

Supplementary Information

Theoretical study of metal/silica interfaces: Ti, Fe, Cr and Ni on β -cristobalite

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1 Supplementary figures

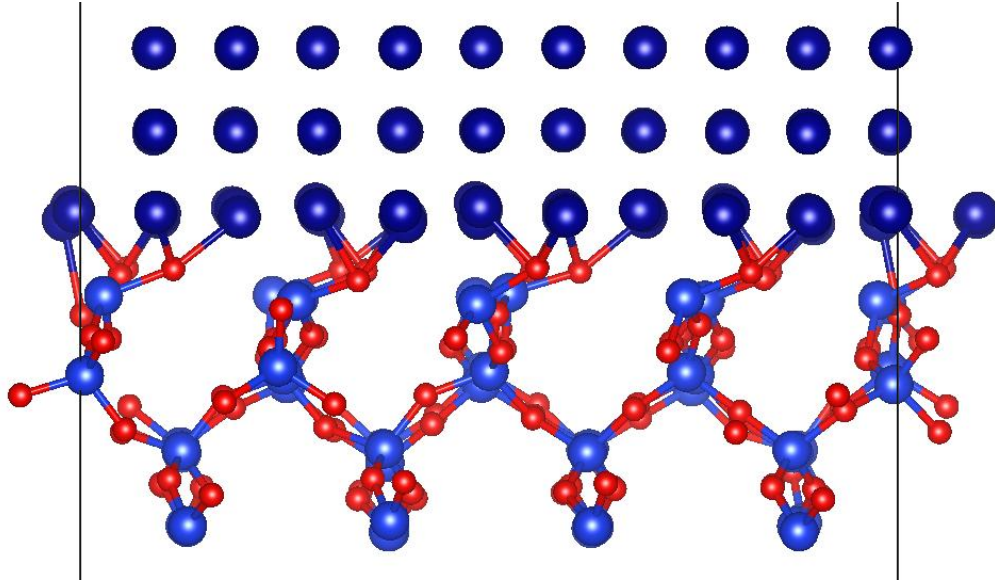


Figure S1: Schematic representation of the optimized structure of the Cr/SiO₂(001) interface with a SiO₂(3 × 4)/Cr(5√2 × 5√2) coincidence cell (see Computational methods in the main text for discussion). Si, O and Cr atoms are shown with large light blue, small red, and large dark blue balls, respectively.

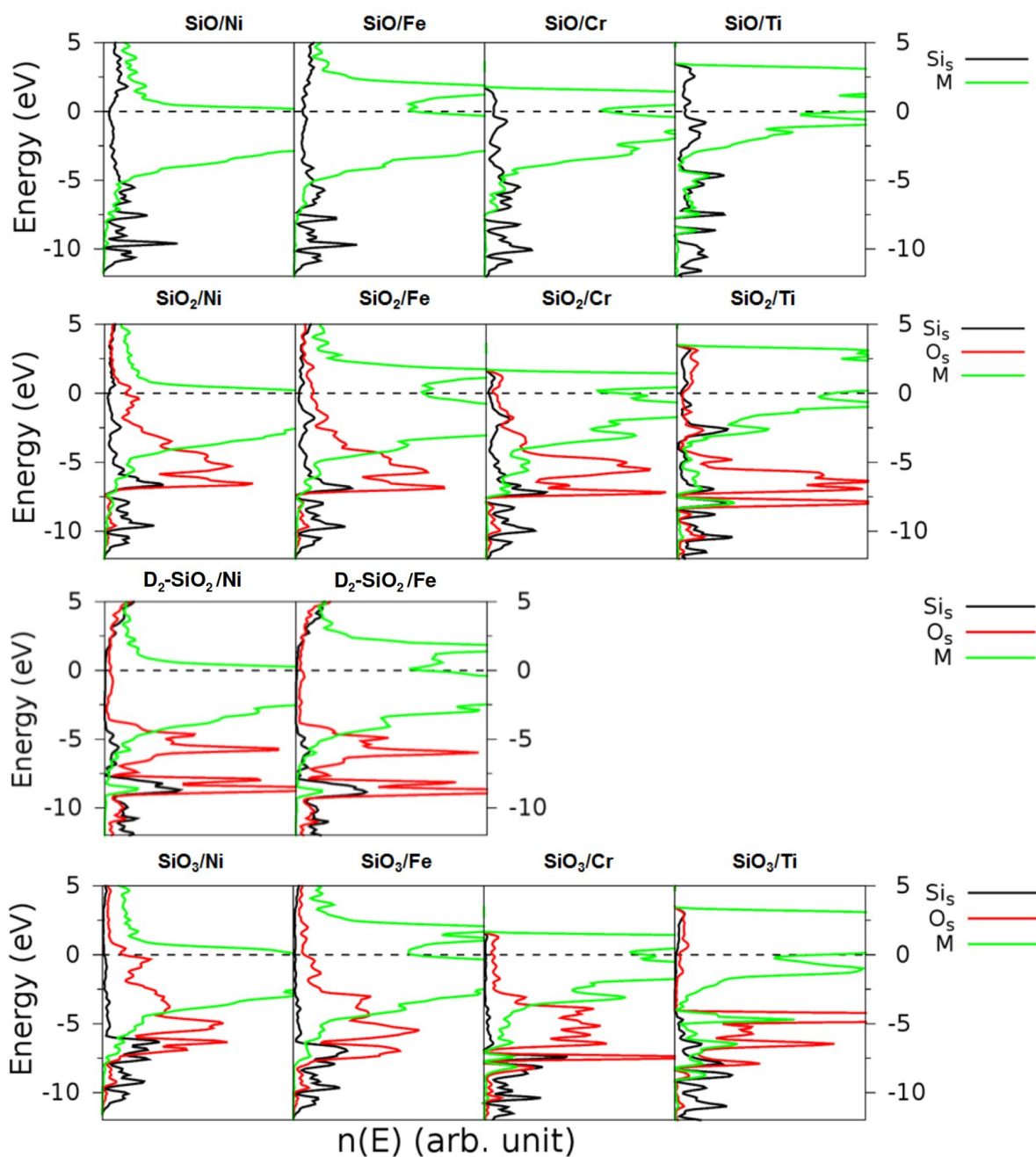


Figure S2: Density of states projected on interfacial Si, O, and M atoms at interfaces between β -cristobalite and transition metals. From left to right: Ni, Fe, Cr and Ti.

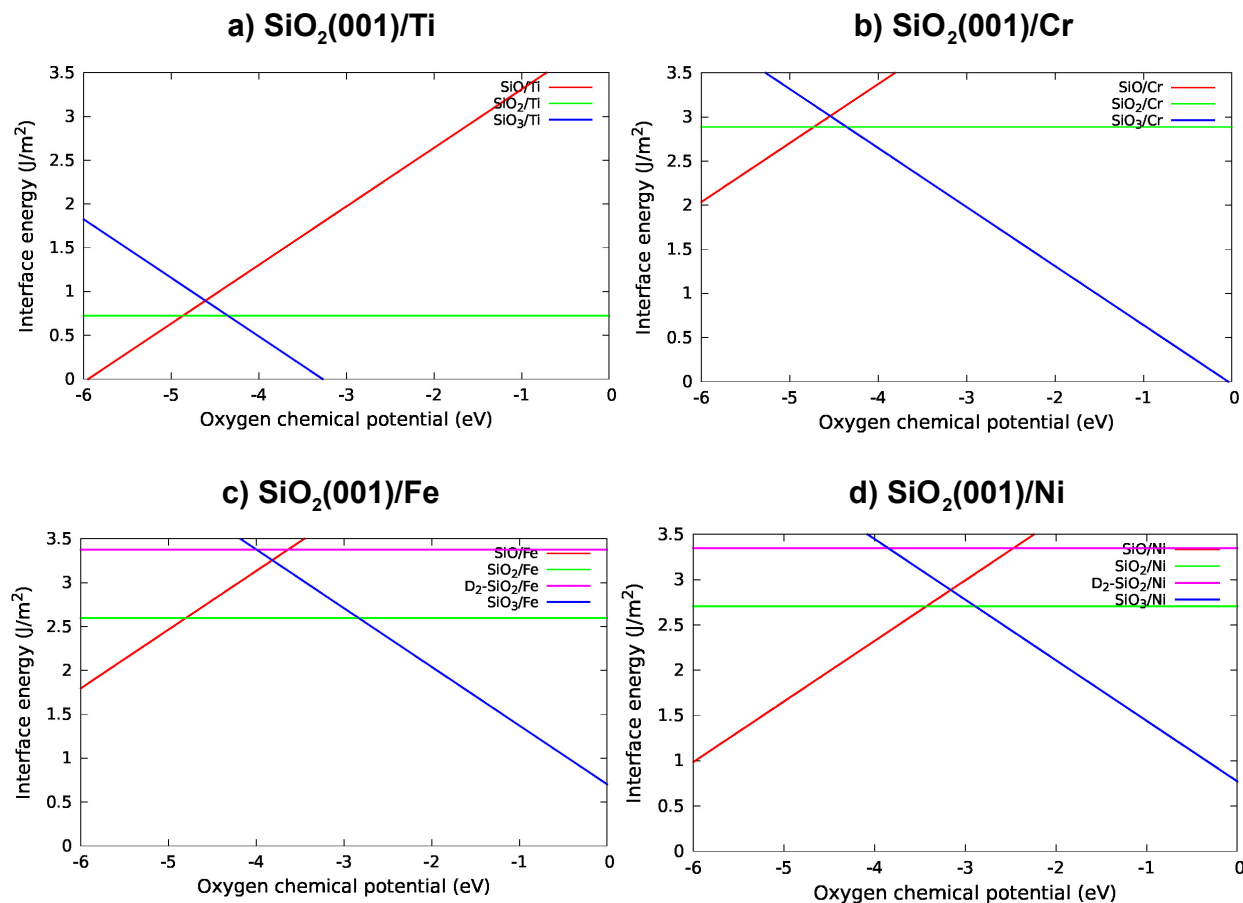


Figure S3: Interface energies as a function of oxygen chemical potential $\Delta\mu_O$: a) Ni/SiO₂(001), b) Fe/SiO₂(001), c) Cr/SiO₂(001) and d) Ti/SiO₂(001).

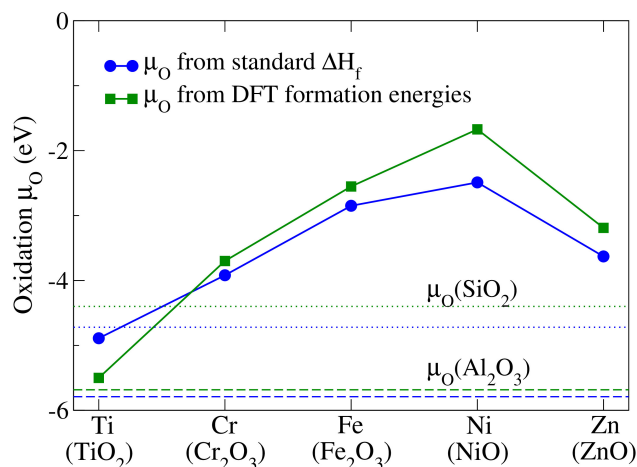


Figure S4: Critical values of oxygen chemical potential $\Delta\mu_O$ at which oxidation of the metallic species considered in this study is thermodynamically favored, deduced from the experimental standard enthalpies of oxide formation $\Delta H_f(298.15 \text{ K})$ per oxygen atom^{1,2} and from DFT formation energy calculations.

