

Supporting Information

for

A Thermodynamic Model of the Surface Hydroxylation of γ - Al_2O_3

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The acidity of surface Lewis sites. NH_3 molecule was used as basic probe to assess the Lewis acidity of the surface site by evaluating its adsorption strength on these sites. The magnitude of the adsorption energy of NH_3 molecule on the surface was used as the descriptor to measure the acidity, and the more negative the energy, the more acidic the site. The results are collected in the Table S1 and Figure S1, which indicated that the lower the coordination number, the more acidic Lewis is, as expected. It is noted that the Al_{IVa} and $\text{Al}_{\text{IVa}'}$ of $\text{Al}_2\text{O}_3(110)$ are equivalent, and the Al_{Vc} and Al_{Vd} sites of $\text{Al}_2\text{O}_3(100)$ are equivalent. Thus, we disregarded the acidity of the $\text{Al}_{\text{IVa}'}$ and Al_{Vd} sites. On the (110) surface, there are three types of sites accessible for NH_3 , i.e. the Al_{III} site, and the Al_{IVa} and Al_{IVb} sites: The adsorption of NH_3 on the Al_{III} site is much stronger (-213 kJ mol^{-1}) than on the two Al_{IVa} and Al_{IVb} sites, suggesting that the Al_{III} site has the strongest Lewis acidity. The adsorption energies on Al_{IVa} and Al_{IVb} sites are close with a difference of 7 kJ mol^{-1} , indicating their similar acidity. Thus, the acidity of the three sites can be ranked as $\text{Al}_{\text{III}} > \text{Al}_{\text{IVa}} > \text{Al}_{\text{IVb}}$. On the (100) surface the adsorption energy of NH_3 on the Al_{Va} site ($-134.1 \text{ kJ mol}^{-1}$) is the lowest, showing the strongest acidity. When adsorbed on the other two sites (Al_{Vb} and Al_{Vc}), the adsorption energies are same (by -103 kJ mol^{-1}), which is the consequence of the similar adsorption mode of NH_3 on these two sites (Figure 1b) and their similar acidity.

Figure S1. The binding strength of NH_3 on the Al sites of Al_2O_3 surfaces: (a) $\text{Al}_2\text{O}_3(110)$, and (b) $\text{Al}_2\text{O}_3(100)$ surfaces.

Figure S2. Total density of states (TDOS) of γ - Al_2O_3 bulk model.

Figure S3. Atom-projected density of states (PDOS) of γ - Al_2O_3 bulk model.

Figure S4. Simulated XRD pattern of γ - Al_2O_3 bulk model.

Table S1. NH_3 adsorption on Al sites of Al_2O_3 (110) and (100) surfaces

Table S2. Experimental IR-bands for CO adsorbed on γ - Al_2O_3 .

The coordinates of γ - Al_2O_3 bulk model.

The coordinates of γ - Al_2O_3 s0(110) model.

The coordinates of γ - Al_2O_3 s0(100) model.

The coordinates of s1a (110) model.

The coordinates of s1b (110) model.

The coordinates of s1c(110) model.

The coordinates of s2a(110) model.

The coordinates of s2b(110) model.

The coordinates of s2c(110) model.
 The coordinates of s3a(110) model.
 The coordinates of s3b(110) model.
 The coordinates of s3c(110) model.
 The coordinates of s3d(110) model.
 The coordinates of s1a(100) model.
 The coordinates of s1b(100) model.
 The coordinates of s1c(100) model.
 The coordinates of s2a(100) model.
 The coordinates of s2b(100) model.
 The coordinates of s2c(100) model.
 The coordinates of s2d(100) model.
 The coordinates of s3a(100) model.
 The coordinates of s3b(100) model.
 The coordinates of s4a(100) model.

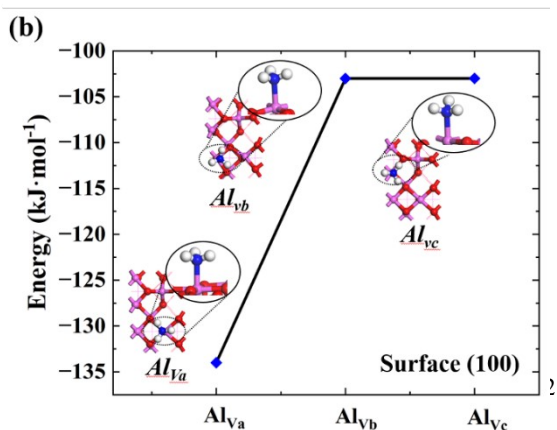
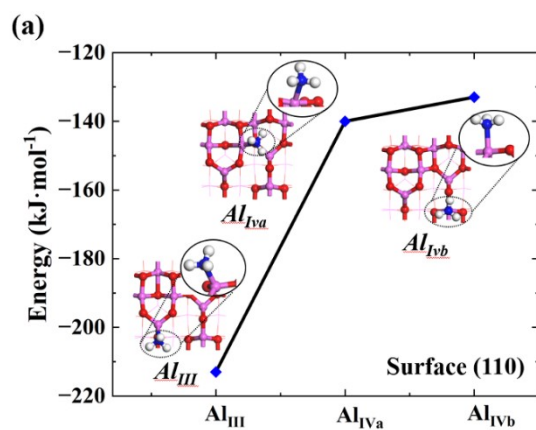


Figure S1. The binding strength of NH₃ on the Al sites of Al₂O₃ surfaces: (a) Al₂O₃(110), and (b) Al₂O₃(100) surfaces

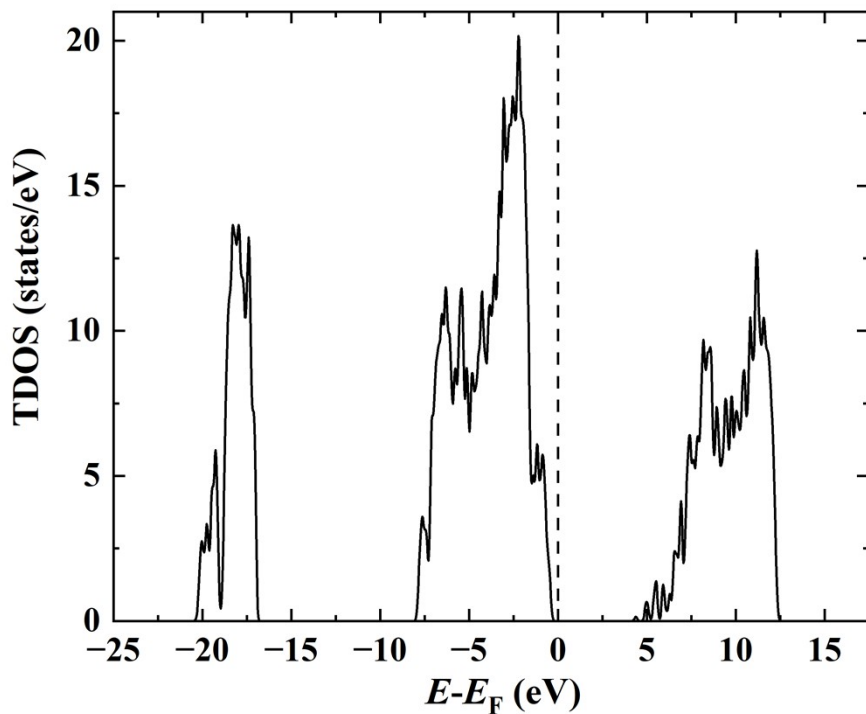


Figure S2. Total density of states (TDOS) of γ -Al₂O₃ bulk model.

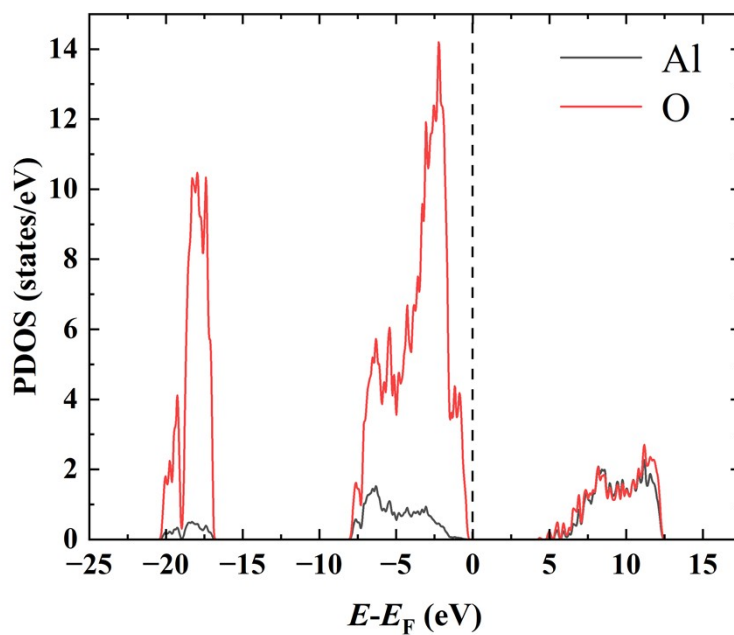


Figure S3. Atom-projected density of states (PDOS) of γ -Al₂O₃ bulk model.

