0.0770262911648248	0.6699832887887189
0.1785560985318786	0.3252838903138182	0.4449488016783190
0.9596783462192544	0.1999470331813505	0.3378634198647517

0.4686598372885507	0.9462438283510590	0.5671041159115667
0.9704438943989956	0.6992049933432581	0.3360146209041805
0.4612383013936233	0.4495536102407344	0.5722444619494855
0.9626992935376795	0.9484638778164488	0.5640305234614000
0.4611276742600350	0.6987881991927856	0.3346649162307175
0.9655721916384289	0.4516649537094151	0.5660742461515623
0.4658498421706384	0.2004637948894252	0.3381544956849271

Table S6 Optimized fractional coordinates of Zr₃-In₂O₃(110) surface.

O In Zr

1.0000000000000000

10.2137000000000011 0.0000000000000000 0.0000000000000000

0.0000000000000000 14.4442999999999984 0.0000000000000000

0.0000000000000000 0.0000000000000000 15.9874000000000045

O In Zr

48 31 1

Selective dynamics

Direct

0.6085130314376889 0.1815443042852970 0.4344215233695581

0.1095143572599503 0.6801554332332203 0.4389540452042276

0.1119235571755236 0.9643886264863795 0.4564536782964743

0.6155919725189041 0.4640478358177008 0.4455278421855437

0.3279391756557578 0.5815266610985488 0.3404890466870635

0.8272659884805668 0.0824036132089090 0.3471668387998894

0.8249026967663836 0.5645214721752039 0.5335176343698722

0.3266626692944860 0.0641560562622397 0.5373086503803838

0.1022464665259393 0.9669766894246630 0.6676045522294183

0.5902197168558052 0.4684138340796453 0.6613693956702296

0.3317147838544213 0.8167263021585905 0.3498967625399347

0.8332631413374636 0.3176972531204796 0.3422910345900488

0.5940872711568971 0.6854980789313910 0.6822276410128030

0.1032642775098447 0.1853117741355407 0.6863957307721228

0.8363713657521338 0.3274954523394515 0.5380420445664392

0.3358272334036523 0.8217743851129402 0.5458113662323282

0.5630490200449794	0.6909331879879580	0.4555609080154211
0.0619786408376100	0.1961720955697507	0.4622923314380978
0.3862311514793551	0.0656460740582615	0.3206684394190016
0.8943132887023599	0.5656498720209124	0.3190699664356795
0.8755316353484911	0.0845791705015433	0.5609122343198700
0.3663389950073165	0.5841253770304649	0.5674704266363475
0.0614325481013441	0.4590074261737580	0.4434150079709449
0.5598150685728369	0.9572842005775563	0.4418814338074541
0.7959402055824101	0.2161872929261814	0.6898258973553725
0.2497860471290857	0.7071788074219785	0.7049625598968342
0.2615868914481031	0.4462749940091072	0.7119542511633911
0.8100199508932936	0.9368796060965072	0.6821625478462917
0.1040242789167669	0.3203266152764432	0.3163795569863326
0.5982144221208789	0.8209915591877934	0.3116920055985617
0.6129597280020027	0.8375505220127464	0.5715758959331746
0.1119760236557366	0.3408590548460155	0.5778018440852174
0.3363269413188474	0.4306437466970712	0.4572538643415164
0.8354497278669554	0.9272388387996880	0.4593841274881746
0.0941857942040875	0.0848166216679789	0.3119817395054509
0.5946728432161461	0.5858263952520918	0.3042713898514371
0.8321795466117835	0.7203082603242468	0.4321827491089324
0.3322007999394878	0.2208547352948300	0.4366276089050263
0.5968468229303877	0.0708961598759511	0.5841139956556352
0.0921206047812925	0.5709216216378776	0.5927883770092166
0.8656933847454715	0.6970357548770071	0.6678691188063545
0.3719221684174530	0.2026405587632320	0.6688862302344231

0.0376205680111080	0.8344958189737779	0.3246958891547423
0.5322200573268997	0.3329781016787788	0.3190263573199568
0.5602490307754066	0.3133862851282717	0.5585930862682085
0.0579564378105647	0.8118419451256643	0.5638476569575397
0.3709045076351969	0.9508625562570322	0.6864850745283870
0.8600077143323372	0.4521190306782269	0.6839352485824584
0.9697051222020970	0.2166761488712719	0.5848829498652591
0.4598843548470384	0.9302976803045271	0.3281745553987234
0.9664480402173528	0.4290643562925834	0.3270261053467875
0.4781355932474225	0.7161116751241484	0.5743282272168908
0.2206798907928754	0.5576580866098821	0.4524501433232762
0.2164065371460923	0.0905187784511605	0.4225369305956197
0.7220706754042645	0.5900222087169115	0.4138272727937961
0.7207659259188004	0.0585094705042923	0.4606594359632958
0.7394537994494712	0.5740619682546572	0.6641596882200423
0.1838765489762455	0.8242677484443933	0.4436036290132196
0.6875668784643812	0.3213504594429619	0.4363352413397970
0.2460787731370676	0.0747007224677743	0.6672641548243037
0.4628685950406741	0.1836639445091167	0.5475623127470612
0.9689663728093876	0.9707551677353411	0.3515175656958836
0.4710052266992912	0.4703028937176538	0.3401518439521998
0.9592546779572575	0.6841821348638442	0.5469038141249108
0.2184340519268341	0.8439453111824894	0.6618525256595388
0.2274258304834198	0.3063838304583524	0.6844626770172473
0.7278270326016931	0.8041583390000656	0.6778187699694033
0.7150783428299098	0.3448017709824209	0.6542252787985126

0.6827567813922883	0.8263481135718588	0.4392327937547746
0.7507224952686364	0.0769179673835196	0.6711849091277839
0.1810216265964975	0.3246577486087689	0.4459679197302455
0.9654066436283761	0.1987765543722154	0.3389605469957896
0.4662697594386452	0.9501646832345721	0.5663426818967862
0.9732017634823149	0.7000041540672405	0.3348802549428618
0.4817086764033626	0.4515223189906039	0.5518081633068110
0.9675832195674662	0.9479176986588582	0.5681372147801333
0.4649769472457950	0.6997509008643177	0.3333521841821521
0.9622260712634179	0.4496199405146807	0.5653916074088577
0.4663176062012516	0.1987759426121594	0.3355498088602615
0.2418435886089796	0.5762612225884310	0.6696431856159880

Table S7 Optimized fractional coordinates of defective Zr₃-In₂O₃(110) surface.