2 Interface data converted to $\text{eV}/\text{\AA}^2$

Table S1: Corresponding to Tab. 4 in the main text. (top) Separation energies E^{sep} ($\text{eV}/\text{\AA}^2$) of metal/silica interfaces as a function of the metal and of the silica surface termination, and minimal separation energy at the oxygen-rich interfaces when considering metal decohesion (SiO_3+M , see text). The separation energy M/M within the metal (i.e. $2E^{\text{surf}}$) is reported for comparison. (bottom) Interface energies E^{int} for the SiO_2 and $\text{D}_2\text{-SiO}_2$ interfaces.

	Ti	Cr	Fe	Ni
Separation energies				
SiO	0.152	0.116	0.077	0.124
SiO_2	0.230	0.189	0.152	0.142
$\text{D}_2\text{-SiO}_2$	–	–	0.022	0.021
SiO_3	0.402	0.360	0.260	0.253
$\text{SiO}_3 + \text{M}$	0.243	0.255	0.169	0.217
M/M	0.267	0.454	0.346	0.333
Interface energies				
SiO_2	0.046	0.180	0.162	0.165
$\text{D}_2 - \text{SiO}_2$	-	-	0.211	0.209

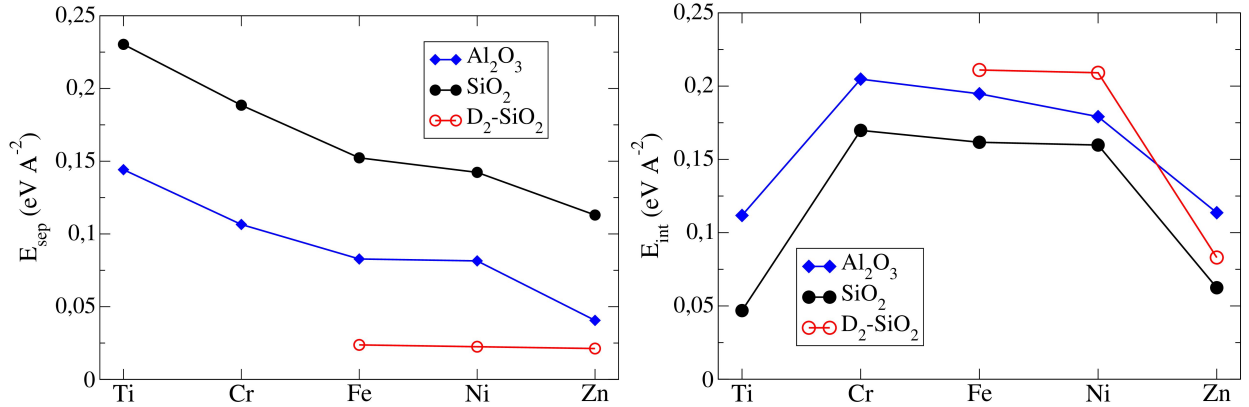


Figure S5: Corresponding to Fig. 5 in the main text. Comparison of the separation energies (top) and interface energies (bottom) at non-polar M/SiO_2 and $\text{M}/\text{Al}_2\text{O}_3$ interfaces.

3 Interface structures

The relaxed structure of the β -cristobalite/metal interfaces discussed in the paper (see section 3.1 in the main text) is given in POSCAR format.

D2-SiO2/Fe

1.0000000000000000

4.8235599999999996 -0.8245061487100001 0.0000000000000000

0.0000000000000000 9.7870400000000011 0.0000000000000000

0.0000000000000000 0.0000000000000000 45.5000000000000000

Si O H Fe
18 38 4 72

Selective dynamics

Direct

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0.5000000000000000	0.5000000000000000	0.0486153846153883	F	F	F
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D2-SiO2/Ni

1.0000000000000000

4.9168000000000003 0.0000000000000000 0.0000000000000000

0.0000000000000000 9.8336000000000006 0.0000000000000000

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Si	O	H	Ni		
18	38	4	72		

Selective dynamics

Direct

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0.5000000000000000	0.5000000000000000	0.0502727272727270	F	F	F
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0.4677025390365258	0.8799628927132803	0.2451537925169042	T	T	T
0.7558950974897914	0.4482575989570770	0.0285311947047582	T	T	T
0.7655907475970949	0.9507043594626339	0.0297431015616249	T	T	T
0.7917789803348881	0.4598857393793804	0.1994096716171173	T	T	T
0.7370501868319672	0.9279169198068972	0.1934468924928137	T	T	T
0.5717613051493688	0.2465521344524496	0.3428748346781608	T	T	T
0.6772631578120958	0.9977161442936135	0.3635947314905977	T	T	T
0.0755872803317442	0.0187053823023344	0.0293393089603751	T	T	T
0.0679746897596367	0.5115669005270645	0.0298213263295182	T	T	T
0.7186969294618064	0.3768792159742207	0.0137885096827834	T	T	T
0.7359698354799307	0.8784805504116775	0.0149742803649837	T	T	T
0.9885954155749331	0.0050257003344396	0.4446128768396491	T	T	T
0.9880903030891180	0.5054975291227639	0.4445131494958667	T	T	T
0.4880252067504173	0.0022774456381382	0.4448911981724813	T	T	T
0.4881729665347230	0.5077336430129810	0.4448327913087730	T	T	T
0.4883228213377994	0.2550617778211249	0.4419499636685882	T	T	T
0.4880440099991600	0.7551030292486443	0.4445815604627105	T	T	T
0.9895436111795790	0.2551722456828063	0.4450357607135977	T	T	T
0.9882904396981608	0.7553736916323071	0.4445490053942502	T	T	T
0.2410659704718839	0.1309089370844481	0.4829873410820809	T	T	T
0.2372957874670700	0.6302182058978194	0.4833948179700929	T	T	T
0.7371816925613497	0.1307906007613117	0.4829717493565956	T	T	T
0.7386014897811051	0.6301593601944139	0.4833875729223204	T	T	T
0.7369077281847763	0.3793847605889935	0.4829416329094584	T	T	T
0.7393383768260254	0.8798226994429663	0.4834079943232762	T	T	T
0.2408973669407175	0.3792318395294893	0.4829198889090922	T	T	T
0.2381790352645770	0.8798984865474824	0.4834590687653858	T	T	T
0.9886605090330354	0.0058899261060078	0.5233069584273432	T	T	T
0.9879147483827740	0.5045634606013865	0.5233185839811374	T	T	T
0.4887142782059337	0.0057441330565713	0.5232807762727077	T	T	T
0.4878935665716199	0.5046808461455030	0.5232846459870509	T	T	T
0.4885809193386427	0.2553540922583406	0.5233262889273088	T	T	T
0.4878245673166099	0.7551105541553297	0.5234123371938313	T	T	T
0.9883795071539381	0.2553451596124450	0.5232303333668676	T	T	T
0.9877775577617718	0.7551279502509477	0.5234544642004663	T	T	T
0.2383339078608609	0.1304628439539390	0.5634077030003363	T	T	T
0.2378027603296174	0.6299313422169757	0.5633688977303702	T	T	T
0.7383014292022392	0.1304754609554147	0.5634218957324318	T	T	T
0.7379311628180412	0.6299610662944781	0.5633569583485594	T	T	T
0.7380805482555806	0.3800324947245467	0.5634491175721256	T	T	T
0.7379413598818325	0.8805182268405902	0.5633817225490605	T	T	T
0.2381478035952988	0.3800103723446402	0.5634534639206551	T	T	T
0.2377749518957730	0.8805552455653028	0.5633358303458730	T	T	T
0.9878639300815343	0.0053401567029106	0.6035073137056163	T	T	T

0.9877796220436219	0.5053940803127082	0.6035150781359508	T	T	T
0.4878108955223771	0.0052808178017790	0.6035107080767125	T	T	T
0.4878469976470208	0.5053954923535687	0.6035140468649364	T	T	T
0.4881506588687261	0.2553068676058244	0.6036284462950421	T	T	T
0.4877641894498501	0.7553485763797605	0.6033643607823035	T	T	T
0.9880665522929196	0.2553385671119174	0.6035394860088212	T	T	T
0.9878477131479561	0.7553618425444407	0.6034647623272077	T	T	T
0.2379362264550392	0.1303041114741506	0.6435744786967168	T	T	T
0.2380473706067459	0.6306498891690743	0.6435534511937070	T	T	T
0.7381395194374339	0.1303562237696921	0.6435650104068777	T	T	T
0.7379267456966248	0.6306289636339278	0.6435538761259084	T	T	T
0.7381709698035240	0.3806529111220636	0.6435701702121923	T	T	T
0.7379479807221734	0.8803718188444464	0.6435552150609964	T	T	T
0.2379983084641832	0.3806480640972366	0.6435715410045545	T	T	T
0.2380314471157689	0.8803706696362652	0.6435630845543034	T	T	T
0.9877694481459687	0.0054360891258132	0.6837591664430152	T	T	T
0.9878464498593634	0.5057455459125821	0.6837421802121236	T	T	T
0.4877646874734201	0.0053822499419665	0.6837643728068629	T	T	T
0.4877892552491959	0.5057004871744842	0.6837458976129489	T	T	T
0.4878187200618419	0.2554970602558834	0.6836062768686003	T	T	T
0.4878479486984000	0.7555778605933477	0.6837932885080463	T	T	T
0.9878645251330435	0.2555552800547806	0.6837250577143452	T	T	T
0.9878069143326195	0.7556018070853674	0.6837722440584764	T	T	T
0.2376003985117713	0.1303880016629429	0.7241046179825733	T	T	T
0.2376579994873250	0.6303773503282464	0.7241877669904997	T	T	T
0.7376295578836970	0.1304146342539234	0.7240938968397583	T	T	T
0.7376789565381586	0.6303865838081796	0.7241911172033672	T	T	T
0.7376822422670122	0.3803729014744385	0.7240941670163089	T	T	T
0.7376774929146143	0.8803565686824164	0.7241885740362448	T	T	T
0.2377055386094944	0.3803702839367797	0.7240892693849368	T	T	T
0.2376793060636094	0.8803535109147441	0.7242080926193600	T	T	T
0.9873826072830462	0.0053051713017497	0.7628598027152046	T	T	T
0.9872207757019141	0.5049401635587364	0.7628431612656061	T	T	T
0.4874535794130338	0.0054077339172376	0.7628528792558555	T	T	T
0.4872334439417664	0.5050048080386037	0.7628414149783495	T	T	T
0.4872077443780907	0.2552337022810010	0.7627278085142860	T	T	T
0.4873358372019621	0.7552156521413598	0.7629235008514630	T	T	T
0.9872691010049962	0.2551394018480073	0.7628031168120919	T	T	T
0.9872451099675620	0.7551766625014097	0.7629148734546235	T	T	T