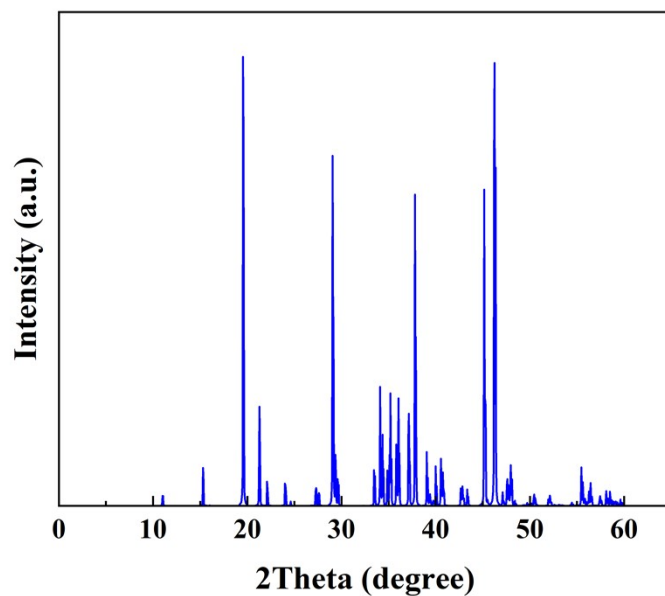


Figure S4. Simulated XRD pattern of γ -Al₂O₃ bulk model.

Table S1. NH₃ adsorption on Al sites of Al₂O₃ (110) and (100) surfaces

Surface	Adsorption site	$d_{\text{Al-N}}$ (Å)	E_{ads} (kJ mol ⁻¹)
(110)	Al _{III}	1.98	-213
	Al _{IVa}	2.04	-140
	Al _{IVb}	2.03	-133
(100)	Al _{Va}	2.05	-134
	Al _{Vb}	2.09	-103
	Al _{Vc}	2.09	-103

Table S2. Experimental IR-bands for CO adsorbed on γ -Al₂O₃.

ω_{exp} (Δ_{exp}) (cm ⁻¹)	Exp.assignment ^{1, 2}
2240-2220(+97/+57)	Defects
2200-2190(+57/47)	III
2184-2173(+41/+30)	IV
2165-2155(+22/+12)	VI
2153-2148(+10/+5)	V

The coordinates of γ -Al₂O₃ bulk model

1.00000000000000

5.5359235677336533 -0.0000000714350437 -0.0025108570170892

-0.0000001076776353 8.3405291938258710 -0.0000000330471680

-0.0859723627445829 -0.0000000307123005 8.0211835243102811

Al O

16 24

Direct

0.3673445374298889 0.0753913177629822 0.6131037137299438

0.6326554714178915 0.9246086832249496 0.3868962852047740

0.6326554544670197 0.5753913028776683 0.3868962444724654

0.3673445513247603 0.4246086960351891 0.6131037540021673

0.1167661798718265 0.5785231810136373 0.8625167898213593

0.8832338267941557 0.4214768231828204 0.1374832137103076

0.8832338220848867 0.0785231727623464 0.1374831921781556

0.1167661817553195 0.9214768255412674 0.8625168020544548

0.3781075397524745 0.7500000107054708 0.1257256420999684

0.6218924654629234 0.2499999899200576 0.8742743567198210

0.8757306899072365 0.7500000022636198 0.1251491228739210

0.1242693112481040 0.2499999996833508 0.8748508745583087

0.6157579360533731 0.7499999770834738 0.7459501279133142

0.3842420694263650 0.2500000208887099 0.2540498715625564

0.8683941972898863 0.2499999884087369 0.4991414851943557

0.1316058108591881 0.7500000138690925 0.5008585173676603

0.8866805559407824 0.4064753417113720 0.8974270111389361

0.1133194427542209 0.5935246509581029 0.1025729880365799

0.1133194648829708 0.9064753425040118 0.1025729895596682

0.8866805551574805 0.0935246600581042 0.8974270105611416

0.6071541179391434 0.9184023062423323 0.6143414038544868

0.3928458877802110 0.0815976912148827 0.3856585966235200

0.3928458440215748 0.4184022715840489 0.3856587362150686

0.6071541578154858 0.5815977301388455 0.6143412629569709

0.3583420378919491 0.4066988031358899 0.8551698692420929

0.6416579760136016 0.5933011979757953 0.1448301241800520

0.6416579941749391 0.9066987951479305 0.1448301856852521

0.3583420088230017 0.0933012045611084 0.8551698144375337

0.1342607589743655 0.9175241615380599 0.6364260673013606

0.8657392474633512 0.0824758421453967 0.3635739253091531

0.8657392425015750 0.4175241723059449 0.3635740118581212

0.1342607658132233 0.5824758449230056 0.6364260014813267

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The coordinates of γ -Al₂O₃ s0(110) model

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0.0000000000000000 8.0254001617000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 24.8878993987999984

Al O

16 24

Selective dynamics

Direct

0.0698238377015936	0.6134038929581769	0.2428356483887615	T	T	T
0.9246100189999993	0.3976500030000025	0.0860299989999973	F	F	F
0.5753899810000007	0.3976500030000025	0.0860299989999973	F	F	F
0.4301761408918040	0.6134039002108533	0.2428355957877695	T	T	T
0.5827844173512409	0.8687944202240446	0.1979009408492679	T	T	T
0.4214699859999982	0.1462399959999985	0.1417900029999970	F	F	F
0.0785299989999970	0.1462399959999985	0.1417900029999970	F	F	F
0.9172155942398524	0.8687943888234366	0.1979009514254522	T	T	T
0.7500000059901997	0.1407450896781373	0.2428220436092425	T	T	T
0.2500000000000000	0.8851500150000007	0.0836400020000028	F	F	F
0.7500000000000000	0.1339599940000014	0.1401000019999969	F	F	F
0.2499999619150052	0.8922511603015536	0.2017149505945133	T	T	T
0.7500000000000000	0.7569500210000015	0.0822699960000008	F	F	F
0.2499999451273337	0.3084867816641775	0.2513331751893689	T	T	T
0.2500000000000000	0.5080299970000013	0.1385000049999974	F	F	F
0.7500000140750985	0.4897272970236625	0.2026167921440816	T	T	T
0.4065400060000002	0.9061499829999988	0.1425700039999995	F	F	F
0.5881962938104262	0.1147032292209145	0.1920157725833679	T	T	T
0.9118037099869263	0.1147032226696469	0.1920157510028447	T	T	T
0.0934600009999969	0.9061499829999988	0.1425700039999995	F	F	F
0.9184399840000026	0.6252700089999976	0.0803600030000027	F	F	F
0.0848541655918334	0.4180613235358231	0.2718510768886389	T	T	T
0.4151460122500314	0.4180611160563437	0.2718508608323527	T	T	T
0.5815600159999974	0.6252700089999976	0.0803600030000027	F	F	F
0.4153878830778492	0.8403466776208970	0.2471281224864339	T	T	T
0.5932800169999979	0.1555200069999998	0.0880500000000026	F	F	F
0.9067199830000021	0.1555200069999998	0.0880500000000026	F	F	F
0.0846120905270666	0.8403466798376769	0.2471281869085377	T	T	T
0.9058477205009887	0.6367536417504406	0.2005103006344014	T	T	T

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The coordinates of $\gamma\text{-Al}_2\text{O}_3$ s0(100) model

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5.5376000404000001	0.0000000000000000	0.0000000000000000
0.0000000000000000	8.3437995910999998	0.0000000000000000
0.0000000000000000	0.0000000000000000	21.3780994415000016

Al O
16 24

Selective dynamics

Direct

0.3464976272088440	0.0912567893220804	0.3323458580770468	T	T	T
0.6144000290000022	0.9425100090000029	0.2470500020000017	F	F	F
0.6144000290000022	0.5932899709999973	0.2470500020000017	F	F	F
0.3465376231868830	0.4443392010636161	0.3323229034489822	T	T	T
0.0518646287603409	0.6037438214145475	0.4220531140016250	T	T	T
0.8691099879999982	0.4393700059999972	0.1534200010000006	F	F	F
0.8691099879999982	0.0964300039999983	0.1534200010000006	F	F	F
0.0518767709573581	0.9319610994649153	0.4220237833525667	T	T	T
0.3641700149999991	0.7678999899999965	0.1490000040000012	F	F	F
0.6188381191431721	0.2678169542839973	0.4267292152638203	T	T	T
0.8617600199999984	0.7678999899999965	0.1487800029999988	F	F	F
0.1052261302856925	0.2678350445994213	0.4265122723457697	T	T	T
0.5572530243990456	0.7677454428549740	0.3880212956104773	T	T	T
0.3682200099999974	0.2678999899999965	0.1971399930000004	F	F	F
0.8483600019999997	0.2678999899999965	0.2891800109999991	F	F	F
0.1114099990000028	0.7678999899999965	0.2898299989999984	F	F	F
0.8750996678890928	0.4193638317707763	0.4422200149126537	T	T	T
0.0996799990000028	0.6113600130000023	0.1403300019999989	F	F	F
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0.8751348919847193	0.1162765638938948	0.4422314107144129	T	T	T
0.5761725247678307	0.9323531913073594	0.3337792947940911	T	T	T
0.3746199910000030	0.0994599980000004	0.2465900030000014	F	F	F
0.3746199910000030	0.4363400040000016	0.2465900030000014	F	F	F
0.5763038802610335	0.6032168816492504	0.3337896317050205	T	T	T
0.3448865178542292	0.4208821706937271	0.4266732964654212	T	T	T