O In Zr In

1.0000000000000000			
10.2136999999999993	0.0000000000000000	0.0000000000000000	
0.0000000000000009	14.4443000000000001	0.0000000000000000	
0.0000000000000010	0.0000000000000010	15.9873999999999992	

O	In	Zr	In
47	21	1	10

Direct

0.6102792875503488	0.1828108140755455	0.4324927636177608
0.1102857668385805	0.6788293338708421	0.4408454507468572
0.1137754987081554	0.9670349854859359	0.4552970892233930
0.6186454213003293	0.4652484581486443	0.4429016959682970
0.3303122283321767	0.5819112905228656	0.3339413079529121
0.8294638308953903	0.0844925967984694	0.3463413595832950
0.8264516637941385	0.5663639319189864	0.5335939582480402
0.3282186130365721	0.0666812189409105	0.5353574220113940
0.1085400186879968	0.9652963055030435	0.6657739875885675
0.5862947016473827	0.4707565205333885	0.6592108712645774
0.3313154774295533	0.8166479730884076	0.3498972259814408
0.8363489709200255	0.3198285113368546	0.3409520691621034
0.5864940130443901	0.6874729771060729	0.6818106685950183
0.1047344109736850	0.1846583369743045	0.6833997477927871
0.8372889158559287	0.3287911008419737	0.5373391154933436
0.3357706243827671	0.8252314930501594	0.5450659937061385
0.5615722752397232	0.6897575024741470	0.4546535034832774

0.0632169852729394	0.1989285636274321	0.4613880414579888
0.3865847076658767	0.0668111045402705	0.3195868363891392
0.8964018230209144	0.5678557264639124	0.3187936670914810
0.8773136228250256	0.0844527607827043	0.5605980997005545
0.3577134884254677	0.5855381255975967	0.5685298972201093
0.0629677526157365	0.4625283155343898	0.4456174842214736
0.5605770658123138	0.9585508780801353	0.4404424010837619
0.7953268067130039	0.2166927670716846	0.6884020475881404
0.2641654629981289	0.4466468654567899	0.7088906918325507
0.8094152859882786	0.9380016815566019	0.6843758309584640
0.1071177196342807	0.3242353244145054	0.3165132495424409
0.5983235508103331	0.8221805041850435	0.3107723994647615
0.6148256711589783	0.8387428596305995	0.5693499590283572
0.1129381876481068	0.3438665165849787	0.5777304347544402
0.3391107588830957	0.4332022351727083	0.4541435971828508
0.8371588822939020	0.9289586420692544	0.4582115249671189
0.0958549566801880	0.0873551683985676	0.3104594851846384
0.5978314503148076	0.5880617553962001	0.3020650517430418
0.8314026683743954	0.7214926798675513	0.4311909952010177
0.3340366897613053	0.2234534999309701	0.4350088055536435
0.5991526419838534	0.0722943600080969	0.5813704309116324
0.0868725375966308	0.5732930617453954	0.6086398300130157
0.8596292033296091	0.6986361750843829	0.6685207362425093
0.3759180684686587	0.2037774123283896	0.6677690572301918
0.0401319678888785	0.8359539080799819	0.3254516400352113
0.5356817924663496	0.3338705386526457	0.3168716394426170

0.5611764396865068	0.3148869543436670	0.5567099702912621
0.0550344296582835	0.8119730868923868	0.5603150323220674
0.3788920272842192	0.9559813865168387	0.6866624265500005
0.8552447534986951	0.4529097989821001	0.6839125993066743
0.9690000930394228	0.2168308897446474	0.5834537931310448
0.4582276311509602	0.9308850793923281	0.3280154821431697
0.9687488025304485	0.4318877125775888	0.3274208688787477
0.4766962701020734	0.7203331723423415	0.5715688675215919
0.2245534697063770	0.5589162742887867	0.4453952234766020
0.2180836671159213	0.0926020199270169	0.4211059031619139
0.7236123225005233	0.5917760521306379	0.4123458629158186
0.7224890864464159	0.0593295406060713	0.4595010541083036
0.7356892902832659	0.5760605302057927	0.6634920953484106
0.1846225172414332	0.8257467585197791	0.4458527294733424
0.6898339091605179	0.3219887799254922	0.4342341603337083
0.2488709102294420	0.0733559953482530	0.6660851968277413
0.4650849160700875	0.1844206782574310	0.5454614942894037
0.9710819018665774	0.9726834184053811	0.3512128242938467
0.4757630549762478	0.4715256363389501	0.3352819963602100
0.9564597843700438	0.6866512497419642	0.5475637703897024
0.2260036273334101	0.8382572288627772	0.6751643730430331
0.2292404376181883	0.3032028948845453	0.6803668464812915
0.7237020187536035	0.8069048108474208	0.6779996368335519
0.7133109111721579	0.3451398053053460	0.6530645332101033
0.6843123100026748	0.8286368534586243	0.4377274394810968
0.2447418027059652	0.5711716422092527	0.6706754335605417

0.7505427106477487	0.0769955913550260	0.6701039084066386
0.1825853706116787	0.3266531460022215	0.4454928795783199
0.9675035371674896	0.2008428641579960	0.3374979402890843
0.4657720510748363	0.9517353778897717	0.5651245493069196
0.9754729560347429	0.7020079252057457	0.3354414295870796
0.4843795155877098	0.4530418209600667	0.5476921958059868
0.9726890912079339	0.9485590975867756	0.5679879223931432
0.4666114350248388	0.7013895302499833	0.3312414210195345
0.9609424394390974	0.4511007524793295	0.5664206967064574
0.4677830414322406	0.1998608631262915	0.3336893787133073

Table S8 Optimized fractional coordinates of In-CO₂ adsorption on In₂O₃(110) surface.