SiO2/Cr

1.0000000000000000

4.9146059090921002 0.0000000000000000 0.0000000000000000

-0.8226153030700000 4.7734674364350003 0.0000000000000000

0.0000000000000000 0.0000000000000000 47.0000000000000000

Si O H Cr

9 19 2 36

Selective dynamics

Direct

0.0920153472392479	0.9227358416598677	0.1845941281409311	T	T	T
0.0484602924408426	0.9509054338972224	0.3331253506619986	T	T	T
0.5000000000000000	0.0000000000000000	0.0694310497034678	F	F	F
0.5934878644617045	0.9170450376069442	0.2214095279246332	T	T	T
0.5444485330028073	0.0778310305176602	0.3712997480430052	T	T	T
0.0650777942406147	0.4286338790653611	0.1470078816329726	T	T	T
0.0735820663291788	0.4383344664662794	0.2957728836377825	T	T	T
0.5613394753034989	0.4990303826051481	0.1088217309606960	T	T	T
0.5813610326025738	0.4187048813156127	0.2586073219765553	T	T	T
0.2379029309531204	0.8710296752521614	0.0497080910192509	T	T	T
0.4152035413495366	0.9809666693739449	0.1938522627262710	T	T	T
0.3597497388560690	0.1004519425717639	0.3421145094428155	T	T	T
0.4054527479522798	0.2247920922480543	0.0917388222451551	T	T	T
0.5318277246177773	0.0898036374718344	0.2497206992737607	T	T	T
0.6968048985843974	0.4126015177097249	0.3810443712339795	T	T	T
0.9928495000258148	0.5968596320594112	0.1753595806620802	T	T	T
0.0482830704181038	0.6296497289629004	0.3237040432975511	T	T	T
0.3719036389072287	0.5654516821494320	0.1356151240243328	T	T	T
0.3930944237625126	0.4688116671562316	0.2858532431638970	T	T	T
0.8536139434482910	0.4400971746477333	0.1209687887947246	T	T	T
0.9002698801233382	0.5213180233057821	0.2685179990089218	T	T	T
0.0511142866267845	0.1043686933641793	0.1564112037284826	T	T	T
0.9516341685078292	0.1183875685123706	0.3058845152596603	T	T	T
0.6225188719876794	0.7579631314002547	0.0867031857991748	T	T	T
0.5155971321835885	0.5880895347915244	0.2302374734790434	T	T	T
0.7756379805100035	0.1380484760503471	0.0507150971052365	T	T	T
0.9166880278443353	0.9965362962133580	0.2121802702663763	T	T	T
0.8297992354074388	0.9495393707040591	0.3599250664837736	T	T	T
0.0752405377611300	0.9671871675836660	0.0500884502577894	T	T	T
0.7759917773048362	0.3092681185314268	0.0398749285223973	T	T	T
0.4193690616957011	0.3983615852621732	0.4115224071197766	T	T	T
0.9537696747578008	0.3251635565853720	0.4122772562939012	T	T	T
0.8567872565866134	0.7890202661270919	0.4033687014802035	T	T	T
0.3098339466965011	0.8641521055067292	0.4126325068956680	T	T	T
0.6303250890811302	0.5968110905234217	0.4512700268753161	T	T	T
0.1060602690946942	0.5728858650832933	0.4527786986541271	T	T	T
0.1124579987883766	0.0726907775435463	0.4530161426311490	T	T	T
0.6258473552448872	0.0809348867981271	0.4512732451289251	T	T	T
0.3769645771028141	0.3420152052670598	0.4947205099104414	T	T	T
0.8570616783151906	0.3248273881730102	0.4946492237500358	T	T	T
0.8701666949698613	0.8344219597124326	0.4957672716269948	T	T	T
0.3686132406975356	0.8310677567323822	0.4948578149366156	T	T	T
0.6238939112865525	0.5885115687105992	0.5379938744055065	T	T	T
0.1106846635011642	0.5721867621667470	0.5379989508794945	T	T	T
0.1201472876086151	0.0878917383788332	0.5375909609412011	T	T	T
0.6050747903673295	0.0743504834772574	0.5381059379844844	T	T	T
0.3748159228863806	0.3410056702026838	0.5810423625357549	T	T	T
0.8596905093866845	0.3241462598876518	0.5808419065743398	T	T	T

0.8741479254988838	0.8403864804249462	0.5807687947156052	T	T	T
0.3572986586706582	0.8247903106150155	0.5807216263644022	T	T	T
0.6236942722141411	0.5904559171075735	0.6236652590801618	T	T	T
0.1070634802537345	0.5743527010218337	0.6237152998525073	T	T	T
0.1254896210362382	0.0911546184072413	0.6237596088784543	T	T	T
0.6087443811717073	0.0732053022826254	0.6237617968119279	T	T	T
0.3762146615882299	0.3427776005425878	0.6666465306487723	T	T	T
0.8573545377109103	0.3238640827520911	0.6667335287943069	T	T	T
0.8778338113938209	0.8439522722247778	0.6667448481034703	T	T	T
0.3582229870740573	0.8232853593485518	0.6667826574410836	T	T	T
0.6296953875905260	0.5960179582325900	0.7096803031464375	T	T	T
0.1085462194361271	0.5746082813720657	0.7097276611231920	T	T	T
0.1297805184152497	0.0967827289862545	0.7096130722018614	T	T	T
0.6078439364074868	0.0742995721642135	0.7097050645575470	T	T	T
0.3795366162473736	0.3449831792381064	0.7514435964727992	T	T	T
0.8491992158046677	0.3157773989096339	0.7510512747945983	T	T	T
0.8786920561727410	0.8446594797056252	0.7513476398938138	T	T	T
0.3487220602188502	0.8167758829756947	0.7509472196989085	T	T	T

SiO2/Fe

1.0000000000000000

4.8983807431150002 0.0000000000000000 0.0000000000000000

-0.8092335810400000 4.7595382108650002 0.0000000000000000

0.0000000000000000 0.0000000000000000 46.0000000000000000

Si O H Fe

9 19 2 36

Selective dynamics

Direct

0.0797249981071994	0.9661243551648071	0.1909151727975110	T	T	T
-0.0071034227946000	0.0515694220325422	0.3435562669776262	T	T	T
0.5000000000000000	0.0000000000000000	0.0709404203491957	F	F	F
0.5854514993667740	0.9542171103699804	0.2289321454221625	T	T	T
0.4836455984194918	0.9077649674520872	0.3820759857981989	T	T	T
-0.0293966555095198	0.4532630017408435	0.1519272573727262	T	T	T
-0.0149547000064447	0.5610188253431903	0.3053515203243924	T	T	T
0.4694400211791404	0.5081071623375377	0.1116148549348393	T	T	T
0.4647890289724656	0.4347430628444979	0.2672493067972808	T	T	T
0.2472122947914195	-0.1542571730407557	0.0506458359052972	T	T	T
0.4038008009161988	0.0074762982994275	0.2004150974500613	T	T	T
0.1863185789247330	0.0145518711285964	0.3720136639241790	T	T	T
0.3874851178788919	0.2487817706427923	0.0890358749342340	T	T	T
0.4984818522078667	0.1183048433153608	0.2575400237433684	T	T	T
-0.0256601159329618	0.6416416648393523	0.1813770732371796	T	T	T
0.0867554980984580	0.8870969712799449	0.3151433560449475	T	T	T
0.1967120730941605	0.5881822032384316	0.1277120376000817	T	T	T
0.1537066295474670	0.4632964294637709	0.2778048461685106	T	T	T
0.6688947273922814	0.4179732995232903	0.1368034262581487	T	T	T
0.6632436800647830	0.5268692145715753	0.2951730211575833	T	T	T

0.0392558316541535	0.1510172259437209	0.1622965930298921	T	T	T
0.0211959588611413	0.3798578025030869	0.3345738360676391	T	T	T
0.6152816936466028	0.7810669607658730	0.0931446709439709	T	T	T
0.5397093720464584	0.6242909080335315	0.2381516667019246	T	T	T
0.3772088913656819	0.5657983963844171	0.3897927514914634	T	T	T
0.7830607359027933	0.1156609587490818	0.0519106380998210	T	T	T
0.9081360052998804	0.0481006968826968	0.2192798366121189	T	T	T
0.6730278845856159	0.9297471392065646	0.3522769188790324	T	T	T
0.0782291194704528	0.9337135077996295	0.0509859425324338	T	T	T
0.7908107432910276	0.2816654088230278	0.0397584620952324	T	T	T
0.1131966646956239	0.0300113872555745	0.4208897281141257	T	T	T
0.6408344442329533	0.0684172057790904	0.4269347303357323	T	T	T
0.6291680493597920	0.5531524263351925	0.4220035967105137	T	T	T
0.1095910161934204	0.5224820429891356	0.4220834740995127	T	T	T
0.3732239744918793	0.2995806447515815	0.4650420645863544	T	T	T
0.8816313061753001	0.3098484912241720	0.4658622630804763	T	T	T
0.8752519519201715	0.8009959369588147	0.4651514175600334	T	T	T
0.3688738332669203	0.7961749003952052	0.4649707339044092	T	T	T
0.1242639592494685	0.0532833611478101	0.5075649789104084	T	T	T
0.6242231916104413	0.0536375556473129	0.5075098447520090	T	T	T
0.6252510270748328	0.5541066955494423	0.5074910616814027	T	T	T
0.1266851512355416	0.5549372649741339	0.5079498201238978	T	T	T
0.3753509972412416	0.3053389214689848	0.5499072510331899	T	T	T
0.8747951063986948	0.3051036821795072	0.5498300007137634	T	T	T
0.8749703120276243	0.8052434625584670	0.5498472412498326	T	T	T
0.3755707272943049	0.8056397740427758	0.5498902712338481	T	T	T
0.1249903878652320	0.0564305667199436	0.5921183830983845	T	T	T
0.6252230835650628	0.0566563639372400	0.5921441456035045	T	T	T
0.6251967511441351	0.5567572346380965	0.5921357315066516	T	T	T
0.1248218263150525	0.5562426754494171	0.5921294892723467	T	T	T
0.3752120282945929	0.3075567978777921	0.6343136523516326	T	T	T
0.8751657678516925	0.3077503350956238	0.6342919227100806	T	T	T
0.8751212823404260	0.8077198051714374	0.6343250484895201	T	T	T
0.3749769422761383	0.8073614863959402	0.6343194393441539	T	T	T
0.1251105109252230	0.0583288926612490	0.6763933089204417	T	T	T
0.6251592467197343	0.0583299134910226	0.6764046038147210	T	T	T
0.6253996821109667	0.5582768532676099	0.6764052341784331	T	T	T
0.1252883998860635	0.5583037437747130	0.6764060492099335	T	T	T
0.3753891089602642	0.3088113760267137	0.7188373303277587	T	T	T
0.8753487457810050	0.3085455982410395	0.7188232595220383	T	T	T
0.8751976371034176	0.8084637248231898	0.7188199415413208	T	T	T
0.3752156798361313	0.8087218511442009	0.7188245698896919	T	T	T
0.1252658788885543	0.0592741608827267	0.7604608222036348	T	T	T
0.6250863139710325	0.0583558953176295	0.7605406105981140	T	T	T
0.6256119386261511	0.5585660682523178	0.7604642838994347	T	T	T
0.1258779221388506	0.5594851017704289	0.7605851694878291	T	T	T