0.6274499889999987	0.6111800070000015	0.1561799939999986	F	F	F
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0.3448868151766408	0.1147647511846388	0.4266247176520125	T	T	T
0.1027672768375795	0.9399704664719631	0.3388718413886856	T	T	T
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0.1028485393205459	0.5957479351419910	0.3388888027825658	T	T	T
0.8323890005928505	0.7678581148593828	0.4320364468149127	T	T	T
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0.2832635844208799	0.7678130896526656	0.4365882715515338	T	T	T
0.6239399910000003	0.2678999899999965	0.1433500050000021	F	F	F
0.5942897341603919	0.2678380012432790	0.3413376904800806	T	T	T
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0.00000000E+00	0.00000000E+00	0.00000000E+00

The coordinates of s1a(110) model

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8.3437995910999998	0.0000000000000000	0.0000000000000000
0.0000000000000000	8.0254001617000004	0.0000000000000000
0.0000000000000000	0.0000000000000000	24.8878993987999984

Al	O	H
16	25	2

Selective dynamics

Direct

0.0752569465471947	0.6109496107602225	0.2426797379882677	T	T	T
0.9246100189999993	0.3976500030000025	0.0860299989999973	F	F	F
0.5753899810000007	0.3976500030000025	0.0860299989999973	F	F	F
0.4250538014162016	0.6208752160514120	0.2403320687333487	T	T	T
0.5824035095414509	0.8702899675877328	0.1970004799023042	T	T	T
0.4214699859999982	0.1462399959999985	0.1417900029999970	F	F	F
0.0785299989999970	0.1462399959999985	0.1417900029999970	F	F	F
0.9186062622804412	0.8661118799730976	0.1980114676060794	T	T	T
0.7505026482516741	0.1361595834904813	0.2428480803452218	T	T	T
0.2500000000000000	0.8851500150000007	0.0836400020000028	F	F	F
0.7500000000000000	0.1339599940000014	0.1401000019999969	F	F	F
0.2487140786695796	0.9005153599494463	0.2015698635921863	T	T	T
0.7500000000000000	0.7569500210000015	0.0822699960000008	F	F	F
0.2531876643929320	0.2699252356411259	0.2658788504555639	T	T	T
0.2500000000000000	0.5080299970000013	0.1385000049999974	F	F	F
0.7495971317636880	0.4900591722685537	0.2016748585137150	T	T	T
0.4065400060000002	0.9061499829999988	0.1425700039999995	F	F	F
0.5889010477546560	0.1142315975191053	0.1921212249674439	T	T	T
0.9105316834456563	0.1178772752656740	0.1927253827550811	T	T	T
0.0934600099999969	0.9061499829999988	0.1425700039999995	F	F	F
0.9184399840000026	0.6252700089999976	0.0803600030000027	F	F	F

0.1059939662847559	0.4228777285199325	0.2731219912559650	T	T	T
0.4271516165095234	0.4207329821270142	0.2706928278842264	T	T	T
0.5815600159999974	0.6252700089999976	0.0803600030000027	F	F	F
0.4153711537378696	0.8435094616892930	0.2471205866039982	T	T	T
0.5932800169999979	0.1555200069999998	0.0880500000000026	F	F	F
0.9067199830000021	0.1555200069999998	0.0880500000000026	F	F	F
0.0851234282790909	0.8389080187259678	0.2467057023926864	T	T	T
0.9068953096952002	0.6324185244504110	0.2018222412671453	T	T	T
0.0824700000000007	0.3725399969999970	0.1378899959999984	F	F	F
0.4175299999999993	0.3725399969999970	0.1378899959999984	F	F	F
0.5943708207667169	0.6372527560553658	0.2005660647024399	T	T	T
0.7500000000000000	0.8851100210000027	0.1414899979999973	F	F	F
0.2501907739187117	0.1412422775917868	0.1999603404367667	T	T	T
0.7501976883903926	0.9143093384648329	0.2471930566284154	T	T	T
0.2500000000000000	0.1213599960000025	0.0871400010000016	F	F	F
0.2500000000000000	0.6510499720000027	0.0816000029999984	F	F	F
0.7284477130886232	0.3473384051444056	0.2560196842390464	T	T	T
0.2512162012085286	0.6195419719822816	0.1990946964074373	T	T	T
0.7500000000000000	0.3809399900000017	0.1380500049999966	F	F	F
0.2915865605797929	0.1284092356768655	0.3157206771781456	T	T	T
0.3139775052786282	0.0126833122342496	0.3073486696700933	T	T	T
0.5425840432949304	0.3776464387618859	0.2717518360596413	T	T	T

0.00000000E+00	0.00000000E+00	0.00000000E+00
0.00000000E+00	0.00000000E+00	0.00000000E+00
0.00000000E+00	0.00000000E+00	0.00000000E+00
0.00000000E+00	0.00000000E+00	0.00000000E+00
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0.00000000E+00	0.00000000E+00	0.00000000E+00
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0.00000000E+00	0.00000000E+00	0.00000000E+00
0.00000000E+00	0.00000000E+00	0.00000000E+00
0.00000000E+00	0.00000000E+00	0.00000000E+00
0.00000000E+00	0.00000000E+00	0.00000000E+00
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0.00000000E+00	0.00000000E+00	0.00000000E+00
0.00000000E+00	0.00000000E+00	0.00000000E+00
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0.00000000E+00	0.00000000E+00	0.00000000E+00
0.00000000E+00	0.00000000E+00	0.00000000E+00
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0.00000000E+00	0.00000000E+00	0.00000000E+00
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The coordinates of s1b(110) model

1.0000000000000000
8.3437995910999998 0.0000000000000000 0.0000000000000000
0.0000000000000000 8.0254001617000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 24.8878993987999984

Al O H
16 25 2

Selective dynamics

Direct

0.0813553901845075	0.6149203457941624	0.2554904336148235	T	T	T
0.9246100189999993	0.3976500030000025	0.0860299989999973	F	F	F
0.5753899810000007	0.3976500030000025	0.0860299989999973	F	F	F
0.4134213156259014	0.6285982609524036	0.2547875674511329	T	T	T
0.5808465332742647	0.8639374165382897	0.1981773663837888	T	T	T
0.4214699859999982	0.1462399959999985	0.1417900029999970	F	F	F
0.0785299989999970	0.1462399959999985	0.1417900029999970	F	F	F
0.9192850306244897	0.8587730171925668	0.1982956954231923	T	T	T
0.7536347639639197	0.1329722210358247	0.2423208076958369	T	T	T
0.2500000000000000	0.8851500150000007	0.0836400020000028	F	F	F
0.7500000000000000	0.1339599940000014	0.1401000019999969	F	F	F

0.2487592297067699	0.9137149678801664	0.2023663562183638	T	T	T
0.7500000000000000	0.7569500210000015	0.0822699960000008	F	F	F
0.2431587207502956	0.3295378697752985	0.2429864948726512	T	T	T
0.2500000000000000	0.5080299970000013	0.1385000049999974	F	F	F
0.7484001193529202	0.4905743637307276	0.2047831150906159	T	T	T
0.4065400060000002	0.9061499829999988	0.1425700039999995	F	F	F
0.5894382664043013	0.1125384834564978	0.1917661225819386	T	T	T
0.9114808484715192	0.1173680642590408	0.1921483169034943	T	T	T
0.093460009999969	0.9061499829999988	0.1425700039999995	F	F	F
0.9184399840000026	0.6252700089999976	0.0803600030000027	F	F	F
0.0725686673152982	0.3969741031922473	0.2742874945247649	T	T	T
0.4275011960847184	0.3958922598588038	0.2734600739906676	T	T	T
0.5815600159999974	0.6252700089999976	0.0803600030000027	F	F	F
0.4118441145076934	0.8540538130469184	0.2444170838460573	T	T	T
0.5932800169999979	0.1555200069999998	0.0880500000000026	F	F	F
0.9067199830000021	0.1555200069999998	0.0880500000000026	F	F	F
0.0881366892652021	0.8450933298786680	0.2441643564744403	T	T	T
0.9109462602649138	0.6287215846391185	0.2088802409254623	T	T	T
0.0824700000000007	0.3725399969999970	0.1378899959999984	F	F	F
0.4175299999999993	0.3725399969999970	0.1378899959999984	F	F	F
0.5863866053207876	0.6321882891765036	0.2100540524730495	T	T	T
0.7500000000000000	0.8851100210000027	0.1414899979999973	F	F	F
0.2501919754980729	0.1495946698014683	0.1987884901123271	T	T	T
0.7514554466397226	0.9124906652601191	0.2475195228115575	T	T	T
0.2500000000000000	0.1213599960000025	0.0871400010000016	F	F	F
0.2500000000000000	0.6510499720000027	0.0816000029999984	F	F	F
0.7225914000505709	0.3406440636717720	0.2570891105541975	T	T	T
0.2517612290459252	0.5619032914457066	0.2074886233241128	T	T	T
0.7500000000000000	0.3809399900000017	0.1380500049999966	F	F	F
0.2548541261209394	0.6498853460842109	0.3081866537857257	T	T	T
0.2519674554275712	0.5550331639883629	0.3325538354963881	T	T	T
0.5444384303861626	0.3557726825610908	0.2683676692587131	T	T	T

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The coordinates of s1c(110) model

1.00000000000000
8.3437995910999998 0.0000000000000000 0.0000000000000000
0.0000000000000000 8.0254001617000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 24.8878993987999984