O In C O

1.0000000000000000		
10.2136999999999993	0.0000000000000000	0.0000000000000000
0.0000000000000009	14.4443000000000001	0.0000000000000000
0.0000000000000010	0.0000000000000010	15.9873999999999992

O In C O

47	32	1	2
----	----	---	---

Direct

0.6091114443259160	0.1819407289191223	0.4347767875663932
0.1085877025047812	0.6831818639680752	0.4362595744337136
0.1110681091181432	0.9618052188377647	0.4536389384306919
0.6091514620516423	0.4651408833231080	0.4538553940510164
0.3243626793625463	0.5833098806828271	0.3482403941823417
0.8256408545526470	0.0810263747706245	0.3433820008608834
0.8246430097337227	0.5643715006844877	0.5343400835480985
0.3281702061716577	0.0608036312404446	0.5337005626676591
0.0981715041114084	0.9731494428607915	0.6624217290682465
0.6019455820117058	0.4673161426789660	0.6665643960616996
0.3321255062819687	0.8183872391272410	0.3471219192060441
0.8287552154360139	0.3174898269449552	0.3447730506003815
0.5982155391501333	0.6870883782208276	0.6832912879675839
0.1041109179701078	0.1846635190478692	0.6830028735475125
0.8358677274004558	0.3282823237529244	0.5380290389650747
0.3349840769628837	0.8186170962744358	0.5447330111166915
0.5652990729592831	0.6948546490255910	0.4529635229933198

0.0611970811725124	0.1938433492410503	0.4591919098605129
0.3893210218363938	0.0662373307043450	0.3176404590939974
0.8899990477257537	0.5650916426435466	0.3178109578359229
0.8735241301881506	0.0851149484287720	0.5568897647319547
0.3725674552169016	0.5879030362180034	0.5657828802655240
0.0611613238414867	0.4579646930762906	0.4401208862747358
0.5608742267441693	0.9563001105195108	0.4391189035723158
0.7984175291183008	0.2146584054105552	0.6888923998676659
0.3144717885539560	0.4307171523197880	0.6754796094182340
0.8108893808620401	0.9369191180998170	0.6792898559493502
0.0982119741337721	0.3182244375642203	0.3130185202079860
0.5973218818769125	0.8203114048047834	0.3083479660931339
0.6132016740148423	0.8366647498436850	0.5699810650396789
0.1082248785572829	0.3367366941623813	0.5736855086916492
0.3336130802279950	0.4275734270838780	0.4602021436313681
0.8349744193310291	0.9267102420156291	0.4560142388556500
0.0930141546278334	0.0833006274024142	0.3098917040451959
0.5906762363984747	0.5824987494785705	0.3072132423048250
0.8320803597079062	0.7190500347541580	0.4331163490962143
0.3305851595932446	0.2188172282454499	0.4354644969236371
0.5973828675443191	0.0678146640616173	0.5823794034716518
0.0997709651127246	0.5696683747453686	0.5826389287857915
0.8707882803547318	0.6968553345881235	0.6685349269606528
0.3758752356671169	0.1942799854683635	0.6674328307764660
0.0329390910516833	0.8329278995121863	0.3198307616622234
0.5298221938713042	0.3340547502096443	0.3219103087441960

0.5590428816950669	0.3120562384236426	0.5623662672471105
0.0566883271014262	0.8119716822704311	0.5660314171797274
0.3694987658065150	0.9485397949333959	0.6842160914349867
0.8712079669868571	0.4514967281335605	0.6843710107506262
0.9687803298845947	0.2169481336668846	0.5816628832348387
0.4617547166408452	0.9305123155107566	0.3251918004168634
0.9619590385561703	0.4284053836832873	0.3274665948930804
0.4823406863059452	0.7119660625599910	0.5728339254139926
0.2209729761121870	0.5590372460460208	0.4639004781523290
0.2151593391115958	0.0896341637480664	0.4204232181560513
0.7179509084030000	0.5879898163746753	0.4168201335694414
0.7201924270694527	0.0582608308983665	0.4574564217114128
0.7453207113258802	0.5728551874573946	0.6655948579454093
0.1836367034921026	0.8229120307003827	0.4392641598526016
0.6826124231924440	0.3253799255322081	0.4402172656713064
0.2469883003461766	0.0749891454800454	0.6638727127891304
0.4655791941065779	0.1818501004824511	0.5458610009596929
0.9682864021475965	0.9694136674292383	0.3476874808636126
0.4645455542480390	0.4702879742689406	0.3513045498361408
0.9640141361188287	0.6804302162225808	0.5471228025191255
0.2138766193198444	0.8525632581224752	0.6531866404756708
0.2327885035676418	0.3005870962640001	0.6755114476079936
0.7310607280005683	0.8032575806074539	0.6751176397359353
0.7207872899083589	0.3458835940345906	0.6547697744326318
0.6830261587417481	0.8249435772410244	0.4363725225012449
0.2463599900497857	0.5746947123437270	0.6826908145407615

0.7517109390430963	0.0769478665347768	0.6682644049053978
0.1797489882328341	0.3249394869084207	0.4423909823569289
0.9623434204161682	0.1984625160925931	0.3375528484194483
0.4681778947284619	0.9480665837140593	0.5635885990577109
0.9701890422563549	0.6980411519878069	0.3354671996560702
0.4621241008161769	0.4467095072920472	0.5701767511689795
0.9639718055051189	0.9485993073963808	0.5639487885432785
0.4624517362234599	0.6980218500281273	0.3334066201430402
0.9673570076633966	0.4507365102122336	0.5644718757678064
0.4673239772735145	0.1996239312668567	0.3359659934266793
0.2291695743188936	0.7448513721766374	0.8651045959577228
0.1927302433915626	0.8080934979580792	0.8246996227836477
0.2652441444558701	0.6823228650342065	0.9054632184937319

Table S9 Optimized fractional coordinates of In-CO₂ adsorption on Zr1-In₂O₃(110) surface.