SiO₂/Ni

1.0000000000000000					
4.9168000000000003	0.0000000000000000	0.0000000000000000			
0.0000000000000000	4.9168000000000003	0.0000000000000000			
0.0000000000000000	0.0000000000000000	45.0000000000000000			
Si	O	H	Ni		
9	19	2	36		

Selective dynamics

Direct

0.0280463982974840	0.0072144362781032	0.1946262291290525	T	T	T
0.0012030430052425	0.0653051628554590	0.3567948889649167	T	T	T
0.5000000000000000	0.0000000000000000	0.0725168741347275	F	F	F
0.5282134673071913	0.0061262144320930	0.2355576769614556	T	T	T
0.5046182500540282	0.9219736312152029	0.3953462285003326	T	T	T
0.0256391391261138	0.5037207797720347	0.1537845430743431	T	T	T
0.0575998130076644	0.5732329446488036	0.3173268821629053	T	T	T
0.5225707295100158	0.4972980879069918	0.1130835670683368	T	T	T
0.5474439537663133	0.5152829658373866	0.2765747772702860	T	T	T
0.2582876167901610	0.1130271742026028	0.0516462183312622	T	T	T
0.2814751256702314	0.1156819600078621	0.2146777678404485	T	T	T
0.2063328798448597	0.0672326787869784	0.3857952433762816	T	T	T
0.6289228774752139	0.2485307675383248	0.0921069641446024	T	T	T
0.6312792239967107	0.2514663873428451	0.2569423628138605	T	T	T
0.1327832326893499	0.7587508979008223	0.1736738338350578	T	T	T
0.1356043377053981	0.8668209705980324	0.3317901750655645	T	T	T
0.2790281666798113	0.3857258193412167	0.1343701471799277	T	T	T
0.3189020603513192	0.4351853730736509	0.3011666405473807	T	T	T
0.7783543330239918	0.6079058506301475	0.1326225748718037	T	T	T
0.8175842114754055	0.6267226023094998	0.2932513006047139	T	T	T
0.9133267869487284	0.2591231075394680	0.1748199652175865	T	T	T
0.9614540383576522	0.3699548146482949	0.3438118894767161	T	T	T
0.4008569154775057	0.7486367984155038	0.0935880977405365	T	T	T
0.4200589097667808	0.7522833133268608	0.2554824506612559	T	T	T
0.4371136938954643	0.5940652608084676	0.4011219775448043	T	T	T
0.7628901896772800	0.8972958549767562	0.0522212149220563	T	T	T
0.7818635912105767	0.8980721363611457	0.2155857200281436	T	T	T
0.7032147866742142	0.9527346099129550	0.3662349338114834	T	T	T
0.0733275036092497	0.0309719254666117	0.0522254789346271	T	T	T
0.7344712230225826	0.7423382630810414	0.0391183946378020	T	T	T
0.1691514321496013	0.0883516551168200	0.4341099405909537	T	T	T
0.6796392042552558	0.0815743308945172	0.4372627626307371	T	T	T
0.6963099851827478	0.5734217714361268	0.4337160947040695	T	T	T
0.1836202704367945	0.5816464891643008	0.4339570941829771	T	T	T
0.4306103045399382	0.3336796757149079	0.4738155024643939	T	T	T
0.9367085459357209	0.3370492576878288	0.4735629324217680	T	T	T
0.9364906365075302	0.8301918272537816	0.4735168353118124	T	T	T
0.4305462233868665	0.8318586566334233	0.4737002191246792	T	T	T
0.1841196873349213	0.0833015705063107	0.5127742325892825	T	T	T
0.6844667573708504	0.0831358610180039	0.5123750050991616	T	T	T
0.6851083789077137	0.5833683361510563	0.5124953046506076	T	T	T

0.1852204820293994	0.5839935984434883	0.5129517874529927	T	T	T
0.4359005841672147	0.3330343833832176	0.5516845110014451	T	T	T
0.9350821515284905	0.3331633057087009	0.5516378391872726	T	T	T
0.9350187209464108	0.8336321236060164	0.5516460695465429	T	T	T
0.4357859641391869	0.8333584204328056	0.5517581793881361	T	T	T
0.1865117728280490	0.0834222387878763	0.5906608046903110	T	T	T
0.6864134653201610	0.0832010423829483	0.5906659965290684	T	T	T
0.6865208897538984	0.5832588451040581	0.5906460967950029	T	T	T
0.1865665709837839	0.5833941975728330	0.5906518218543181	T	T	T
0.4366900239377738	0.3332885102179086	0.6296792700558685	T	T	T
0.9367031401561062	0.3333525164098639	0.6296614978330485	T	T	T
0.9367682107947700	0.8332962879668152	0.6296729984061649	T	T	T
0.4366947188976621	0.8333512631991847	0.6296811551815745	T	T	T
0.1863148684923281	0.0834010145390428	0.6687692498111879	T	T	T
0.6862474030862945	0.0833203465338796	0.6687659883807041	T	T	T
0.6864290517221002	0.5833351100256542	0.6687476837053808	T	T	T
0.1865694511065887	0.5833784944987181	0.6687409054068424	T	T	T
0.4356543189638873	0.3333671575573422	0.7080190091313162	T	T	T
0.9355955703633339	0.3333546698612567	0.7080180700478569	T	T	T
0.9355980945844102	0.8333290960024712	0.7080193786941759	T	T	T
0.4356468030640387	0.8333021314677574	0.7080114297533688	T	T	T
0.1852941485434405	0.0832373774329749	0.7456189447323882	T	T	T
0.6850925028060901	0.0833547575484849	0.7456250722688160	T	T	T
0.6853124668129990	0.5833374934695793	0.7456269686845675	T	T	T
0.1853541029352179	0.5832212293375442	0.7456334288175485	T	T	T

SiO2/Ti

1.0000000000000000

4.7798483894599997 0.0000000000000000 0.0000000000000000

0.0000000000000000 4.9897544099999998 0.0000000000000000

0.0000000000000000 0.0000000000000000 55.0000000000000000

Si O H Ti

9 19 2 24

Selective dynamics

Direct

0.0218059612834693	0.0066582188442226	0.1584228440638853	T	T	T
0.9818976973627684	0.0477236365420168	0.2915446391439644	T	T	T
0.5000000000000000	0.0000000000000000	0.0593319879284167	F	F	F
0.5223121035697886	0.9951195450026091	0.1927358404565851	T	T	T
0.4927269318399325	0.9003517637376746	0.3246038967589584	T	T	T
0.0371359351897738	0.5062624379539216	0.1257110373992134	T	T	T
0.0722684105436855	0.5562143909833424	0.2596369186137721	T	T	T
0.5351136970313348	0.4943625396616795	0.0916439481783584	T	T	T
0.5650101561931322	0.5027795670312969	0.2256191515320083	T	T	T
0.2447744319319654	0.1304478892413101	0.0442838490864474	T	T	T
0.2621744491633891	0.1121659924938712	0.1770048123920489	T	T	T
0.1721703286072156	0.0539464578435300	0.3169485801754917	T	T	T
0.6433911942220263	0.2435892666189190	0.0749686642744649	T	T	T

0.6393934374454773	0.2373920227648085	0.2096930771850438	T	T	T
0.6101732710901828	0.1685573492040007	0.3427160528033326	T	T	T
0.1425736565355962	0.7628663347273417	0.1416483237061996	T	T	T
0.1339898905238641	0.8427523789368294	0.2727148296507877	T	T	T
0.2964150752474879	0.3834204225930549	0.1101371600356629	T	T	T
0.3503715064199397	0.4261704215147404	0.2474597740427171	T	T	T
0.7955338494393231	0.6130370156533615	0.1072880347142515	T	T	T
0.8497180712976373	0.6143836223623680	0.2379350962160629	T	T	T
0.9160926722027725	0.2629269409048121	0.1424606206797066	T	T	T
0.9605670711753334	0.3464673071620936	0.2799982164420882	T	T	T
0.4061283647747373	0.7407364808441059	0.0756056086366641	T	T	T
0.4258590925737877	0.7383231777538768	0.2089704231248319	T	T	T
0.7552535942944161	0.8967073801553838	0.0410102234878380	T	T	T
0.7623597850346329	0.8887969972559659	0.1741485853993439	T	T	T
0.6687891190319846	0.9535094310416525	0.2986617886648801	T	T	T
0.0633164941654059	0.0345301088696388	0.0423681860868683	T	T	T
0.7426300487593238	0.7149217582951692	0.0346691720926344	T	T	T
0.5342232801712825	0.5286272896166864	0.3555265898657254	T	T	T
0.0237435502299306	0.1334575275959295	0.3529885990423764	T	T	T
0.0404493796568701	0.6601170841803068	0.3795979618848975	T	T	T
0.5360833970154175	0.9961481719944416	0.3800391148346023	T	T	T
0.5544315573593366	0.5032311554324025	0.4068904960600577	T	T	T
0.0517870750270433	0.1582053835713495	0.4048873300162370	T	T	T
0.0586904123415408	0.6648273489928158	0.4321446484171432	T	T	T
0.5566345071559908	0.0004885635176635	0.4321984721570900	T	T	T
0.5574168460840738	0.5031368781348675	0.4588039316489727	T	T	T
0.0569910229127402	0.1663719317128951	0.4578910540704655	T	T	T
0.0585258093538741	0.6679067025923686	0.4845689586090103	T	T	T
0.5580696673975822	0.0029438611621160	0.4845994227058128	T	T	T
0.5596645997117591	0.5043327665769866	0.5109848062021456	T	T	T
0.0593976101667053	0.1690969058854677	0.5106238641401077	T	T	T
0.0601726791557553	0.6687354081269987	0.5370790619913066	T	T	T
0.5598692168085790	0.0048520205296327	0.5371008090376108	T	T	T
0.5603256508874637	0.5061755035498123	0.5634947145661968	T	T	T
0.0600711484961352	0.1685870038258983	0.5633661121537301	T	T	T
0.0606422221209471	0.6683118557137888	0.5895550580612436	T	T	T
0.5604026862010585	0.0064462861299646	0.5896069805696840	T	T	T
0.5608274469210457	0.4996791571095969	0.6148767972246816	T	T	T
0.0605749474615678	0.1755741822051533	0.6148098978070706	T	T	T
0.0609768289550985	0.6373347249375527	0.6396018911443164	T	T	T
0.5605350915760994	0.0378514368210574	0.6396408420896336	T	T	T