Al O H
16 25 2

Selective dynamics

Direct

0.0709632996926307 0.6139606955840093 0.2430159139446462 T T T

0.9246100189999993	0.3976500030000025	0.0860299989999973	F	F	F
0.5753899810000007	0.3976500030000025	0.0860299989999973	F	F	F
0.4295288787406997	0.6183285959697891	0.2417855077226319	T	T	T
0.5831585407930906	0.8705551265112965	0.1965174858242033	T	T	T
0.4214699859999982	0.1462399959999985	0.1417900029999970	F	F	F
0.0785299989999970	0.1462399959999985	0.1417900029999970	F	F	F
0.9180589110307588	0.8695825788868834	0.1970568467407650	T	T	T
0.7441284429652991	0.1241844074442125	0.2518900644937305	T	T	T
0.2500000000000000	0.8851500150000007	0.0836400020000028	F	F	F
0.7500000000000000	0.1339599940000014	0.1401000019999969	F	F	F
0.2502848076912204	0.8983262291097038	0.2024910000957496	T	T	T
0.7500000000000000	0.7569500210000015	0.0822699960000008	F	F	F
0.2558830927093838	0.3107589468963168	0.2521594592588831	T	T	T
0.2500000000000000	0.5080299970000013	0.1385000049999974	F	F	F
0.7500618625245046	0.5016286750115930	0.1971835161687110	T	T	T
0.4065400060000002	0.9061499829999988	0.1425700039999995	F	F	F
0.5887403647427648	0.1136203651682088	0.1928100456504122	T	T	T
0.9094214129517716	0.1173746192467384	0.1938451132778527	T	T	T
0.093460009999969	0.9061499829999988	0.1425700039999995	F	F	F
0.9184399840000026	0.6252700089999976	0.0803600030000027	F	F	F
0.0901783662833931	0.4197681183712302	0.2729598335904659	T	T	T
0.4253235350418358	0.4212017280738315	0.2717677931118048	T	T	T
0.5815600159999974	0.6252700089999976	0.0803600030000027	F	F	F
0.4155705608520067	0.8415807313126970	0.2467925081325811	T	T	T
0.5932800169999979	0.1555200069999998	0.0880500000000026	F	F	F
0.9067199830000021	0.1555200069999998	0.0880500000000026	F	F	F
0.0858093257378546	0.8396136031018323	0.2468562262711166	T	T	T
0.9125088808068419	0.6343742980808073	0.1983454529405005	T	T	T
0.0824700000000007	0.3725399969999970	0.1378899959999984	F	F	F
0.4175299999999993	0.3725399969999970	0.1378899959999984	F	F	F
0.5889723462428377	0.6373701920423425	0.1974716003004684	T	T	T
0.7500000000000000	0.8851100210000027	0.1414899979999973	F	F	F
0.2516683361542747	0.1440240028952869	0.2025030750522862	T	T	T
0.7513222669020316	0.8972400890802474	0.2432673420438507	T	T	T
0.2500000000000000	0.1213599960000025	0.0871400010000016	F	F	F
0.2500000000000000	0.6510499720000027	0.0816000029999984	F	F	F
0.7347685521861105	0.3590834669054993	0.2509776386827133	T	T	T
0.2505257683338571	0.6091549319335458	0.2009326583631977	T	T	T
0.7500000000000000	0.3809399900000017	0.1380500049999966	F	F	F
0.6966319057684011	0.1323416512759391	0.3200991958686157	T	T	T
0.6817179258660991	0.0229143949633078	0.3357790195583975	T	T	T
0.6322850080500072	0.3759774905361719	0.2712389600391351	T	T	T

0.00000000E+00 0.00000000E+00 0.00000000E+00

1.0000000000000000
 8.3437995910999998 0.0000000000000000 0.0000000000000000
 0.0000000000000000 8.0254001617000004 0.0000000000000000
 0.0000000000000000 0.0000000000000000 24.8878993987999984

Al O H
 16 26 4

Selective dynamics

Direct

0.0898322641446169	0.6120466703686336	0.2502632472897309	T	T	T
0.9246100189999993	0.3976500030000025	0.0860299989999973	F	F	F
0.5753899810000007	0.3976500030000025	0.0860299989999973	F	F	F
0.4115947742997674	0.6157559440850235	0.2505170869680327	T	T	T
0.5851395392413192	0.8696341842290213	0.1966423634288827	T	T	T
0.4214699859999982	0.1462399959999985	0.1417900029999970	F	F	F
0.0785299989999970	0.1462399959999985	0.1417900029999970	F	F	F
0.9196797930952842	0.8635468501068265	0.2000431034176972	T	T	T
0.7545389137865147	0.1374333774809943	0.2421293494886991	T	T	T
0.2500000000000000	0.8851500150000007	0.0836400020000028	F	F	F
0.7500000000000000	0.1339599940000014	0.1401000019999969	F	F	F
0.2445291610491659	0.8886771836209265	0.1971014647205959	T	T	T
0.7500000000000000	0.7569500210000015	0.0822699960000008	F	F	F
0.2483932297676694	0.2554598499451343	0.2594177470488503	T	T	T
0.2500000000000000	0.5080299970000013	0.1385000049999974	F	F	F
0.7496467230642682	0.4947115985449163	0.2037323479724063	T	T	T
0.4065400060000002	0.9061499829999988	0.1425700039999995	F	F	F
0.5899615310391143	0.1136404073349943	0.1919323726224863	T	T	T
0.9108199295586928	0.1167133066490983	0.1921774291122389	T	T	T
0.0934600099999969	0.9061499829999988	0.1425700039999995	F	F	F
0.9184399840000026	0.6252700089999976	0.0803600030000027	F	F	F
0.0926745773539975	0.3958115281451157	0.2651564540917297	T	T	T
0.4243400807170062	0.3914205288157117	0.2643295479677616	T	T	T
0.5815600159999974	0.6252700089999976	0.0803600030000027	F	F	F
0.4162546639717609	0.8639104298972682	0.2470901940312743	T	T	T
0.5932800169999979	0.1555200069999998	0.0880500000000026	F	F	F
0.9067199830000021	0.1555200069999998	0.0880500000000026	F	F	F
0.0865931344219643	0.8507032386045759	0.2463367818659823	T	T	T
0.9116641998848739	0.6326880076038588	0.2080360179128858	T	T	T
0.0824700000000007	0.3725399969999970	0.1378899959999984	F	F	F
0.4175299999999993	0.3725399969999970	0.1378899959999984	F	F	F
0.5876143345884175	0.6401554479181256	0.2096825586425399	T	T	T
0.7500000000000000	0.8851100210000027	0.1414899979999973	F	F	F
0.2504988450136820	0.1349450977861151	0.1963492710588935	T	T	T
0.7497362596244822	0.9167406530004218	0.2483215109621133	T	T	T


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0.00000000E+00  0.00000000E+00  0.00000000E+00
0.00000000E+00  0.00000000E+00  0.00000000E+00
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0.00000000E+00  0.00000000E+00  0.00000000E+00

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The coordinates of s2b(110) model

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  0.0000000000000000    8.0254001617000004    0.0000000000000000
  0.0000000000000000    0.0000000000000000    24.8878993987999984