O In Zr In C O

1.0000000000000000
 10.2136999999999993 0.0000000000000000 0.0000000000000000
 0.0000000000000009 14.4443000000000001 0.0000000000000000
 0.0000000000000010 0.0000000000000010 15.9873999999999992

O In Zr In C O

47 11 1 20 1 2

Direct

0.6098481282871878 0.1825639202036043 0.4353633945893160
 0.1091149015861139 0.6827906400327025 0.4354456878660807
 0.1108636309613575 0.9634629680302975 0.4503234713472434
 0.6082856149411022 0.4661367140316200 0.4543651706804296
 0.3241154691544046 0.5823493950044010 0.3480967782058311
 0.8240947777220723 0.0813785540976957 0.3408408976242883
 0.8248664540100206 0.5641987075746649 0.5338857202541928
 0.3187384381862934 0.0606951738774364 0.5388281251801017
 0.1077545915437765 0.9750492062116910 0.6532077833840479
 0.6025803085992748 0.4678471055833490 0.6671999030771789
 0.3318261473450249 0.8169449737274919 0.3477554223141982
 0.8292787034068273 0.3182683894258168 0.3432274866256341
 0.6006572097119984 0.6873290876714573 0.6825791121571686
 0.1121264268012767 0.1749346656521526 0.6760746755825666
 0.8357578931636642 0.3287159621871335 0.5368834498115692
 0.3372356424492872 0.8219649663616405 0.5464815675473287

0.5655625731342240	0.6949658196308419	0.4525153183083165
0.0603699289686399	0.1937870595390328	0.4574205708169002
0.3861197603424899	0.0659192265077426	0.3208284772132967
0.8909011977496423	0.5646431952491592	0.3177320486929213
0.8707250740267337	0.0838786120497466	0.5547547509528078
0.3722576472463139	0.5894936949052867	0.5659971323957049
0.0616241619388453	0.4565501447295777	0.4406063623328989
0.5582559632731345	0.9566960408445506	0.4398308481050220
0.8017989941835780	0.2143130810977970	0.6862880037171846
0.3109992057766220	0.4331440615194835	0.6759790029467384
0.8158454956409459	0.9364086634161958	0.6774709472809732
0.1005510415406680	0.3183124876328893	0.3130457289688475
0.5968445683381056	0.8205201944374835	0.3079371722888429
0.6170641929281119	0.8363996222781991	0.5697849318428303
0.1058402116100355	0.3343499413278499	0.5750547165807639
0.3332765940888620	0.4271463691851073	0.4618515162398248
0.8343663062856010	0.9267102837279678	0.4527664903532596
0.0908018319267907	0.0845208339348871	0.3062973528777840
0.5904746044856768	0.5824018019077183	0.3067493555109285
0.8325812328348001	0.7186689808168287	0.4318151744821469
0.3318917461156405	0.2166822495646824	0.4385498533728809
0.5922550835998152	0.0674963161690076	0.5838438472218567
0.0991965553303710	0.5697089943083848	0.5819749177889992
0.8738256833038029	0.6961336991746812	0.6679403629980497
0.3727800784777228	0.1926788571387640	0.6662759566627717
0.0338784316696032	0.8329873468946113	0.3188805822625112

0.5298986216765051	0.3343347965581882	0.3237900443516605
0.5597843107733375	0.3137837409549085	0.5634302725417492
0.0566419638494632	0.8127234795548236	0.5623898132274517
0.3676024446220444	0.9530194953228996	0.6869191883476790
0.8721923656219442	0.4514003861042827	0.6842104398371799
0.9669247762368751	0.2151871098066956	0.5799123463174033
0.4598533751890118	0.9296873507209181	0.3250921371284918
0.9640072754653279	0.4285174295622071	0.3264624415502673
0.4842763629907836	0.7126870508333581	0.5725018286655951
0.2203282434467276	0.5586286532959402	0.4632395145336762
0.2132357656239085	0.0900808099098079	0.4166971987407035
0.7187569436520951	0.5877966970704930	0.4157928775439750
0.7196033329703496	0.0577435361458931	0.4546783980120410
0.7467026712954729	0.5730059609704806	0.6653389619996564
0.1829362347846108	0.8235932258293432	0.4391585012488174
0.6834536454064375	0.3269268588792140	0.4389749723385316
0.2552043534407252	0.0695682162348636	0.6586724543282507
0.4695574147639502	0.1843558869097252	0.5454160090919670
0.9673337475151644	0.9696328189831954	0.3440048550324374
0.4643405559916867	0.4704661932641478	0.3513332692880350
0.9634318355215029	0.6807579400410255	0.5450979284703318
0.2122173933102603	0.8411817154703355	0.6580910464591551
0.2322646523884389	0.3009510453485431	0.6747849005998088
0.7350521798089243	0.8026813660963381	0.6750330226730661
0.7222282714281424	0.3463953044313417	0.6544349059678702
0.6835687613812899	0.8245234808664587	0.4347649265968200

0.2444520607364438	0.5793984891796600	0.6806309663474372
0.7516037547875610	0.0759492345449039	0.6673817327759725
0.1800074316663479	0.3242106577117633	0.4426044715563091
0.9610278521902113	0.1990425275723377	0.3351544964772782
0.4705052702573795	0.9449301973274212	0.5646468612509968
0.9712585334625837	0.6980168248636490	0.3338244876798082
0.4623853019134489	0.4483533089906176	0.5709245299922611
0.9635610820544519	0.9478242301150267	0.5606986430873229
0.4622584510062325	0.6975201536773009	0.3329251726050141
0.9670235641609777	0.4505573755778400	0.5639867987129267
0.4671159301217667	0.1995964508618012	0.3359826997339900
0.2227486392762425	0.7498855331384161	0.8838806425205453
0.1820513456449594	0.8203039262647889	0.8575350556740626
0.2634507808799897	0.6795625333474085	0.9095911182312229

Table S10 Optimized fractional coordinates of In-CO₂ adsorption on Zr₃-In₂O₃(110) surface.