SiO3/Cr

1.0000000000000000

4.9146059090921002 0.0000000000000000 0.0000000000000000

-0.8226153030700000 4.7734674364350003 0.0000000000000000

0.0000000000000000 0.0000000000000000 47.0000000000000000

Si O H Cr

9 20 2 36
 Selective dynamics
 Direct

0.0744253891199449	0.9589288236735456	0.1839798862923558	T	T	T
0.0126420775114724	0.0743873200040781	0.3309406315290104	T	T	T
0.5000000000000000	0.0000000000000000	0.0694310497034678	F	F	F
0.5777217158495631	0.9515699145912393	0.2202759212788905	T	T	T
0.5248149309843768	0.0246461696050773	0.3699186238492445	T	T	T
0.9563745250155833	0.4429995259562318	0.1469982207082481	T	T	T
0.0988570127078106	0.5866594172258317	0.2931615164518675	T	T	T
0.4583659417746802	0.5083561268602637	0.1085749213738794	T	T	T
0.5775589326092359	0.4508481291933890	0.2569050846815770	T	T	T
0.2474383713736898	0.8397642204637208	0.0499473069237197	T	T	T
0.3995072035120515	0.0163486274110696	0.1926453045783774	T	T	T
0.2363228046634447	0.0781793487862714	0.3561847312581676	T	T	T
0.3884240457906927	0.2538977818594432	0.0859395695653404	T	T	T
0.5067778579749529	0.1201928683496050	0.2486520950228339	T	T	T
0.6546521206505247	0.3052221546096234	0.3879514218757194	T	T	T
0.9799616494587653	0.6300197239014409	0.1759894742701889	T	T	T
0.0987686864019963	0.9071636444009599	0.3032898746641024	T	T	T
0.1756982545310066	0.5783661818899191	0.1227841293654848	T	T	T
0.4043509518428223	0.5295787940322114	0.2843311313906867	T	T	T
0.6486846588829067	0.4186091521558737	0.1340271576220076	T	T	T
0.9031923706556526	0.5252550910111324	0.2652063704691514	T	T	T
0.0195686201346987	0.1359007943860036	0.1558723919110676	T	T	T
0.9919860551357971	0.3904520241976783	0.3204588633099945	T	T	T
0.6109103758504659	0.7861046102381621	0.0918593531942022	T	T	T
0.5098415897560855	0.6207800230266685	0.2285657254046569	T	T	T
0.4781581473912269	0.7731355186952484	0.3942771991860923	T	T	T
0.7837886294030270	0.1103743264573680	0.0508801271780541	T	T	T
0.9018716048272921	0.0386827210111420	0.2116178153428478	T	T	T
0.7143116824068017	0.9363349918095523	0.3441127426807284	T	T	T
0.0797541623820095	0.9282751915511014	0.0498548747867460	T	T	T
0.8013772881786139	0.2842708579431275	0.0401344195298066	T	T	T
0.3678016117780842	0.4101575124673573	0.4186196458375875	T	T	T
0.8921774346532914	0.3247812690787910	0.4210136022929305	T	T	T
0.7781862655354317	0.8395405694542291	0.4247182940052951	T	T	T
0.2306199970411527	0.8730066723486445	0.4253558654862744	T	T	T
0.5598741289101667	0.6038472730587472	0.4631617421723604	T	T	T
0.0662949333047038	0.6067218522099438	0.4639702103901513	T	T	T
0.1057042511646458	0.1299544595475268	0.4654665996342686	T	T	T
0.5974848494671505	0.1283157993565496	0.4630327339303619	T	T	T
0.3321288039244408	0.3676568915800544	0.5071969782780315	T	T	T
0.8206930587683132	0.3605979362803353	0.5066716213851166	T	T	T
0.8228918644042054	0.8614830689246915	0.5066772360247498	T	T	T
0.3285981742986834	0.8619386571875154	0.5065063098901206	T	T	T
0.5759728913676128	0.6132071223066120	0.5498877514249472	T	T	T
0.0755807079235922	0.6128254823200407	0.5497367513642715	T	T	T
0.0779447803909576	0.1125839753499775	0.5492959164150903	T	T	T

0.5788912387875556	0.1140732115975140	0.5498635338206981	T	T	T
0.3253689920848473	0.3613371304716253	0.5925912626334906	T	T	T
0.8284664401522690	0.3622776134683363	0.5925127059347162	T	T	T
0.8256085615968232	0.8611107581026829	0.5925943444861801	T	T	T
0.3267641399635721	0.8648205436645355	0.5925314809339142	T	T	T
0.5757782278469108	0.6111744690643306	0.6352380439510199	T	T	T
0.0792738886769300	0.6149942408810034	0.6353831858339873	T	T	T
0.0754993403060524	0.1108439531125356	0.6355086393925262	T	T	T
0.5793705900390762	0.1149105327001934	0.6353838462840855	T	T	T
0.3228942637026151	0.3583041151454509	0.6783112720948168	T	T	T
0.8319111454070693	0.3684075756028733	0.6783362409243239	T	T	T
0.8239678613944221	0.8590627596376947	0.6783185675430659	T	T	T
0.3336074629995736	0.8676094014951374	0.6783172531368606	T	T	T
0.5706880570252082	0.6053697941864371	0.7212320660517477	T	T	T
0.0836942231775168	0.6186709009574543	0.7211774283811749	T	T	T
0.0702644796954601	0.1046760839218663	0.7210536954781830	T	T	T
0.5832679429229444	0.1188320040441653	0.7211763485434801	T	T	T
0.3233254304954798	0.3590563171929446	0.7628436344285774	T	T	T
0.8442158195152913	0.3763204494837424	0.7626339015767130	T	T	T
0.8197803427750046	0.8555503788893688	0.7627563348869444	T	T	T
0.3420494871047097	0.8777321732590266	0.7626702647688006	T	T	T

SiO3/Fe

1.0000000000000000

4.8983807431150002 0.0000000000000000 0.0000000000000000

-0.8092335810400000 4.7595382108650002 0.0000000000000000

0.0000000000000000 0.0000000000000000 46.0000000000000000

Si	O	H	Fe
9	20	2	36

Selective dynamics

Direct

0.0199456134794929	0.9996720384255511	0.1916401560467165	T	T	T
0.0063180027502980	0.0451822206970149	0.3494832072741261	T	T	T
0.5000000000000000	0.0000000000000000	0.0709404203491957	F	F	F
0.5174756745915303	0.0158429458370861	0.2309783488456034	T	T	T
0.4988162619589431	0.0737216423739326	0.3877731467053991	T	T	T
0.0213274343932568	0.4928100495538885	0.1515882568278926	T	T	T
0.0132830202001060	0.5318565347310127	0.3100242432565068	T	T	T
0.5227704712168304	0.5028286257775179	0.1119234780132672	T	T	T
0.5201388464937082	0.5265075911242647	0.2709143315719942	T	T	T
0.2753530124089707	0.0644622613887265	0.0476400358976505	T	T	T
0.2927490959144876	0.1348575133468088	0.2101776401962638	T	T	T
0.2888241405399512	0.2012170337419406	0.3655303660916474	T	T	T
0.6227031501589977	0.2719591684121951	0.0904921463380788	T	T	T
0.6266223811625906	0.2772463485421994	0.2523995909152177	T	T	T
0.6092305655462766	0.3287225310304294	0.4112356000237654	T	T	T
0.1306536217980465	0.7493625121667122	0.1736726464544773	T	T	T
0.1104238506769448	0.7817341569825516	0.3332492014571287	T	T	T

0.2666500614834035	0.3810320590043830	0.1332681254775920	T	T	T
0.2709146237920947	0.4216514499736093	0.2936516965434208	T	T	T
0.7953239218504180	0.6150597645893185	0.1313882305680849	T	T	T
0.7987866848320593	0.6602522558619768	0.2886523808924295	T	T	T
0.8926479971810650	0.2193817988013009	0.1706841373915822	T	T	T
0.8712428275961202	0.2515261254140668	0.3275044513367149	T	T	T
0.4045109934488451	0.7442013262404217	0.0935634269808716	T	T	T
0.3862188050151403	0.7469232308467824	0.2506386730355104	T	T	T
0.3325859097097776	0.8161613758590391	0.4070000765142794	T	T	T
0.7557692715361455	0.9161825732851838	0.0508763492030226	T	T	T
0.7648864597097429	0.8962661761121637	0.2137100587845069	T	T	T
0.7553359116191345	0.9492695225719530	0.3725532924724462	T	T	T
0.0701821696311740	0.0142874524406267	0.0504311813126179	T	T	T
0.6952562587856903	0.8304266673571092	0.0322936608495397	T	T	T
0.2814509363009279	0.2065410973950677	0.4427114115274833	T	T	T
0.8034662451226282	0.2118250108615172	0.4444281811539881	T	T	T
0.7055626533177062	0.6926194506164265	0.4394162671598565	T	T	T
0.1961675997114085	0.6806175215190606	0.4426807345052737	T	T	T
0.5033355936777468	0.4530951640817023	0.4847651871023047	T	T	T
0.0044354799727770	0.4517940556159559	0.4857649734173108	T	T	T
0.0001439704927364	0.9471464957245743	0.4843431013555346	T	T	T
0.5022719635266952	0.9495587597302517	0.4841775868191434	T	T	T
0.2566249500869588	0.2053549816256250	0.5269422241795212	T	T	T
0.7560307021087382	0.2057944206415030	0.5270155298428634	T	T	T
0.7555349001633260	0.7075112365744900	0.5269285990306543	T	T	T
0.2564259863535554	0.7075092856303584	0.5270912126964973	T	T	T
0.5096614847964673	0.4624081887796265	0.5689432118655233	T	T	T
0.0096363115331499	0.4623872121956438	0.5689051872517084	T	T	T
0.0093539512565570	0.9620088658203230	0.5689951738133345	T	T	T
0.5092874603714037	0.9620926412974029	0.5690608727141324	T	T	T
0.2624578258429509	0.2167987156931943	0.6109422827300435	T	T	T
0.7625208242556809	0.2166458766879131	0.6109323784832057	T	T	T
0.7629103420013266	0.7165286747839659	0.6109568370395095	T	T	T
0.2626977567749336	0.7165117680261304	0.6109831588084376	T	T	T
0.5150942319613279	0.4695160976280732	0.6529734019072606	T	T	T
0.0150694447303295	0.4695755722051089	0.6529846419092209	T	T	T
0.0150584379002439	0.9696975150938414	0.6529531119318790	T	T	T
0.5151445627840943	0.9695367186928578	0.6529455882736528	T	T	T
0.2667774210671183	0.2212179610065093	0.6950301625757334	T	T	T
0.7668573818551820	0.2214947477897269	0.6950322984571216	T	T	T
0.7667323543612952	0.7214789798298540	0.6950364015965746	T	T	T
0.2666247847474352	0.7212374865741751	0.6950226520201923	T	T	T
0.5177283927931526	0.4717108969843338	0.7374268037710294	T	T	T
0.0177486961766746	0.4717631110479417	0.7374316777230661	T	T	T
0.0178138904001841	0.9717655515991765	0.7374360670181801	T	T	T
0.5177726387247574	0.9716926101050731	0.7374299465450065	T	T	T
0.2685534551489752	0.2222319957658598	0.7792492981229913	T	T	T
0.7684820233087919	0.2214038061460997	0.7792909066643716	T	T	T
0.7681588231195420	0.7212740663201842	0.7792514599658489	T	T	T