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Selective dynamics

Direct

```

0.0841855648052192  0.6270113024511315  0.2548905306241897  T  T  T
0.9246100189999993  0.3976500030000025  0.0860299989999973  F  F  F
0.5753899810000007  0.3976500030000025  0.0860299989999973  F  F  F
0.4184222946347593  0.6201417114018729  0.2548281200227245  T  T  T
0.5826465386120699  0.8599620357541375  0.1970697321736367  T  T  T
0.4214699859999982  0.1462399959999985  0.1417900029999970  F  F  F
0.0785299989999970  0.1462399959999985  0.1417900029999970  F  F  F
0.9193491219599075  0.8712996287950024  0.1987810522198341  T  T  T
0.7225893557502002  0.1293548056613232  0.2501669255766760  T  T  T
0.2500000000000000  0.8851500150000007  0.0836400020000028  F  F  F
0.7500000000000000  0.1339599940000014  0.1401000019999969  F  F  F
0.2503276531006308  0.9152169219869716  0.2021086758159636  T  T  T
0.7500000000000000  0.7569500210000015  0.0822699960000008  F  F  F
0.2366773564056255  0.3317585753245445  0.2418554596645580  T  T  T
0.2500000000000000  0.5080299970000013  0.1385000049999974  F  F  F
0.7564483192389833  0.4981540706725582  0.2009572435866714  T  T  T
0.4065400060000002  0.9061499829999988  0.1425700039999995  F  F  F
0.5872556640063086  0.1181747393551281  0.1915828831434654  T  T  T
0.9101607929041974  0.1122740153912436  0.1919819423885604  T  T  T
0.0934600009999969  0.9061499829999988  0.1425700039999995  F  F  F

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0.5729292560740127	0.8694187809805126	0.1935114125148644	T	T	T
0.4214699859999982	0.1462399959999985	0.1417900029999970	F	F	F
0.0785299989999970	0.1462399959999985	0.1417900029999970	F	F	F
0.9256212391263796	0.8659653377065645	0.1929590765069010	T	T	T
0.7617426848393830	0.1422043796893680	0.2503252516482498	T	T	T
0.2500000000000000	0.8851500150000007	0.0836400020000028	F	F	F
0.7500000000000000	0.1339599940000014	0.1401000019999969	F	F	F
0.2496860718024783	0.9076410371748581	0.2055744772157155	T	T	T
0.7500000000000000	0.7569500210000015	0.0822699960000008	F	F	F
0.2511916521057877	0.2806933329792403	0.2671986390519584	T	T	T
0.2500000000000000	0.5080299970000013	0.1385000049999974	F	F	F
0.7458544439568442	0.5010204260877253	0.1973994980735820	T	T	T
0.4065400060000002	0.9061499829999988	0.1425700039999995	F	F	F
0.5937721777078986	0.1087287116006880	0.1936702164076055	T	T	T
0.9079580370789082	0.1139602208271610	0.1935784052141163	T	T	T
0.0934600099999969	0.9061499829999988	0.1425700039999995	F	F	F
0.9184399840000026	0.6252700089999976	0.0803600030000027	F	F	F
0.0920853079338396	0.4239468557478874	0.2718285710472435	T	T	T
0.4251464009239925	0.4179139668074101	0.2689126305295255	T	T	T
0.5815600159999974	0.6252700089999976	0.0803600030000027	F	F	F
0.4177509233608027	0.8396523836653571	0.2468943426832033	T	T	T
0.5932800169999979	0.1555200069999998	0.0880500000000026	F	F	F
0.9067199830000021	0.1555200069999998	0.0880500000000026	F	F	F
0.0798508296507540	0.8399687556901294	0.2466218330988524	T	T	T
0.9074034799504952	0.6354250846971325	0.1989861522955974	T	T	T
0.0824700000000007	0.3725399969999970	0.1378899959999984	F	F	F
0.4175299999999993	0.3725399969999970	0.1378899959999984	F	F	F
0.5875007823227270	0.6398846661363500	0.1969697995712371	T	T	T
0.7500000000000000	0.8851100210000027	0.1414899979999973	F	F	F
0.2498392443206823	0.1425342219318515	0.1993324767960760	T	T	T
0.7493865978807582	0.8981313022459136	0.2438452901503003	T	T	T
0.2500000000000000	0.1213599960000025	0.0871400010000016	F	F	F
0.2500000000000000	0.6510499720000027	0.0816000029999984	F	F	F
0.7119925046736549	0.3628198764331196	0.2512890372173505	T	T	T
0.2481633398951426	0.6215477137098481	0.1983807678691375	T	T	T
0.7500000000000000	0.3809399900000017	0.1380500049999966	F	F	F
0.8143070554239004	0.1037240665923453	0.3165165665784693	T	T	T
0.2624353953995370	0.1277733928500939	0.3151886557879811	T	T	T
0.8351795709018303	0.1982646393025355	0.3396522255447723	T	T	T
0.1724747173107773	0.0530899440554947	0.3204469870840838	T	T	T
0.5840071346670058	0.3764431827170010	0.2627890655846804	T	T	T
0.7570834953253200	0.8547240271866360	0.2803093292616080	T	T	T

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The coordinates of s3a(110) model

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0.0000000000000000 8.0254001617000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 24.8878993987999984

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Selective dynamics

Direct

0.0882095082292809	0.6118385536726566	0.2498016684076817	T	T	T
0.9246100189999993	0.3976500030000025	0.0860299989999973	F	F	F
0.5753899810000007	0.3976500030000025	0.0860299989999973	F	F	F
0.4113702685557820	0.6201399199299257	0.2508223093176655	T	T	T
0.5822701079374099	0.8656208045398434	0.1989301001550916	T	T	T
0.4214699859999982	0.1462399959999985	0.1417900029999970	F	F	F
0.0785299989999970	0.1462399959999985	0.1417900029999970	F	F	F
0.9142003422505641	0.8758264289647912	0.1970430651104517	T	T	T
0.7238781986095907	0.1341579348227892	0.2502072188079885	T	T	T
0.2500000000000000	0.8851500150000007	0.0836400020000028	F	F	F
0.7500000000000000	0.1339599940000014	0.1401000019999969	F	F	F
0.2548385814697020	0.8905685463402622	0.1968253914255639	T	T	T
0.7500000000000000	0.7569500210000015	0.0822699960000008	F	F	F
0.2329317134862529	0.2525964067235423	0.2596065055467830	T	T	T
0.2500000000000000	0.5080299970000013	0.1385000049999974	F	F	F
0.7561053365322673	0.5037338407919344	0.1994532277187875	T	T	T
0.4065400060000002	0.9061499829999988	0.1425700039999995	F	F	F
0.5882735263236228	0.1180067278823981	0.1918512959431040	T	T	T
0.9099665912806195	0.1125822082094245	0.1920923729295437	T	T	T
0.0934600099999969	0.9061499829999988	0.1425700039999995	F	F	F
0.9184399840000026	0.6252700089999976	0.0803600030000027	F	F	F
0.0740154083596784	0.3947770474293463	0.2647938764007601	T	T	T
0.4089903984583089	0.3886644411754779	0.2685752593070569	T	T	T
0.5815600159999974	0.6252700089999976	0.0803600030000027	F	F	F
0.4141712778418106	0.8536143336101545	0.2459783964664882	T	T	T
0.5932800169999979	0.1555200069999998	0.0880500000000026	F	F	F
0.9067199830000021	0.1555200069999998	0.0880500000000026	F	F	F
0.0854601560371889	0.8601732698911427	0.2474090017939485	T	T	T
0.9176346481253408	0.6441851048890380	0.2066434011703186	T	T	T
0.0824700000000007	0.3725399969999970	0.1378899959999984	F	F	F
0.4175299999999993	0.3725399969999970	0.1378899959999984	F	F	F
0.5873501790645222	0.6302395677492727	0.2087226155823292	T	T	T

0.7500000000000000	0.1339599940000014	0.1401000019999969	F	F	F
0.2458257381485057	0.8903667973851556	0.1965849287660876	T	T	T
0.7500000000000000	0.7569500210000015	0.0822699960000008	F	F	F
0.2399058359695989	0.2532127187332064	0.2595650123465154	T	T	T
0.2500000000000000	0.5080299970000013	0.1385000049999974	F	F	F
0.7571885012005070	0.5047224965431729	0.1993100169445679	T	T	T
0.4065400060000002	0.9061499829999988	0.1425700039999995	F	F	F
0.5888166529680255	0.1179281115611465	0.1920255279483189	T	T	T
0.9092436969686598	0.1123465798934250	0.1924345768629949	T	T	T
0.0934600009999969	0.9061499829999988	0.1425700039999995	F	F	F
0.9184399840000026	0.6252700089999976	0.0803600030000027	F	F	F
0.0829333524476976	0.4002564199400954	0.2650638800153547	T	T	T
0.4195336277561034	0.3821205165253619	0.2668242873301087	T	T	T
0.5815600159999974	0.6252700089999976	0.0803600030000027	F	F	F
0.4168260150490446	0.8601306060787092	0.2465755539841733	T	T	T
0.5932800169999979	0.1555200069999998	0.0880500000000026	F	F	F
0.9067199830000021	0.1555200069999998	0.0880500000000026	F	F	F
0.0900290465630043	0.8551368870624870	0.2468526726685719	T	T	T
0.9185920217791204	0.6413919006487346	0.2056910290998848	T	T	T
0.0824700000000007	0.3725399969999970	0.1378899959999984	F	F	F
0.4175299999999993	0.3725399969999970	0.1378899959999984	F	F	F
0.5885095492006157	0.6355381297574961	0.2092743572664551	T	T	T
0.7500000000000000	0.8851100210000027	0.1414899979999973	F	F	F
0.2491068440234612	0.1362332931608466	0.1963775275832645	T	T	T
0.7483350558008207	0.9104496331520533	0.2465360323404548	T	T	T