O In Zr In C O

1.0000000000000000		
10.2136999999999993	0.0000000000000000	0.0000000000000000
0.0000000000000009	14.4443000000000001	0.0000000000000000
0.0000000000000010	0.0000000000000010	15.9873999999999992

O	In	Zr	In	C	O
47	21	1	10	1	2

Direct

0.6102945579902306	0.1830594574700455	0.4324105866453565
0.1102588833082892	0.6787221003036478	0.4414327399899445
0.1137073103593357	0.9670738988040625	0.4549839040592716
0.6184605427234491	0.4655081378137330	0.4431854659369180
0.3301322099208716	0.5819034441789361	0.3343906576382373
0.8294699251446928	0.0845354132116788	0.3462407112456549
0.8268663272085262	0.5665910899208337	0.5338791399687265
0.3285931082582978	0.0668367501533063	0.5347785417338192
0.1081634823758494	0.9669022532968998	0.6648107500121766
0.5865171927571744	0.4709161393082263	0.6597788250091827
0.3310378425416708	0.8165318958932763	0.3495547312980398
0.8364783736244785	0.3199502258011601	0.3410960644449864
0.5860000972694659	0.6877144227373556	0.6823472575674485
0.1037487987815298	0.1840814078908869	0.6834756616414104
0.8369016512896961	0.3289992991716258	0.5373032637223487
0.3358563368263235	0.8257718037294929	0.5447274435009549

0.5612562856981622	0.6895740156982526	0.4547200329649944
0.0632053975937320	0.1986817590146659	0.4611133542786591
0.3866894412844727	0.0668383420980975	0.3195066277157587
0.8962823865279432	0.5678181922929130	0.3187051776281870
0.8767453515092215	0.0846289780477705	0.5603617373934434
0.3580351823006651	0.5860688068716073	0.5698912278838457
0.0632034585901801	0.4629028378247984	0.4459002776593189
0.5607472861249029	0.9585133499843312	0.4402415825105654
0.7950849675920639	0.2167140160730199	0.6884638709838913
0.2677555754053189	0.4429642394194389	0.7052282760086266
0.8090771101330893	0.9380314835661803	0.6845369450217273
0.1072391812606660	0.3244272782480807	0.3164885218349944
0.5982149312855153	0.8220762902193230	0.3106767914802054
0.6147364376975102	0.8385017292354124	0.5692391721595725
0.1119007773449632	0.3428889639245715	0.5771647102585863
0.3391521301424850	0.4333993648116776	0.4547166300769341
0.8369130479122014	0.9290069191746337	0.4579751882987860
0.0958465094531075	0.0873814642859004	0.3102071020189270
0.5976248672439500	0.5879903194767564	0.3019195069318386
0.8313907965431609	0.7213612357908817	0.4312644955817617
0.3340614014663894	0.2237064904519532	0.4348339942252772
0.5994987518358654	0.0724083447002227	0.5810525328401366
0.0865869413655248	0.5728262076318024	0.6112280076094679
0.8596435509135505	0.6986304217781764	0.6692642750811399
0.3765142777986099	0.2028309493354777	0.6676257894986874
0.0400904263963762	0.8358395185955152	0.3252843289158846

0.5356875964756899	0.3340050205927287	0.3167419202453285
0.5608770532544783	0.3151855707863603	0.5568398008064225
0.0544004083282821	0.8123602715863978	0.5599787733686916
0.3797727331675533	0.9573930345472470	0.6864195581667006
0.8552807754719658	0.4528208331204704	0.6840541848838685
0.9684733394501175	0.2167766992293525	0.5830710683247567
0.4580801374023093	0.9308083066137003	0.3279975288977560
0.9689071216719630	0.4320047370669962	0.3276672024244980
0.4758531686664449	0.7201390858263176	0.5716432835808548
0.2252624067384321	0.5591943141116333	0.4463443799755912
0.2181162540866701	0.0926314814064035	0.4209088317948780
0.7235856310469457	0.5917977279750425	0.4123157167922568
0.7223974666907356	0.0594130040768394	0.4593238645716999
0.7356859454668707	0.5760937304297945	0.6635958003073686
0.1845302601092832	0.8257942425617899	0.4457390647132290
0.6896840724836185	0.3222931558489417	0.4342535807985307
0.2493845319576228	0.0738489831227631	0.6656456095259244
0.4654903560752942	0.1844527491228168	0.5451066848419516
0.9710725723216517	0.9726838506036005	0.3510407038995410
0.4755776716619102	0.4715423451395767	0.3355452951998139
0.9569538432577606	0.6866300038770206	0.5481044752091044
0.2262537865411925	0.8408733302175960	0.6748604224742566
0.2288778159337555	0.3012266137086463	0.6792213534296215
0.7234164955988097	0.8069778164046291	0.6778729528970122
0.7132347991023305	0.3451565835827011	0.6530181657707469
0.6842674561101620	0.8284603028370253	0.4376494732239296

0.2448708488530616	0.5685754715095521	0.6731856372736609
0.7504365158686360	0.0770264250973482	0.6700932128095864
0.1826193977817878	0.3267384564048830	0.4453394378716080
0.9674714507748222	0.2008431177360832	0.3374529513552723
0.4661658845188944	0.9519375836948599	0.5648528822124154
0.9756389965107460	0.7018660547583755	0.3356941432140827
0.4840885259328078	0.4535439562405207	0.5483342382842542
0.9723778497287884	0.9488993986576246	0.5674504261825138
0.4664725401097133	0.7013066239537418	0.3313198440744096
0.9611179549134728	0.4511138579847193	0.5665779994525462
0.4678353883960882	0.1999310132095798	0.3335879970670099
0.2192027972029159	0.6922967901585286	0.8554026164307919
0.2122972461897115	0.7562793250512164	0.8993124012453068
0.2263777923472372	0.6218988729099352	0.8171706151265161

Table S11 Optimized fractional coordinates of bt-CO₂ direct adsorption on In₂O₃(110) surface.