0.2682481675721178	0.7220292038296776	0.7792861858905411	T	T	T
--------------------	--------------------	--------------------	---	---	---

SiO3/Ni

1.0000000000000000		
4.9168000000000003	0.0000000000000000	0.0000000000000000
0.0000000000000000	4.9168000000000003	0.0000000000000000
0.0000000000000000	0.0000000000000000	45.0000000000000000

Si	O	H	Ni
9	20	2	36

Selective dynamics

Direct

0.0022535812804502	0.9943966274219861	0.1953710338501700	T	T	T
0.0110511608981552	0.9986348309552969	0.3602125191933094	T	T	T
0.5000000000000000	0.0000000000000000	0.0725168741347275	F	F	F
0.5030626377402815	0.9947989389753417	0.2364626635581435	T	T	T
0.5122934853991119	0.9883731980286442	0.4024625213037263	T	T	T
0.0045422887830140	0.4955256186235769	0.1543378847631304	T	T	T
0.0129190605773059	0.4993293941720149	0.3187816027718426	T	T	T
0.5040940881736327	0.4977870893510442	0.1134080856981265	T	T	T
0.5105837009868354	0.4946076760261642	0.2775770239815122	T	T	T
0.2676641170586898	0.1059783474112086	0.0499134955209422	T	T	T
0.2489949715539227	0.1018455988865716	0.2164539453851349	T	T	T
0.2577948280222200	0.0862644575629701	0.3820717589773262	T	T	T
0.6174707787650341	0.2495510967928072	0.0927633102721597	T	T	T
0.6150240217962332	0.2456922491817851	0.2566461758385237	T	T	T
0.5727466410392958	0.2397857963540035	0.4253969092244945	T	T	T
0.1139319091357807	0.7450230487265901	0.1749236607161153	T	T	T
0.1167093574213618	0.7548271413081601	0.3387067072684521	T	T	T
0.2542101467638985	0.3859259305746907	0.1337791856198024	T	T	T
0.2636058875470520	0.3869932904167856	0.2986164645203296	T	T	T
0.7537892119491384	0.6058495731886780	0.1340307875825584	T	T	T
0.7633474081692027	0.6005969471577453	0.2978038667461581	T	T	T
0.8962122676192251	0.2450833593692105	0.1748103737083716	T	T	T
0.9093650941052942	0.2555458298024972	0.3403927290172784	T	T	T
0.3916392340846904	0.7498113879541698	0.0933376972167255	T	T	T
0.3993461935629011	0.7457961456263006	0.2574072283633517	T	T	T
0.4610489031820968	0.7312551221034218	0.4249184193646247	T	T	T
0.7709165934744502	0.8976627649780612	0.0535466620892828	T	T	T
0.7491029310172516	0.8852771306439027	0.2154054287234553	T	T	T
0.7590552470687503	0.8973909526278542	0.3806171554311972	T	T	T
0.0791559683373555	0.0337373182373123	0.0516468862404363	T	T	T
0.7442842446760132	0.7467654856679931	0.0398539073684199	T	T	T
0.2898878329133283	0.2353088202112540	0.4573093564251300	T	T	T
0.8053356064343549	0.2288830432028045	0.4576068128253162	T	T	T
0.7468542203852846	0.7277194378756161	0.4568943915003327	T	T	T
0.2323368667723646	0.7329378542229964	0.4575192774362823	T	T	T
0.5195272381124579	0.4810963446752256	0.4970396964268623	T	T	T
0.0191455167161308	0.4811663580781885	0.4962134710797370	T	T	T

0.0192950864366804	0.9807057838455411	0.4963476285314561	T	T	T
0.5194969047672029	0.9805377573516809	0.4968083036757489	T	T	T
0.2679095503454069	0.2309152615402660	0.5356238143402251	T	T	T
0.7686269748625554	0.2312378442908079	0.5357177645306038	T	T	T
0.7697231015506238	0.7316186223316873	0.5356537284067879	T	T	T
0.2688283548820560	0.7312477259296886	0.5357234713297234	T	T	T
0.5187646807185738	0.4809447450578595	0.5747932751150483	T	T	T
0.0187842125604596	0.4809745063487804	0.5747971590512969	T	T	T
0.0188426303973837	0.9809411823774478	0.5747752330861525	T	T	T
0.5187629515717603	0.9809199074986958	0.5748427678109219	T	T	T
0.2682428387710450	0.2311270937947297	0.6137849132447015	T	T	T
0.7679262998980557	0.2311560456083611	0.6137838733273467	T	T	T
0.7678459353265533	0.7311423372646644	0.6137913491947303	T	T	T
0.2681178288946894	0.7311480595012909	0.6137818800957996	T	T	T
0.5186330477837707	0.4807326338011239	0.6527876633331363	T	T	T
0.0185948539728560	0.4806961288679332	0.6527038211117218	T	T	T
0.0185591152714280	0.9807011092184688	0.6527249376329174	T	T	T
0.5185802620365719	0.9807282800474075	0.6527734547333515	T	T	T
0.2686410013609382	0.2307151203151284	0.6918349440072757	T	T	T
0.7686344363702989	0.2306853966398121	0.6918328172305002	T	T	T
0.7686493617820249	0.7306813412799188	0.6918362779976891	T	T	T
0.2686291554855167	0.7306942527380880	0.6918334255674037	T	T	T
0.5199138672034845	0.4797715532131450	0.7310441781261929	T	T	T
0.0199416174596533	0.4797386668125497	0.7310773891655049	T	T	T
0.0199588129809526	0.9797284714136874	0.7310592256562570	T	T	T
0.5199388472832586	0.9797877049297321	0.7310555386861769	T	T	T
0.2703716898057871	0.2295054999636164	0.7686347189137781	T	T	T
0.7701835045536979	0.2295289382403523	0.7686182718382747	T	T	T
0.7702067656223202	0.7295307217001505	0.7686275211623317	T	T	T
0.2704708418876934	0.7295503641334937	0.7686205893475815	T	T	T

SiO3/Ti

1.0000000000000000

4.9897544099999998 0.0000000000000000 0.0000000000000000

0.0000000000000000 4.7798483894599997 0.0000000000000000

0.0000000000000000 0.0000000000000000 55.0000000000000000

Si O H Ti

9 20 2 24

Selective dynamics

Direct

0.0092316207215006	0.9689263257495213	0.1604567916869115	T	T	T
0.0935883165548077	0.9169158099720818	0.2892486303461084	T	T	T
0.5000000000000000	0.0000000000000000	0.0593319879284167	F	F	F
0.5158473525790441	0.0513485793470707	0.1934546403669231	T	T	T
0.5936631569211102	0.1114138474785662	0.3162437621687459	T	T	T
0.0143271340724809	0.4638110487829223	0.1262432841740946	T	T	T
0.9740148735253911	0.4158448146778539	0.2579711417347568	T	T	T
0.5166278422063826	0.4991414713381985	0.0934472868969607	T	T	T

0.4757972705645273	0.5426748438912909	0.2266293500954788	T	T	T
0.2645409071726235	0.0965300821111015	0.0409620789583087	T	T	T
0.2623774830997405	0.0934023149946483	0.1753487048289628	T	T	T
0.4061797765193589	0.9937456261356346	0.2940503555436109	T	T	T
0.6243594476327203	0.2641550487916433	0.0743194350955392	T	T	T
0.5918482127410485	0.3589366508252141	0.2039768084807747	T	T	T
0.5767269573190816	0.4440668901945557	0.3184910211455829	T	T	T
0.1093170481307766	0.6874878458304678	0.1467373826612643	T	T	T
0.0715017496049413	0.5899571494336513	0.2818677025599072	T	T	T
0.2734505778670453	0.3743480761537583	0.1099597028181165	T	T	T
0.1793951698765213	0.4415936435961569	0.2351446653071321	T	T	T
0.7720988591975058	0.5951919429721499	0.1099502664113459	T	T	T
0.6785891286064256	0.5202504692409278	0.2496548464492463	T	T	T
0.90135444484201503	0.1884147557223201	0.1401050969958320	T	T	T
0.9654003750613143	0.0898226670201581	0.2665105592780819	T	T	T
0.3953745859799795	0.7646904283783655	0.0785842257210234	T	T	T
0.4448137672313166	0.8623731864278525	0.2171695546000691	T	T	T
0.4738531015752372	0.9701110004273801	0.3418906447047618	T	T	T
0.7637683452037507	0.8832429975246541	0.0440185321635340	T	T	T
0.7640667376689336	0.9068964547452438	0.1790753304506012	T	T	T
0.9119537877610071	0.9945583280953869	0.3139472061762305	T	T	T
0.0802106490856929	0.0205370040285544	0.0427451508199184	T	T	T
0.7363355910929030	0.7231305985623493	0.0333574671685000	T	T	T
0.5093690890352249	0.5509268029175090	0.3520073948124747	T	T	T
0.0864110813700023	0.0222704358883092	0.3533592824904872	T	T	T
0.9802118362014696	0.5303022140960394	0.3786808661109546	T	T	T
0.6322285572816781	0.0400771904055830	0.3795398987967076	T	T	T
0.4824029030076460	0.5304178207888199	0.4048744427356965	T	T	T
0.1309448771371393	0.0310627861642061	0.4052437699479086	T	T	T
0.9755165584183203	0.5296656813675753	0.4312629446189717	T	T	T
0.6355099990852082	0.0314604334415023	0.4315387081353705	T	T	T
0.4733992881488973	0.5326431418966564	0.4573118304742749	T	T	T
0.1355702818208826	0.0320582052667291	0.4576719780185599	T	T	T
0.9722546308810749	0.5335259724544841	0.4836150822111094	T	T	T
0.6364350186090064	0.0334156103505094	0.4836860528260871	T	T	T
0.4713958721044165	0.5344136799546675	0.5098093940507482	T	T	T
0.1354763640945222	0.0348361226310274	0.5099182096154991	T	T	T
0.9715390156302490	0.5356603256775756	0.5361259614085441	T	T	T
0.6348448207708870	0.0358698377028333	0.5361660754014324	T	T	T
0.4722894005182710	0.5365738137605547	0.5624864700013887	T	T	T
0.1339106940728598	0.0362938608735277	0.5625304707295768	T	T	T
0.9723855624034172	0.5366125624242244	0.5886438189899152	T	T	T
0.6339653449060521	0.0367533734044017	0.5886490997812714	T	T	T
0.4653821934672635	0.5370142631868262	0.6138530026648397	T	T	T
0.1409220301352789	0.0369239573730766	0.6138880481323525	T	T	T
0.0036363101622854	0.5369346838927456	0.6386709931991206	T	T	T
0.6028667681710189	0.0371997429961439	0.6386701095586105	T	T	T