0.2500000000000000	0.1213599960000025	0.0871400010000016	F	F	F
0.2500000000000000	0.6510499720000027	0.0816000029999984	F	F	F
0.7923687725578720	0.3546875935844528	0.2503577838350342	T	T	T
0.2584877877429751	0.6262036730662505	0.1995400101251368	T	T	T
0.7500000000000000	0.3809399900000017	0.1380500049999966	F	F	F
0.2641488655658424	0.6444527628811767	0.3042808492218451	T	T	T
0.2672737472306176	0.0917699263584495	0.3072363234635042	T	T	T
0.6134635680185480	0.1784648879844656	0.3084584907844389	T	T	T
0.2575071481047217	0.5531253579959610	0.3298573584353615	T	T	T
0.1815700338628621	0.0080333012965742	0.3057630465290489	T	T	T
0.5463077345748254	0.0959477936892875	0.3259513523943594	T	T	T
0.9200403120631309	0.3645917843599002	0.2583758446869862	T	T	T
0.5082554097262325	0.3087590394597251	0.2866251204566158	T	T	T
0.3877885729575514	0.9409410203101053	0.2762038211009115	T	T	T

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0.00000000E+00	0.00000000E+00	0.00000000E+00
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The coordinates of s3c(110) model

1.0000000000000000

8.3437995910999998	0.0000000000000000	0.0000000000000000
0.0000000000000000	8.0254001617000004	0.0000000000000000
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Selective dynamics

Direct

0.0808553738607140	0.6154052061857537	0.2390881282793852	T	T	T
0.9246100189999993	0.3976500030000025	0.0860299989999973	F	F	F
0.5753899810000007	0.3976500030000025	0.0860299989999973	F	F	F
0.4527510408101590	0.6232684631573135	0.2530587896490386	T	T	T
0.5724970356922324	0.8630628538010289	0.1914249708461331	T	T	T
0.4214699859999982	0.1462399959999985	0.1417900029999970	F	F	F
0.0785299989999970	0.1462399959999985	0.1417900029999970	F	F	F
0.9231953881427399	0.8723275346930530	0.1957426170872672	T	T	T
0.7186609436363839	0.1394137206747481	0.2506103908230042	T	T	T
0.2500000000000000	0.8851500150000007	0.0836400020000028	F	F	F
0.7500000000000000	0.1339599940000014	0.1401000019999969	F	F	F
0.2514724809949623	0.8969079027462683	0.2022640229625671	T	T	T
0.7500000000000000	0.7569500210000015	0.0822699960000008	F	F	F
0.2287408949804383	0.2668789493221136	0.2627540642433489	T	T	T
0.2500000000000000	0.5080299970000013	0.1385000049999974	F	F	F
0.7518613593039233	0.5038282608482018	0.1970854315151179	T	T	T
0.4065400060000002	0.9061499829999988	0.1425700039999995	F	F	F
0.5892927614027776	0.1140013716314599	0.1917666130444156	T	T	T
0.9037956637409326	0.1070236133587416	0.1942998466064965	T	T	T
0.0934600009999969	0.9061499829999988	0.1425700039999995	F	F	F
0.9184399840000026	0.6252700089999976	0.0803600030000027	F	F	F
0.0731862880289401	0.4187137082760535	0.2683436824788433	T	T	T
0.4045267296469225	0.4027098269577351	0.2703177558954048	T	T	T
0.5815600159999974	0.6252700089999976	0.0803600030000027	F	F	F
0.4190089224455134	0.8508953891266877	0.2445390192780928	T	T	T
0.5932800169999979	0.1555200069999998	0.0880500000000026	F	F	F
0.9067199830000021	0.1555200069999998	0.0880500000000026	F	F	F
0.0850009168459045	0.8409552557244356	0.2472948610903716	T	T	T
0.9113593467015227	0.6424355267791302	0.1982483122566372	T	T	T
0.0824700000000007	0.3725399969999970	0.1378899959999984	F	F	F
0.4175299999999993	0.3725399969999970	0.1378899959999984	F	F	F
0.5875014206822686	0.6343292349343589	0.1968033558798933	T	T	T

0.7500000000000000	0.8851100210000027	0.1414899979999973	F	F	F
0.2448433026692849	0.1399142342973298	0.1986262512778072	T	T	T
0.7455362993477931	0.9022447127956402	0.2478609913345739	T	T	T
0.2500000000000000	0.1213599960000025	0.0871400010000016	F	F	F
0.2500000000000000	0.6510499720000027	0.0816000029999984	F	F	F
0.7839023688308561	0.3578424443658915	0.2501056881800540	T	T	T
0.2624195558779753	0.6141364776447058	0.2020873087485395	T	T	T
0.7500000000000000	0.3809399900000017	0.1380500049999966	F	F	F
0.5951285704796921	0.6670523655417202	0.3059644302990835	T	T	T
0.2289558665820329	0.1250575923591136	0.3145749763356451	T	T	T
0.5994005132393151	0.1699101181498761	0.3078896140365768	T	T	T
0.6368286801694324	0.5805587634733894	0.3292561685684631	T	T	T
0.9064398540482959	0.3735559115815932	0.2617786321174547	T	T	T
0.1893490848019500	0.0128902818449985	0.3084447507824616	T	T	T
0.4885818301930289	0.3317057666551739	0.2898024060988139	T	T	T
0.5195235222566901	0.0865754276412779	0.3179175472671966	T	T	T
0.7095982926817805	0.8204314836749321	0.2770450150991009	T	T	T

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0.00000000E+00	0.00000000E+00	0.00000000E+00
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0.00000000E+00	0.00000000E+00	0.00000000E+00
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0.00000000E+00	0.00000000E+00	0.00000000E+00
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0.7500000000000000	0.1339599940000014	0.1401000019999969	F	F	F
0.2452313508584123	0.8906332979616517	0.1968687619428261	T	T	T
0.7500000000000000	0.7569500210000015	0.0822699960000008	F	F	F
0.2689848517793462	0.2529604637046847	0.2595752247832108	T	T	T
0.2500000000000000	0.5080299970000013	0.1385000049999974	F	F	F
0.7443197823268457	0.5034798813698993	0.1995214282430602	T	T	T
0.4065400060000002	0.9061499829999988	0.1425700039999995	F	F	F
0.5901448973429623	0.1128286313243116	0.1921040548702058	T	T	T
0.9118542515580165	0.1179551755976324	0.1917586481070020	T	T	T
0.0934600009999969	0.9061499829999988	0.1425700039999995	F	F	F
0.9184399840000026	0.6252700089999976	0.0803600030000027	F	F	F
0.0926478406870115	0.3882249818793146	0.2685758140714319	T	T	T
0.4273905060947693	0.3956715750300421	0.2647984467013753	T	T	T
0.5815600159999974	0.6252700089999976	0.0803600030000027	F	F	F
0.4148864664613482	0.8604027560843898	0.2473721564718874	T	T	T
0.5932800169999979	0.1555200069999998	0.0880500000000026	F	F	F
0.9067199830000021	0.1555200069999998	0.0880500000000026	F	F	F
0.0860434387004322	0.8534456090367311	0.2460537388411735	T	T	T
0.9132450190690936	0.6298206875872709	0.2087970031789550	T	T	T
0.0824700000000007	0.3725399969999970	0.1378899959999984	F	F	F
0.4175299999999993	0.3725399969999970	0.1378899959999984	F	F	F
0.5830837272865348	0.6443993288168055	0.2066693687908065	T	T	T
0.7500000000000000	0.8851100210000027	0.1414899979999973	F	F	F
0.2511602943007528	0.1360329307858403	0.1967962727305928	T	T	T
0.7500971256828554	0.9101750029822945	0.2461281878777717	T	T	T
0.2500000000000000	0.1213599960000025	0.0871400010000016	F	F	F
0.2500000000000000	0.6510499720000027	0.0816000029999984	F	F	F
0.7150292523418658	0.3528841436679477	0.2508287517631994	T	T	T
0.2511351282581952	0.6253718988635105	0.1997628984651331	T	T	T
0.7500000000000000	0.3809399900000017	0.1380500049999966	F	F	F
0.2542832367650155	0.6452447911074758	0.3043683924395741	T	T	T
0.2927445076988269	0.0915610193990526	0.3074757109206164	T	T	T
0.8940432327697415	0.1671959074094691	0.3089816602083639	T	T	T
0.2578789463151471	0.5532346593521039	0.3297500779004115	T	T	T
0.5870562573089221	0.3606339429941013	0.2592719866407186	T	T	T
0.2005977346687449	0.0166565837502865	0.3095262182954198	T	T	T
0.3895142439493192	0.9445976815798643	0.2773645253542666	T	T	T
0.0053834702289266	0.3177925494185238	0.2866984956575034	T	T	T
0.9430001153500469	0.0677746691999433	0.3238516726708390	T	T	T

0.00000000E+00	0.00000000E+00	0.00000000E+00
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The coordinates of s1a(100) model

1.0000000000000000
5.5376000404000001 0.0000000000000000 0.0000000000000000
0.0000000000000000 8.3437995910999998 0.0000000000000000
0.0000000000000000 0.0000000000000000 21.3780994415000016

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Selective dynamics

Direct

0.3450179072710856	0.0915578038629060	0.3309024551575166	T	T	T
0.6144000290000022	0.9425100090000029	0.2470500020000017	F	F	F
0.6144000290000022	0.5932899709999973	0.2470500020000017	F	F	F
0.3546115796572606	0.4437883359170529	0.3331970941596234	T	T	T
0.0963116905876642	0.6136156394610290	0.4231474266540118	T	T	T
0.8691099879999982	0.4393700059999972	0.1534200010000006	F	F	F
0.8691099879999982	0.0964300039999983	0.1534200010000006	F	F	F
0.0703430469428060	0.9383298459595576	0.4212119929034998	T	T	T