O In C O

1.000000000000000		
10.213699999999993	0.000000000000000	0.000000000000000
0.0000000000000009	14.444300000000001	0.000000000000000
0.0000000000000010	0.0000000000000010	15.987399999999992

O In C O

47	32	1	2
----	----	---	---

Direct

0.6084690587952035	0.1838017386999686	0.4327237510684133
0.1079684759895802	0.6845498411455422	0.4386789118438360
0.1095635346019860	0.9653325609011817	0.4535961181184223
0.6092511777524131	0.4670550753765417	0.4541046509130552
0.3233509475070132	0.5854596512705298	0.3501688692166418
0.8254550430449735	0.0832709352599055	0.3433170617779497
0.8259160993633862	0.5663989995105753	0.5344796341222922
0.3276642538037153	0.0646813294781423	0.5314980383863275
0.0949467933344737	0.9785726425403772	0.6627753000207726
0.6031481524961878	0.4685213386868018	0.6660169611995801
0.3290250199435969	0.8206136785117810	0.3481146941892552
0.8282230189612090	0.3201742788548366	0.3435901150882854
0.6012401054567842	0.6870855171789427	0.6829938060342026
0.1016906340455488	0.1858643208391079	0.6823386874740791
0.8353195046985638	0.3297537916686596	0.5367422604965059
0.3343943174400577	0.8252797825630005	0.5449860251730266

0.5606410715671140	0.6960939633688876	0.4576227722416627
0.0607641148380010	0.1971075645070103	0.4583927581405056
0.3884995866074149	0.0682817960341885	0.3171906753369894
0.8887318262973990	0.5678815974145726	0.3191816322830794
0.8733001998612085	0.0870940674984590	0.5560048817835282
0.3698503668634283	0.5874121796548979	0.5714358979253077
0.0613563111895397	0.4600838944388908	0.4396573504464824
0.5598682906744979	0.9587250325139973	0.4395812517363589
0.7990743538008811	0.2161369212234712	0.6881448750728107
0.3240418556293397	0.4240537474085296	0.6771808675876647
0.8108216281044348	0.9383986316368262	0.6782314433118820
0.0973767524967984	0.3212722500425631	0.3123534090499615
0.5953017177819842	0.8214136857493608	0.3113052435777400
0.6102793554426155	0.8391927831994971	0.5726205069495311
0.1077396388086575	0.3393944514740566	0.5735621509770671
0.3338517626039236	0.4299825350737350	0.4612367003449134
0.8330978218126168	0.9284379340240592	0.4561094184831854
0.0920561259502150	0.0858470536226345	0.3092319104750114
0.5896751124116663	0.5860381274859846	0.3092873956578381
0.8301070485220546	0.7215692568146234	0.4348912060538102
0.3299416024012746	0.2223337410862283	0.4337263407888048
0.5983361547557613	0.0712411792953039	0.5810737896237481
0.0992658697124419	0.5683463183446567	0.5846824384368727
0.8719850867659839	0.6986530524075351	0.6682552004482025
0.3764505593285115	0.1969640868086642	0.6655596822804273
0.0325804990096872	0.8346437523392357	0.3218819404369598

0.5290816782751795	0.3369647810416613	0.3218439511685359
0.5609616044349842	0.3132631920628103	0.5609150377159473
0.0576863996969173	0.8153304279287211	0.5660447672462992
0.3704587223997582	0.9589386840148979	0.6832486988712876
0.8717714088192692	0.4523827225727763	0.6837478361399757
0.9675378304415774	0.2185320122158475	0.5804082658379800
0.4596964625392131	0.9320905192459069	0.3263881248112293
0.9612686933789151	0.4314501599857142	0.3269321120544135
0.4744140149312320	0.7155240104196025	0.5785047984776687
0.2208427744046844	0.5607917421568690	0.4657136858798693
0.2144592075782809	0.0923988623028596	0.4193057573081723
0.7159528170051713	0.5917238002025154	0.4190148831171842
0.7196002315173928	0.0601066914458764	0.4570282064201874
0.7466336269388429	0.5746085098927426	0.6658203308430012
0.1830594486078680	0.8258598384903235	0.4423993291677993
0.6822024229985272	0.3267862669141618	0.4387785884419008
0.2470504364365848	0.0786533032754335	0.6621270313181797
0.4656398585432875	0.1840179762091053	0.5440498973398762
0.9676157189952661	0.9714056521329970	0.3481396496334262
0.4642581989702201	0.4731361233338043	0.3513742417939644
0.9656953916481315	0.6832361128386192	0.5485175115765111
0.2147615458692205	0.8613555782500962	0.6559656129076641
0.2308900039026817	0.2990725233739661	0.6740444948389657
0.7314037285987370	0.8043425562841402	0.6756661381071545
0.7211382843723314	0.3468901407210790	0.6545294236354102
0.6797922616406122	0.8265791131037925	0.4397295315375052

0.2423682745603409	0.5555215747395812	0.6826713332117896
0.7519454810971521	0.0782672980487176	0.6675807831469170
0.1792696197890850	0.3275844921883585	0.4417350209142011
0.9616861495459094	0.2008985768508972	0.3367852228490316
0.4675175771442253	0.9517474543240569	0.5637420128145375
0.9690823923610972	0.7004767872095679	0.3375440506887336
0.4676047011793222	0.4484678322144493	0.5676371603009951
0.9630323879526395	0.9501307838299016	0.5636122615714237
0.4604508925088022	0.7009187954680662	0.3366446256319579
0.9643156574102826	0.4518521214934090	0.5625250977865022
0.4663572170527779	0.2019274666584315	0.3346246162374489
0.2192932229664544	0.6827460521645045	0.7599812474040130
0.1487697644290092	0.7004698038610110	0.8185553619943013
0.2879830385858881	0.7397745745790649	0.7126266746850746

Table S12 Optimized fractional coordinates of bt-CO₂ direct adsorption on Zr1-In₂O₃(110) surface.