SiO/Cr

1.0000000000000000

4.9146059090921002 0.0000000000000000 0.0000000000000000

-0.8226153030700000 4.7734674364350003 0.0000000000000000

0.0000000000000000 0.0000000000000000 45.0000000000000000

Si O H Cr
9 18 2 36

Selective dynamics

Direct

0.9806698107950069	0.9158039676964975	0.1918325028003451	T	T	T
0.0888782908574512	0.9273948847787921	0.3442988988720046	T	T	T
0.5000000000000000	0.0000000000000000	0.0725168741347275	F	F	F
0.5019812031342070	0.0510699541175796	0.2295802937402058	T	T	T
0.5800054643257582	0.0518128526082577	0.3850312194507808	T	T	T
0.0758415637505507	0.4316074961880005	0.1526735253585869	T	T	T
0.9849000078926196	0.4103094429101120	0.3055140276485417	T	T	T
0.5690121504907495	0.4993412559458292	0.1132213931032098	T	T	T
0.5061610784770352	0.5493249717621538	0.2677079494040555	T	T	T
0.2355126979492255	0.8688737983727606	0.0523714777403725	T	T	T
0.1758418354325428	0.9794262644941440	0.2211181184818471	T	T	T
0.3993858357901985	0.0780047953987051	0.3539207984872235	T	T	T
0.4069769266140142	0.2243837592671412	0.0959486394711675	T	T	T
0.5783015365901178	0.3822561451055293	0.2379640460221424	T	T	T
0.9802195647112342	0.5949615292674935	0.1814354647129335	T	T	T
0.1015092695512791	0.6093756711036846	0.3335579878502273	T	T	T
0.3815423820062733	0.5745080161128371	0.1410664090323408	T	T	T
0.1814343296341150	0.4619576313928135	0.2762825152878250	T	T	T
0.8612687473059566	0.4327149706241471	0.1253840976709739	T	T	T
0.6833036858031107	0.4759304327495641	0.2962074710354230	T	T	T
0.0880967560857542	0.1128470600467253	0.1634266335970835	T	T	T
0.9716819353528479	0.0895515038564625	0.3167294962830240	T	T	T
0.6283783736968687	0.7574500800198862	0.0899673001414385	T	T	T
0.5679003445357083	0.8811839871309601	0.2594199267727220	T	T	T
0.7733958367325897	0.1403605507943269	0.0527506573023544	T	T	T
0.6741435997824468	0.9695276896704854	0.2010680745011371	T	T	T
0.8682885896477472	0.9186045301962693	0.3723292263563920	T	T	T
0.0742452819535160	0.9669946275013430	0.0525350464630918	T	T	T
0.7728685631308565	0.3123050625599504	0.0415836192112664	T	T	T
0.2940011579901949	0.3092373291672104	0.4238600541255408	T	T	T
0.7639508818714944	0.3505137524600528	0.4262175671526407	T	T	T
0.9250837131027723	0.8246890387787218	0.4178058410410728	T	T	T
0.3700866105892118	0.7868022944561304	0.4264553350295657	T	T	T
0.6355123750163827	0.6069421037644744	0.4689157287341246	T	T	T
0.1130359428547507	0.5833563141444031	0.4685456199998868	T	T	T
0.0885946203670613	0.0771164448482864	0.4663566762267735	T	T	T
0.5971975704462338	0.0838661908933105	0.4675550290718675	T	T	T
0.3545453122144337	0.3321657553993660	0.5126778678370272	T	T	T
0.8470472102345212	0.3240267393455269	0.5125004712374874	T	T	T
0.8579393432436859	0.8397309301645208	0.5129956505441839	T	T	T

0.3468100285069369	0.8307755068232012	0.5123423797699473	T	T	T
0.6055790563874410	0.5865568261322736	0.5571051282332746	T	T	T
0.1010518979492403	0.5803106459967182	0.5573246502075051	T	T	T
0.1050979222661539	0.0862376051422160	0.5576699291834615	T	T	T
0.5988841635505153	0.0800848058823149	0.5576747637319244	T	T	T
0.3531519702518509	0.3351938822340088	0.6022283370595218	T	T	T
0.8472984929639793	0.3303839602798249	0.6021901825643852	T	T	T
0.8551130778583911	0.8347249989650010	0.6021759053924569	T	T	T
0.3501110110229462	0.8286635215277798	0.6022392189715973	T	T	T
0.6058810431673223	0.5862559538451606	0.6470733569930545	T	T	T
0.1011127907684610	0.5816166903629281	0.6469671340526943	T	T	T
0.1056724351758120	0.0867188215597778	0.6467665840896615	T	T	T
0.6007547525986041	0.0811162331522723	0.6468469987951622	T	T	T
0.3595895685480883	0.3390903003567587	0.6917463217033486	T	T	T
0.8496408488457092	0.3281451432221942	0.6917536455678430	T	T	T
0.8577066764801060	0.8382667343238381	0.6917723053379632	T	T	T
0.3475851515513995	0.8291916676257216	0.6917340760050621	T	T	T
0.6114667873944910	0.5911821226618628	0.7363955293335422	T	T	T
0.0986794343018715	0.5779805680014789	0.7364990878594853	T	T	T
0.1118442576215628	0.0916290258355801	0.7366083183621228	T	T	T
0.5982577265674962	0.0776512018418956	0.7365777419329262	T	T	T
0.3607168188493688	0.3398681348578947	0.7799953857237156	T	T	T
0.8400451827078967	0.3221860640285357	0.7798999330167860	T	T	T
0.8657376986971741	0.8435098405539350	0.7799068966563496	T	T	T
0.3429796208923008	0.8209952765012858	0.7799590465880399	T	T	T

SiO/Fe

1.0000000000000000		
4.8983807431150002	0.0000000000000000	0.0000000000000000
-0.8092335810400000	4.7595382108650002	0.0000000000000000
0.0000000000000000	0.0000000000000000	45.0000000000000000

Si	O	H	Fe
9	18	2	36

Selective dynamics

Direct

0.0067728748654119	0.9948063488658150	0.1954342331274290	T	T	T
0.0074514051592516	0.9963288732757007	0.3564416795108087	T	T	T
0.5000000000000000	0.0000000000000000	0.0725168741347275	F	F	F
0.5068608815593620	0.9961056237759820	0.2355474809634970	T	T	T
0.5086864887698042	0.9911099491217215	0.3973672738850169	T	T	T
0.0082841455154963	0.4948690913368807	0.1545943142791657	T	T	T
0.0097737562283626	0.4978600378658413	0.3161953573242542	T	T	T
0.5074979962464923	0.5004517058304430	0.1142179833396639	T	T	T
0.5089383052877636	0.4966285636056185	0.2762347457096297	T	T	T
0.2833117374387868	0.0699667758099025	0.0480040406733551	T	T	T
0.2702056604917260	0.1177434702375990	0.2162598478956284	T	T	T
0.2782462256792542	0.1315828881168386	0.3765953922934742	T	T	T
0.6173085360214685	0.2698158304495593	0.0930230113089578	T	T	T

0.6305754810417170	0.2621251300935015	0.2563423864810233	T	T	T
0.1286992219008098	0.7595390346112794	0.1757174476907579	T	T	T
0.1364740412730612	0.7650607406177414	0.3367781145158233	T	T	T
0.2443106720286963	0.3761753302726021	0.1350190916473579	T	T	T
0.2451069835872204	0.3727991873512480	0.2969925306331049	T	T	T
0.7734341830431646	0.6144281210242895	0.1349773349863099	T	T	T
0.7744097285217677	0.6204467100922102	0.2967569809065651	T	T	T
0.8860830884699311	0.2289067893989127	0.1754367917342492	T	T	T
0.8833980608336987	0.2338853429383008	0.3372242512672159	T	T	T
0.3925199628355358	0.7406451949488186	0.0948868843526611	T	T	T
0.3850323051710092	0.7314125134250276	0.2565928703167941	T	T	T
0.7636004011456663	0.9169707089851684	0.0532687705019583	T	T	T
0.7414718050303293	0.8733125768529604	0.2160579795342912	T	T	T
0.7317922731394049	0.8543544811848989	0.3754182467102893	T	T	T
0.0785059014896845	0.0243816943913941	0.0511748417582183	T	T	T
0.7085553898674704	0.7994103427159658	0.0359589245225962	T	T	T
0.2454844702673213	0.2421614589637642	0.4337054417555848	T	T	T
0.7525880667846110	0.2445657450534640	0.4363787018051326	T	T	T
0.7615338481159668	0.7382427104506775	0.4341232156412786	T	T	T
0.2549133220612489	0.7362434545607002	0.4362099575792939	T	T	T
0.5031181394623090	0.4895586041417062	0.4779257260775509	T	T	T
0.0038422752189575	0.4900912508392850	0.4780597380718490	T	T	T
0.0036171413830530	0.9900991734478524	0.4779660377489918	T	T	T
0.5030579632142391	0.9896437345598272	0.4780278605077939	T	T	T
0.2530291804960356	0.2393110098465243	0.5210548937782846	T	T	T
0.7526990182513629	0.2389478334634063	0.5212070348409910	T	T	T
0.7534888679522780	0.7392185151011859	0.5210339089242169	T	T	T
0.2538438245387411	0.7396743967614796	0.5212197650528196	T	T	T
0.5029943770138914	0.4889127095897905	0.5640717698168629	T	T	T
0.0029572439082486	0.4888649217752743	0.5640554318626982	T	T	T
0.0030084698479342	0.9889200335135868	0.5640615340000608	T	T	T
0.5030382111827336	0.9889574997419004	0.5640998641367787	T	T	T
0.2528190875401535	0.2384892435431993	0.6069932211239788	T	T	T
0.7528742901145549	0.2388316383432070	0.6070109409756910	T	T	T
0.7526379290344849	0.7388530173032350	0.6069897957006845	T	T	T
0.2525870688619563	0.7385189379566270	0.6070126586299338	T	T	T
0.5027630867406003	0.4886415940882358	0.6499444882401590	T	T	T
0.0027286616522915	0.4886350790802609	0.6499180077432243	T	T	T
0.0027616592627169	0.9886309587350723	0.6499404881813717	T	T	T
0.5027822273497975	0.9886282260444261	0.6499424401819809	T	T	T
0.2530799924105054	0.2384558086558357	0.6930307796472661	T	T	T
0.7532436834844702	0.2387125307137694	0.6930460244590151	T	T	T
0.7531706691662094	0.7386453874954029	0.6930362522858999	T	T	T
0.2530155305918242	0.7383704790385934	0.6930452099240654	T	T	T
0.5029321633769896	0.4884772961712542	0.7364289379098068	T	T	T
0.0029729283135040	0.4884662009114464	0.7364066963599001	T	T	T
0.0029262955312532	0.9884646867161351	0.7364316203833425	T	T	T
0.5029131495505865	0.9884816915594214	0.7363975362626434	T	T	T
0.2527004625745164	0.2384008563099798	0.7792045355920365	T	T	T