0.3641700149999991	0.7678999899999965	0.1490000040000012	F	F	F
0.5848430125535113	0.2350791873303545	0.4353959777081340	T	T	T
0.8617600199999984	0.7678999899999965	0.1487800029999988	F	F	F
0.0946463030858275	0.2727943002134717	0.4249000136680036	T	T	T
0.5830662883638966	0.7691010141540434	0.3870951639847524	T	T	T
0.3682200009999974	0.2678999899999965	0.1971399930000004	F	F	F
0.8483600019999997	0.2678999899999965	0.2891800109999991	F	F	F
0.1114099990000028	0.7678999899999965	0.2898299989999984	F	F	F
0.9109661066158323	0.4439110490614115	0.4529802140326313	T	T	T
0.0996799990000028	0.6113600130000023	0.1403300019999989	F	F	F
0.0996799990000028	0.9244400259999992	0.1403300019999989	F	F	F
0.8727453982394227	0.1185350217246553	0.4402756388707493	T	T	T
0.5797461398763448	0.9343544366721502	0.3335805973128083	T	T	T
0.3746199910000030	0.0994599980000004	0.2465900030000014	F	F	F
0.3746199910000030	0.4363400040000016	0.2465900030000014	F	F	F
0.5867417404756948	0.6028885378387863	0.3336421535956583	T	T	T
0.3353877250254430	0.4243354184958123	0.4219803400498535	T	T	T
0.6274499889999987	0.6111800070000015	0.1561799939999986	F	F	F
0.6274499889999987	0.9246199729999987	0.1561799939999986	F	F	F
0.3207297282743222	0.1058254156978048	0.4252127058208711	T	T	T
0.1043742974254059	0.9404131667516213	0.3374987705291790	T	T	T
0.8478800059999969	0.1003699970000014	0.2383099939999980	F	F	F
0.8478800059999969	0.4354299900000029	0.2383099939999980	F	F	F
0.1109554655582666	0.5982882951528273	0.3392166318103195	T	T	T

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The coordinates of s1b(100) model

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5.537600404000001	0.0000000000000000	0.0000000000000000
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0.0000000000000000	0.0000000000000000	21.3780994415000016

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Selective dynamics

Direct

0.3482623704670835	0.0948337732497410	0.3287537863849512	T	T	T
0.6137099860000035	0.9423900250000017	0.2445400060000011	F	F	F
0.6137099860000035	0.5931699870000031	0.2445400060000011	F	F	F
0.3419784233316276	0.4487001427603537	0.3309308845744489	T	T	T
0.0430413729130917	0.5883560145133206	0.4291571739600703	T	T	T
0.8684200049999973	0.4392499920000006	0.1509100050000001	F	F	F
0.8684200049999973	0.0963099969999988	0.1509100050000001	F	F	F
0.0613172630101643	0.9382274900098727	0.4183577580313091	T	T	T
0.3634800020000029	0.7677800060000024	0.1464899930000030	F	F	F
0.6091039929560342	0.2639738578852180	0.4233033390442929	T	T	T
0.8610699769999997	0.7677800060000024	0.1462700069999983	F	F	F
0.0950356745807316	0.2666447841212668	0.4225759293065147	T	T	T
0.5858631146904835	0.7734216459789183	0.3822272716970053	T	T	T
0.3675299880000011	0.2677800060000024	0.1946299969999998	F	F	F
0.8476700189999988	0.2677800060000024	0.2866699989999972	F	F	F
0.1107200099999971	0.7677800060000024	0.2873199880000001	F	F	F
0.8537748676078247	0.4097805060004716	0.4370516968495712	T	T	T
0.0989900099999971	0.6112400290000011	0.1378200050000018	F	F	F
0.0989900099999971	0.9243199829999966	0.1378200050000018	F	F	F
0.8709165811887765	0.1118548073984876	0.4385751594590811	T	T	T
0.5848515950968003	0.9377723206131622	0.3302293478690098	T	T	T
0.3739300069999985	0.0993399990000015	0.2440800070000009	F	F	F

0.3739300069999985	0.4362199899999979	0.2440800070000009	F	F	F
0.5795374114060393	0.6049104250864351	0.3309261393634143	T	T	T
0.3356151053776856	0.4192695527339884	0.4219301270447781	T	T	T
0.6267600059999978	0.6110600230000003	0.1536699979999980	F	F	F
0.6267600059999978	0.9244999889999974	0.1536699979999980	F	F	F
0.3383166590359924	0.1165683074756989	0.4233065572349626	T	T	T
0.1119092004303321	0.9398889677040851	0.3358871020827559	T	T	T
0.8471900219999995	0.1002499980000024	0.2357999979999974	F	F	F
0.8471900219999995	0.4353100060000017	0.2357999979999974	F	F	F
0.1078258885710221	0.6037557773172113	0.3421128477705166	T	T	T
0.8524855925773229	0.7710336225683403	0.4285108053140831	T	T	T
0.1035000010000005	0.2677800060000024	0.1457300040000007	F	F	F
0.3302840433788263	0.7985076306453364	0.4359601234709575	T	T	T
0.6232500079999994	0.2677800060000024	0.1408399939999967	F	F	F
0.5901092268453335	0.2673684023919939	0.3378687857822442	T	T	T
0.3687900010000007	0.7677800060000024	0.2343900050000016	F	F	F
0.1136141257704711	0.2684045052429230	0.3338673538630432	T	T	T
0.8477600220000028	0.7677800060000024	0.2389599979999986	F	F	F
0.1547563453719803	0.6111888722140719	0.5101610922552670	T	T	T
0.0358366120130814	0.6541497589105991	0.5390032667871416	T	T	T
0.3085612292918699	0.7349211100601742	0.4778971078628446	T	T	T

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0.5856119244628912	0.7625137177556787	0.3822504018796745	T	T	T
0.3675299880000011	0.2677800060000024	0.1946299969999998	F	F	F
0.8476700189999988	0.2677800060000024	0.2866699989999972	F	F	F
0.1107200009999971	0.7677800060000024	0.2873199880000001	F	F	F
0.8703216113311827	0.4232253157904652	0.4387099514077989	T	T	T
0.0989900009999971	0.6112400290000011	0.1378200050000018	F	F	F
0.0989900009999971	0.9243199829999966	0.1378200050000018	F	F	F
0.8537301349424015	0.1252415722134584	0.4368892808350275	T	T	T
0.5802688929492339	0.9310116282434436	0.3309565997528394	T	T	T
0.3739300069999985	0.0993399990000015	0.2440800070000009	F	F	F
0.3739300069999985	0.4362199899999979	0.2440800070000009	F	F	F
0.5839414490419473	0.5982749078644873	0.3302285316342479	T	T	T
0.3371386819910192	0.4193851346079894	0.4233486606226394	T	T	T
0.6267600059999978	0.6110600230000003	0.1536699979999980	F	F	F
0.6267600059999978	0.9244999889999974	0.1536699979999980	F	F	F
0.3359383917880268	0.1165968438509677	0.4220335296492496	T	T	T
0.1085193165763064	0.9315476646691219	0.3421920249647948	T	T	T
0.8471900219999995	0.1002499980000024	0.2357999979999974	F	F	F
0.8471900219999995	0.4353100060000017	0.2357999979999974	F	F	F
0.1110656964700507	0.5956108421000023	0.3358930863890347	T	T	T
0.8520037671501388	0.7640974861477654	0.4286414263686883	T	T	T
0.1035000010000005	0.2677800060000024	0.1457300040000007	F	F	F
0.3294789853374542	0.7376289857784193	0.4359687291819581	T	T	T
0.6232500079999994	0.2677800060000024	0.1408399939999967	F	F	F
0.5900492550133625	0.2687430541620388	0.3379496066780804	T	T	T
0.3687900010000007	0.7677800060000024	0.2343900050000016	F	F	F
0.1137655676377123	0.2671265330705716	0.3338442774272618	T	T	T
0.8477600220000028	0.7677800060000024	0.2389599979999986	F	F	F
0.1536868304400737	0.9248587899266366	0.5103979674601820	T	T	T
0.3092038652214227	0.7996400308276593	0.4781382450509145	T	T	T
0.0339670809010301	0.8835929280763596	0.5393914396947235	T	T	T

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0.6137099860000035	0.5931699870000031	0.2445400060000011	F	F	F
0.3324730283512352	0.4398971187034989	0.3307670074626787	T	T	T
0.0517759421501785	0.6044278058034008	0.4205439409793698	T	T	T
0.8684200049999973	0.4392499920000006	0.1509100050000001	F	F	F
0.8684200049999973	0.0963099969999988	0.1509100050000001	F	F	F
0.0097863132788420	0.9301570037441029	0.4162293482608453	T	T	T
0.3634800020000029	0.7677800060000024	0.1464899930000030	F	F	F
0.6489115814021331	0.2891413114506747	0.4240712769362440	T	T	T
0.8610699769999997	0.7677800060000024	0.1462700069999983	F	F	F
0.1343603749173861	0.2802925910441219	0.4623990876570290	T	T	T
0.5386383393021753	0.7651012512211643	0.3843773041229225	T	T	T
0.3675299880000011	0.2677800060000024	0.1946299969999998	F	F	F
0.8476700189999988	0.2677800060000024	0.2866699989999972	F	F	F
0.1107200009999971	0.7677800060000024	0.2873199880000001	F	F	F
0.8839767567321880	0.4285602005267237	0.4472767130624318	T	T	T
0.0989900009999971	0.6112400290000011	0.1378200050000018	F	F	F
0.0989900009999971	0.9243199829999966	0.1378200050000018	F	F	F
0.9049282462003629	0.1234835212175554	0.4419876065321656	T	T	T
0.5663686006126627	0.9362201345074003	0.3330273334089687	T	T	T
0.3739300069999985	0.0993399990000015	0.2440800070000009	F	F	F
0.3739300069999985	0.4362199899999979	0.2440800070000009	F	F	F
0.5663242539684150	0.6024509475448957	0.3309545112557313	T	T	T