O In Zr In C O

1.0000000000000000		
10.2136999999999993	0.0000000000000000	0.0000000000000000
0.0000000000000009	14.4443000000000001	0.0000000000000000
0.0000000000000010	0.0000000000000010	15.9873999999999992

O	In	Zr	In	C	O
47	11	1	20	1	2

Direct

0.6089155580447762	0.1844852286429631	0.4334007758926425
0.1083177177693073	0.6853155907618728	0.4396662426090639
0.1087790325437481	0.9663142060725063	0.4519781328326461
0.6086073915352970	0.4678610693283292	0.4544369636907664
0.3227047519614465	0.5850923944333206	0.3507040707820742
0.8241112974388074	0.0833479356935844	0.3409989316231071
0.8253181428112712	0.5664108191162632	0.5349725882461724
0.3177696971531128	0.0638193728755939	0.5374525104999224
0.1016660910282136	0.9844300440896225	0.6542746124454223
0.6035782523416550	0.4693202372379531	0.6671425054261862
0.3302751451188489	0.8196561312286891	0.3490667608578475
0.8296567203143973	0.3205353380441495	0.3425546274555836
0.6029175491021574	0.6874542064858168	0.6843501922227173
0.1087508878253718	0.1786134359313654	0.6776730812615553

0.8347670711079609	0.3304290164853288	0.5362381939482276
0.3360215388838836	0.8277349444918943	0.5473744981159475
0.5609546054085905	0.6961633985564114	0.4575994411103353
0.0601803727673317	0.1962314821724626	0.4576115583199876
0.3854154938650862	0.0678985905024826	0.3211600866057088
0.8897446803958154	0.5673546066302469	0.3197880653694334
0.8685304141628880	0.0869081031288462	0.5546803903471551
0.3696644689733652	0.5882425218699406	0.5726423480159821
0.0617807809777230	0.4589979487511511	0.4404936827957052
0.5577881004383098	0.9591076152529643	0.4407061419262686
0.8018812831524447	0.2164470796607808	0.6869249903994226
0.3224485888314418	0.4242518680258767	0.6784714923918045
0.8139634746823212	0.9385465519942213	0.6770991975629809
0.1005053450726723	0.3206658654557146	0.3131163649123882
0.5959981288963380	0.8216021384871310	0.3112423876133857
0.6135333989747301	0.8383789334570562	0.5733341981195126
0.1050379989234091	0.3372207006184009	0.5750052648324964
0.3335939052475052	0.4294227077395287	0.4628550236682034
0.8319416707748487	0.9285848284327256	0.4536928109548521
0.0900793039133269	0.0862960902192239	0.3065732669434230
0.5894461937952709	0.5860001243342690	0.3090225384432249
0.8313401884798128	0.7213701179301162	0.4346721726869840
0.3313599690163307	0.2196204455764051	0.4377443263308002

0.5917646461901336	0.0710614801229849	0.5836775347747112
0.0992451746137469	0.5682287250156525	0.5849910139897775
0.8745214323682979	0.6982692208232314	0.6686803225790737
0.3731989784207136	0.1955487916975229	0.6648394881839959
0.0341170420425400	0.8348164760564355	0.3218961117308448
0.5289027657627235	0.3373810417510032	0.3236162368372976
0.5621788324966993	0.3148406772806877	0.5624306896437061
0.0566085917165906	0.8168226535016796	0.5663722174158000
0.3663721537330939	0.9621192462869322	0.6866928261861018
0.8731502901071051	0.4523547586703728	0.6843386111986467
0.9650605175996426	0.2175940580532353	0.5792508530434606
0.4594686992241230	0.9316020923088465	0.3259394694826045
0.9640628674632109	0.4313268596779586	0.3261567440896805
0.4774499500715063	0.7146145516539508	0.5789649670151029
0.2204192670691031	0.5605881013569325	0.4660503657496719
0.2126271975068337	0.0922486843801120	0.4163134836646250
0.7173117623430924	0.5911941535125131	0.4180875146934979
0.7187146071220791	0.0600554857807567	0.4542708313353385
0.7481347937402328	0.5747183476247252	0.6669738554462623
0.1821543502208365	0.8268317070067837	0.4406952230948462
0.6834569033940655	0.3284082984226032	0.4375619577806427
0.2557479763416748	0.0762114829243510	0.6571846478974150
0.4697302234962387	0.1870093269633976	0.5433787407268749

0.9663271928613155	0.9714598798238155	0.3449865595768215
0.4634643685889119	0.4734137925497839	0.3513035098475348
0.9650065232009234	0.6830720255436996	0.5478918710178657
0.2108621153114538	0.8589122437642430	0.6547755145852939
0.2283020572426707	0.2999632243703159	0.6748038303481418
0.7343832115603895	0.8038424628562216	0.6773023888441276
0.7224262768137292	0.3479111203019397	0.6552071615351546
0.6804470502586785	0.8256874576230052	0.4385833083326820
0.2415145531755404	0.5566488501137212	0.6833474067590252
0.7505072003075410	0.0783979344110158	0.6679933219490813
0.1796275382074005	0.3267551482189904	0.4425405050454907
0.9610453910638564	0.2012055226598329	0.3349369918340162
0.4715150095571905	0.9485104284127392	0.5649198213088937
0.9703199858658185	0.7002158817958964	0.3365350687799926
0.4685402022382829	0.4497921465735564	0.5682392230135331
0.9591458953558963	0.9503481444864901	0.5612442006648910
0.4606589739531019	0.7003046367069830	0.3361298392230105
0.9637032009788156	0.4520037530003510	0.5624635478986336
0.4654816923662272	0.2022852732542585	0.3344793082166001
0.2171570221965589	0.6828272872387360	0.7619910304713939
0.1463224048140672	0.6998727473966513	0.8205797255207160
0.2856878993075322	0.7417921283098751	0.7156917214072148

Table S13 Optimized fractional coordinates of bt-CO₂ direct adsorption on Zr3-In₂O₃(110) surface.