0.7527031244759357	0.2383500835943408	0.7791935344963932	T	T	T
0.7523944762853247	0.7382986503487814	0.7792012016823975	T	T	T
0.2523634418434497	0.7383528662890768	0.7791943700727941	T	T	T

SiO/Ni

1.0000000000000000

4.9168000000000003	0.0000000000000000	0.0000000000000000
0.0000000000000000	4.9168000000000003	0.0000000000000000
0.0000000000000000	0.0000000000000000	45.0000000000000000

Si	O	H	Ni
9	18	2	36

Selective dynamics

Direct

0.0022107613063173	0.9907244383065111	0.1951871081837059	T	T	T
0.0085965361657232	0.9853509419386419	0.3596775450773210	T	T	T
0.5000000000000000	0.0000000000000000	0.0725168741347275	F	F	F
0.5015560306584541	0.9867738986899166	0.2361799387521668	T	T	T
0.5079961631583138	0.9887461224681300	0.4032967134034216	T	T	T
0.0062530372060482	0.4925078405359352	0.1542149803267840	T	T	T
0.0020120078353955	0.4847182391368954	0.3184178930879125	T	T	T
0.5055024053693209	0.4975771269276976	0.1133427356856578	T	T	T
0.5021178560992963	0.4847335925370242	0.2772592000665597	T	T	T
0.2672320592198648	0.1041983901033522	0.0498811886636449	T	T	T
0.2479524011042018	0.0982269176010678	0.2163937436769383	T	T	T
0.2694939903358628	0.0869862253175792	0.3792559352208838	T	T	T
0.6185982480172743	0.2511607943305412	0.0924267219468160	T	T	T
0.6128075567442604	0.2346371163162121	0.2568700657149042	T	T	T
0.1158342466932608	0.7415155133723197	0.1748535683502576	T	T	T
0.1102148969350680	0.7335835536585166	0.3390632419349047	T	T	T
0.2561549352553739	0.3834487394103419	0.1336554432201537	T	T	T
0.2494171287291739	0.3772423101957442	0.2974591263117677	T	T	T
0.7557393784084337	0.6040508815875465	0.1339665852002022	T	T	T
0.7494559401337288	0.5921716517449742	0.2982331894086102	T	T	T
0.8973370658407839	0.2415858728325444	0.1745770263542194	T	T	T
0.8986996204931200	0.2352429741138622	0.3392989039807958	T	T	T
0.3923171319121974	0.7515369905151635	0.0936160801979332	T	T	T
0.3964402729408571	0.7346949843438662	0.2565819528784580	T	T	T
0.7703818544980855	0.8960017052844331	0.0535640493652492	T	T	T
0.7480600133538997	0.8807329534576742	0.2150120075312584	T	T	T
0.7559297794385653	0.8846066714153560	0.3806554155503055	T	T	T
0.0787246346584153	0.0320216251243328	0.0516435575489392	T	T	T
0.7431238743170416	0.7451817092739362	0.0398619615862733	T	T	T
0.2650163394458757	0.2438206288195749	0.4403891543123496	T	T	T
0.7575615261120419	0.2329740032294439	0.4395375032177630	T	T	T
0.7717680822409163	0.7305931212260158	0.4401669579512613	T	T	T
0.2769799989937454	0.7404950058910730	0.4395830090439524	T	T	T
0.5192353317277030	0.4868397191362563	0.4785888329001005	T	T	T
0.0183503650018430	0.4865667851056314	0.4781913652686809	T	T	T

0.0184245491771794	0.9863988143562317	0.4780928581948485	T	T	T
0.5190236645213842	0.9863560480970859	0.4787070251178316	T	T	T
0.2688095653278716	0.2360800596700478	0.5175242134877699	T	T	T
0.7697899080500009	0.2355387863100670	0.5176685072855111	T	T	T
0.7698734434574404	0.7356734809323213	0.5176107336409476	T	T	T
0.2688448006131816	0.7359552223905740	0.5176317877917579	T	T	T
0.5196363712865766	0.4856697772778911	0.5566713681555511	T	T	T
0.0197236673663590	0.4857161038829632	0.5566723563196386	T	T	T
0.0197644759701498	0.9858295439652847	0.5567001526793646	T	T	T
0.5196376506936483	0.9857325379073654	0.5566059436003474	T	T	T
0.2698645795084370	0.2361033219052349	0.5956609075746850	T	T	T
0.7696180051471343	0.2360305803158802	0.5956301677685439	T	T	T
0.7697628555518344	0.7360796550519728	0.5956592118957650	T	T	T
0.2700578534020883	0.7362703113332760	0.5956385465034272	T	T	T
0.5198933139040820	0.4872612734554875	0.6346032474606669	T	T	T
0.0198117203273268	0.4873852845201126	0.6345766694388048	T	T	T
0.0198718120326485	0.9874328793475199	0.6345746465246169	T	T	T
0.5199878572512653	0.9873115501008850	0.6345996376672579	T	T	T
0.2697840389118948	0.2390374513528424	0.6736123931368905	T	T	T
0.7697748404623068	0.2390301645876751	0.6736303205561290	T	T	T
0.7698078623914276	0.7390655014707644	0.6736231493687033	T	T	T
0.2698217564768751	0.7390528191241460	0.6736052175148589	T	T	T
0.5198087164144305	0.4904505199759915	0.7127664900682981	T	T	T
0.0199134079978957	0.4904274188608401	0.7127650211071586	T	T	T
0.0199327985310184	0.9904337635172386	0.7127595441717657	T	T	T
0.5198295991886405	0.9903830637841731	0.7127511882799318	T	T	T
0.2698469553022739	0.2410455035581230	0.7503133477509771	T	T	T
0.7697942886555298	0.2410387639217112	0.7503141709971254	T	T	T
0.7698139198575394	0.7410971948251367	0.7503064595266158	T	T	T
0.2697975825840782	0.7411996103584619	0.7503234675051834	T	T	T

SiO/Ti

1.0000000000000000

4.9897544099999998 0.0000000000000000 0.0000000000000000

0.0000000000000000 4.7798483894599997 0.0000000000000000

0.0000000000000000 0.0000000000000000 47.0000000000000000

Si	O	H	Ti
9	18	2	24

Selective dynamics

Direct

0.0204560750167246	0.9942864228299015	0.1869561744020132	T	T	T
0.0296493596819118	0.0312149363222147	0.3424114703055494	T	T	T
0.5000000000000000	0.0000000000000000	0.0694310497034678	F	F	F
0.5173070799992630	0.9883128217201502	0.2250380852022786	T	T	T
0.4850855690924547	0.8303610217912052	0.3812890480453390	T	T	T
0.0196643394944047	0.4924746607629658	0.1470793701291697	T	T	T
0.0143437652632485	0.5308658161484274	0.3029827146709749	T	T	T
0.5163067943395774	0.4982982134959641	0.1090858020049765	T	T	T

0.5091751698006419	0.4906848188739872	0.2649075910746674	T	T	T
0.2639078541357804	0.1068828875891867	0.0484941866568533	T	T	T
0.2724707095535379	0.1102345182630131	0.2056779114678875	T	T	T
0.2920133186281930	0.1057356636719220	0.3628712604349573	T	T	T
0.6282551373350600	0.2567377335277570	0.0877330391131963	T	T	T
0.6244934343170385	0.2291666991568917	0.2465925042201036	T	T	T
0.1335248597733525	0.7436350470641102	0.1669622778540756	T	T	T
0.1292859987404071	0.8121727920014195	0.3180817240817504	T	T	T
0.2714485122056089	0.3748146010243332	0.1283957237723143	T	T	T
0.2579795264649576	0.3916065729240756	0.2846739368992175	T	T	T
0.7711458548114365	0.6067576970077084	0.1277852700692534	T	T	T
0.7569144465660429	0.6155115962179281	0.2835322922795100	T	T	T
0.9032621621067776	0.2437354206600588	0.1670859989373170	T	T	T
0.9134477955991613	0.3096042548376090	0.3270756220167428	T	T	T
0.3919181238278071	0.7572615380233216	0.0909140565388711	T	T	T
0.3969713676854667	0.7290356285470097	0.2433340818665286	T	T	T
0.7622502339280857	0.8876830065381753	0.0509466239861283	T	T	T
0.7727652899763200	0.8805811903264740	0.2063934711036310	T	T	T
0.7989936611822728	0.8881299461252468	0.3627175326402039	T	T	T
0.0803895112345927	0.0282193612616339	0.0501705762776083	T	T	T
0.7355816720794266	0.7272463282274586	0.0385025235430092	T	T	T
0.3422848497970747	0.3488217197794157	0.4017687784014115	T	T	T
0.8393449218217128	0.3807365224326631	0.4331552614209926	T	T	T
0.5038945185210011	0.8829028639261125	0.4347555750240417	T	T	T
0.9754674228224758	0.8758555413652260	0.4039743583152173	T	T	T
0.3369258555496017	0.3812818250560213	0.4633070567509634	T	T	T
0.8327562294906699	0.3803628265997858	0.4942317494307602	T	T	T
0.4953854596672329	0.8814079348240966	0.4954000834161576	T	T	T
0.9966942915333306	0.8794449432777895	0.4646620000519306	T	T	T
0.3305140055700519	0.3835943815174758	0.5251057804020078	T	T	T
0.8294110173063913	0.3845444518342802	0.5558294835206112	T	T	T
0.4943937644656202	0.8847058227238307	0.5563762413710762	T	T	T
0.9949202902753527	0.8825547322137979	0.5257922973336449	T	T	T
0.3277499686931193	0.3859963804260573	0.5866273027526461	T	T	T
0.8272643210029074	0.3874729849561547	0.6173441508788287	T	T	T
0.4906974856841373	0.8875449012520846	0.6176842344603841	T	T	T
0.9926896911496357	0.8861341856394560	0.5868933152618823	T	T	T
0.3273800554858610	0.3886736136969233	0.6483332722929944	T	T	T
0.8266842876458398	0.3893794884625663	0.6789514781367316	T	T	T
0.4888425221357053	0.8893552036692967	0.6791514239730319	T	T	T
0.9890854062676624	0.8885857782847069	0.6485019937538965	T	T	T
0.3192987322913439	0.3898794175520450	0.7085154667217921	T	T	T
0.8575312987203318	0.3897254384915740	0.7375464200961659	T	T	T
0.4562520499289633	0.8901742368207195	0.7376438454333396	T	T	T
0.9948625197669685	0.8896850672957655	0.7086117720000829	T	T	T

References

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- (2) Cox, J. D.; Wagman, D. D.; Medvedev, V. A. *CODATA Key Values for Thermodynamics*; Hemisphere Publishing Corp.: New York, 1984.