O	In	Zr	In	C	O
1.0000000000000000					
10.2136999999999993	0.0000000000000000				0.0000000000000000
0.0000000000000009	14.4443000000000001				0.0000000000000000
0.0000000000000010	0.0000000000000010				15.9873999999999992

O	In	Zr	In	C	O
47	21	1	10	1	2

Direct

0.6089391584802151	0.1832215242632301	0.4324231271352099
0.1099005032714492	0.6810155829789972	0.4414425594746682
0.1117132124651637	0.9660098036527071	0.4551490484676434
0.6160915255106182	0.4660204735154483	0.4453985858506760
0.3279019113579681	0.5836136550155037	0.3411729012400146
0.8281421065518797	0.0838681794503132	0.3448693144731413
0.8261218565475493	0.5660136667758359	0.5332973141469575
0.3280825584555491	0.0654012763085002	0.5342202263759208
0.0996655099154817	0.9738986905775018	0.6646173453423888
0.5910570189034947	0.4700157272475367	0.6615674788751752
0.3320328828791506	0.8182954634329530	0.3493543763190900
0.8342540189943620	0.3198014243686990	0.3411589281421897
0.5950041299817485	0.6872074045331124	0.6820127397193126
0.1013224683167497	0.1843646987268387	0.6836778867574052
0.8352692863423785	0.3284728011700078	0.5364549439660106
0.3360868738173373	0.8245867000838771	0.5451926274602144

0.5625610886014207	0.6922721909394011	0.4553678841728543
0.0622962734662049	0.1975221101148489	0.4600770373418245
0.3867696729885923	0.0671767825537002	0.3192183952007744
0.8944552205721341	0.5675374252217592	0.3188095896292658
0.8741838758563770	0.0861267320455544	0.5581681110096088
0.3649380110054130	0.5860170579554723	0.5712961560464550
0.0626335865246369	0.4616680120837582	0.4434213026694762
0.5609179018944548	0.9586899807624731	0.4398956949584686
0.7963565400891953	0.2169897275210843	0.6882801746295359
0.2731242696602738	0.4361708444332658	0.7084773359273216
0.8104672956845379	0.9381703925398107	0.6796951142170555
0.1048585812654110	0.3228420717591947	0.3154305884134071
0.5984265157512704	0.8220020430188157	0.3107366372536561
0.6130495315252221	0.8387469450063351	0.5706977818535779
0.1108386205145147	0.3410199418987278	0.5761132084940412
0.3372431805394459	0.4324653658194476	0.4577830994844367
0.8355309341748322	0.9285041951582041	0.4569548582991978
0.0948309042826476	0.0863222192041321	0.3099826357499044
0.5948300618748176	0.5875126888028021	0.3040474811043302
0.8329034001346827	0.7217604183148218	0.4324122013378402
0.3325357384581554	0.2228103379501410	0.4349633942570792
0.5979211083117569	0.0723596578417641	0.5819441809395846
0.0911914527133736	0.5685569418915780	0.5992386479738737
0.8663068057501626	0.6983811524862570	0.6672897003797862
0.3744094553811942	0.2012230077362669	0.6669784801363291
0.0393893047571373	0.8351348553602207	0.3250744522621506

0.5324763354703922	0.3351728105015735	0.3189019098135736
0.5600401915443878	0.3149269375758378	0.5578777990228321
0.0585314822488579	0.8140026376922710	0.5645723427715490
0.3727637191361615	0.9559159492861380	0.6845317707971256
0.8600077429297751	0.4520789322349154	0.6831142810004457
0.9680914707264479	0.2174490764563211	0.5819644020584041
0.4601880778425106	0.9316400150551402	0.3265344430525598
0.9673927507387616	0.4314341186131988	0.3265657401516628
0.4773374633124595	0.7172856298083299	0.5743168859014155
0.2232838073079895	0.5595224952948671	0.4539743778385598
0.2168219365801030	0.0920254707753509	0.4205297199284029
0.7222926630150311	0.5919535231820990	0.4136891244881540
0.7211995682448294	0.0600240029566799	0.4580586724796959
0.7407601527054957	0.5752990949044522	0.6645911171307836
0.1845243046346228	0.8260291147564732	0.4431842863786399
0.6871968878128535	0.3232423220750433	0.4345656168696452
0.2480219250771421	0.0771551453731154	0.6643928002268015
0.4646155416142649	0.1847486976483156	0.5449306764505530
0.9699017815396684	0.9720897701586497	0.3495255943363570
0.4711241069442130	0.4724831786927273	0.3399539741281031
0.9606569614638043	0.6851901734611107	0.5475975193843524
0.2180537449468240	0.8549895071046814	0.6595139718057326
0.2266996478164083	0.3008439497555283	0.6806766899272586
0.7284340086582300	0.8054019088768403	0.6771263067528258
0.7146535576617232	0.3455835894538702	0.6536029909050740
0.6828008537088415	0.8273767276659022	0.4383197186823781

0.2403540769420207	0.5628547004045944	0.6743576863080053
0.7510477470157113	0.0780077982865807	0.6694909193870086
0.1815308992237076	0.3264758138098092	0.4446445254466129
0.9659930084655483	0.2005581030635427	0.3367774341056000
0.4683052689964147	0.9520112155504977	0.5641396941285801
0.9744744658385478	0.7009835327971772	0.3354176046196686
0.4829358746969593	0.4537264857423013	0.5519870391500612
0.9657091728910906	0.9495621728482473	0.5656430262442799
0.4651665203347954	0.7014462710378427	0.3326882988907822
0.9605063933526893	0.4500125093992430	0.5640484245918378
0.4663055636408893	0.2005983776618438	0.3336765439752706
0.2016835673474373	0.6770825804234217	0.7726415709311064
0.1547765314743685	0.7250417296458843	0.8269712059143433
0.2629758725290582	0.7171837594486820	0.7015697465361327