0.3442175611841759	0.4280053427989417	0.4233036637126188	T	T	T
0.6267600059999978	0.6110600230000003	0.1536699979999980	F	F	F
0.6267600059999978	0.9244999889999974	0.1536699979999980	F	F	F
0.4019424919252585	0.1343482631437884	0.4396333314957513	T	T	T
0.0981985374265010	0.9429208699300203	0.3362720682276865	T	T	T
0.8471900219999995	0.1002499980000024	0.2357999979999974	F	F	F
0.8471900219999995	0.4353100060000017	0.2357999979999974	F	F	F
0.0952656377243708	0.5987368796733988	0.3372475398101349	T	T	T
0.8115835006203562	0.7645267812819275	0.4289299005218484	T	T	T
0.1035000010000005	0.2677800060000024	0.1457300040000007	F	F	F
0.2660883010244534	0.7811037432920563	0.4342178274549023	T	T	T
0.6232500079999994	0.2677800060000024	0.1408399939999967	F	F	F
0.5962759772523953	0.2675059356573568	0.3404119230247156	T	T	T
0.3687900010000007	0.7677800060000024	0.2343900050000016	F	F	F
0.1214649150274288	0.2654457925704968	0.3318574669195478	T	T	T
0.8477600220000028	0.7677800060000024	0.2389599979999986	F	F	F
0.2113329135226553	0.2725148725969591	0.5414527244393913	T	T	T
0.1078194144520434	0.3149170952218787	0.5738232340145810	T	T	T
0.4426657263605502	0.0495706944572079	0.4692911570688468	T	T	T

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 0.0000000000000000 8.3437995910999998 0.0000000000000000
 0.0000000000000000 0.0000000000000000 21.3780994415000016

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Selective dynamics

Direct

0.3315177894723014	0.0954639176660962	0.3304216529160284	T	T	T
0.6144000290000022	0.9425100090000029	0.2470500020000017	F	F	F
0.6144000290000022	0.5932899709999973	0.2470500020000017	F	F	F
0.3439031687767223	0.4393034673920424	0.3318047150716475	T	T	T
0.0709109237613314	0.6120722867080725	0.4197389579130951	T	T	T
0.8691099879999982	0.4393700059999972	0.1534200010000006	F	F	F
0.8691099879999982	0.0964300039999983	0.1534200010000006	F	F	F
0.0781513837550781	0.9304325338085087	0.4206248889997094	T	T	T
0.3641700149999991	0.7678999899999965	0.1490000040000012	F	F	F
0.6166890113670999	0.1937539447595681	0.4309276288886641	T	T	T
0.8617600199999984	0.7678999899999965	0.1487800029999988	F	F	F
0.1072798029118161	0.2636875703620293	0.4504152803490669	T	T	T
0.5746023602918721	0.7682911526142444	0.3855285507060388	T	T	T
0.3682200009999974	0.2678999899999965	0.1971399930000004	F	F	F
0.8483600019999997	0.2678999899999965	0.2891800109999991	F	F	F
0.1114099990000028	0.7678999899999965	0.2898299989999984	F	F	F
0.8901723734039723	0.4394503411369650	0.4438240140206555	T	T	T
0.0996799990000028	0.6113600130000023	0.1403300019999989	F	F	F
0.0996799990000028	0.9244400259999992	0.1403300019999989	F	F	F
0.8908796706793459	0.0982729208595448	0.4420792192154381	T	T	T
0.5742024304707325	0.9361688283616599	0.3338284633029530	T	T	T
0.3746199910000030	0.0994599980000004	0.2465900030000014	F	F	F
0.3746199910000030	0.4363400040000016	0.2465900030000014	F	F	F
0.5781134730506285	0.5999917041873656	0.3338220498978258	T	T	T
0.3145212216450316	0.4409250648393249	0.4256625219365564	T	T	T
0.6274499889999987	0.6111800070000015	0.1561799939999986	F	F	F
0.6274499889999987	0.9246199729999987	0.1561799939999986	F	F	F
0.3282689232807793	0.1002630024810298	0.4247960053231509	T	T	T
0.1004949839606520	0.9387549332659562	0.3371364974314314	T	T	T
0.8478800059999969	0.1003699970000014	0.2383099939999980	F	F	F
0.8478800059999969	0.4354299900000029	0.2383099939999980	F	F	F
0.1050603862281350	0.5961572153640873	0.3372179422657703	T	T	T
0.8480964148759228	0.7702638543637336	0.4303327316493306	T	T	T
0.1041899989999990	0.2678999899999965	0.1482400000000013	F	F	F
0.3042768470018176	0.7683822100497618	0.4350911341694784	T	T	T
0.6239399910000003	0.2678999899999965	0.1433500050000021	F	F	F

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The coordinates of s2b(100) model

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Selective dynamics

Direct

0.3426395386897571	0.0881514444709641	0.3313332481874796	T	T	T
0.6144000290000022	0.9425100090000029	0.2470500020000017	F	F	F
0.6144000290000022	0.5932899709999973	0.2470500020000017	F	F	F
0.3569947617672034	0.4421898199997256	0.3325520247446691	T	T	T
0.1005090786889011	0.6127491696114469	0.4217415390700815	T	T	T
0.8691099879999982	0.4393700059999972	0.1534200010000006	F	F	F
0.8691099879999982	0.0964300039999983	0.1534200010000006	F	F	F
0.0710955021492074	0.9406744050606425	0.4274983925805019	T	T	T
0.3641700149999991	0.7678999899999965	0.1490000040000012	F	F	F
0.5835325977166222	0.2395723425440759	0.4346031200226445	T	T	T
0.8617600199999984	0.7678999899999965	0.1487800029999988	F	F	F
0.0924884394584910	0.2727317605316323	0.4230414094356351	T	T	T
0.5916002637577310	0.7669477584887933	0.3859896851808584	T	T	T
0.3682200009999974	0.2678999899999965	0.1971399930000004	F	F	F
0.8483600019999997	0.2678999899999965	0.2891800109999991	F	F	F
0.1114099990000028	0.7678999899999965	0.2898299989999984	F	F	F
0.9089832216171576	0.4445642155363481	0.4516850001803385	T	T	T
0.0996799990000028	0.6113600130000023	0.1403300019999989	F	F	F
0.0996799990000028	0.9244400259999992	0.1403300019999989	F	F	F
0.8686630873670422	0.1232711871041184	0.4391256376564862	T	T	T

0.9836764734555367	0.5851877081269843	0.4262587319504446	T	T	T
0.8691099879999982	0.4393700059999972	0.1534200010000006	F	F	F
0.8691099879999982	0.0964300039999983	0.1534200010000006	F	F	F
0.0619961508841102	0.9357411111008695	0.4205001729773794	T	T	T
0.3641700149999991	0.7678999899999965	0.1490000040000012	F	F	F
0.6296860118486354	0.2381112344042196	0.4241432754521766	T	T	T
0.8617600199999984	0.7678999899999965	0.1487800029999988	F	F	F
0.1138588770021076	0.2542630375252602	0.4556560780634782	T	T	T
0.5706393076100990	0.7802537710083838	0.3832531027755386	T	T	T
0.3682200009999974	0.2678999899999965	0.1971399930000004	F	F	F
0.8483600019999997	0.2678999899999965	0.2891800109999991	F	F	F
0.1114099990000028	0.7678999899999965	0.2898299989999984	F	F	F
0.8576560827461913	0.3942758514292808	0.4401713663111440	T	T	T
0.0996799990000028	0.6113600130000023	0.1403300019999989	F	F	F
0.0996799990000028	0.9244400259999992	0.1403300019999989	F	F	F
0.8758193502688204	0.0994179034249792	0.4466296794845284	T	T	T
0.5781463054653644	0.9414379546973543	0.3319879682115390	T	T	T
0.3746199910000030	0.0994599980000004	0.2465900030000014	F	F	F
0.3746199910000030	0.4363400040000016	0.2465900030000014	F	F	F
0.5749694617412910	0.6040117734941294	0.3350672721970160	T	T	T
0.3719775015207732	0.4019659310959427	0.4289448106727477	T	T	T
0.6274499889999987	0.6111800070000015	0.1561799939999986	F	F	F
0.6274499889999987	0.9246199729999987	0.1561799939999986	F	F	F
0.3395865854285008	0.1115300440920517	0.4237218681268398	T	T	T
0.1052823322148743	0.9382346292999428	0.3380634478053484	T	T	T
0.8478800059999969	0.1003699970000014	0.2383099939999980	F	F	F
0.8478800059999969	0.4354299900000029	0.2383099939999980	F	F	F
0.1088003082730940	0.6014459991948653	0.3465801866779263	T	T	T
0.8360288687241902	0.7732808821699014	0.4293780680902145	T	T	T
0.1041899989999990	0.2678999899999965	0.1482400000000013	F	F	F
0.3290935681600280	0.8076014875428806	0.4395264082634602	T	T	T
0.6239399910000003	0.2678999899999965	0.1433500050000021	F	F	F
0.5919542500971677	0.2655368655627633	0.3402261606334541	T	T	T
0.3694800139999970	0.7678999899999965	0.2369000019999987	F	F	F
0.1180713161372046	0.2717826304328192	0.3344922211799365	T	T	T
0.8484500049999966	0.7678999899999965	0.2414699939999991	F	F	F
0.1532538582718992	0.5981730072056540	0.5000039429013303	T	T	T
0.1908273653939823	0.2841733830922991	0.5355404728729555	T	T	T
0.3720001114112335	0.4896061093794653	0.4606332807004938	T	T	T
0.1462754966017333	0.5055519428320512	0.5288887388660320	T	T	T
0.1111402579115832	0.2225697501117636	0.5678395467769662	T	T	T
0.3062900098870140	0.7327845106745366	0.4768576021995635	T	T	T

0.00000000E+00 0.00000000E+00 0.00000000E+00

0.00000000E+00 0.00000000E+00 0.00000000E+00

The coordinates of s2d(100) model

1.0000000000000000

5.5376000404000001	0.0000000000000000	0.0000000000000000
0.0000000000000000	8.3437995910999998	0.0000000000000000
0.0000000000000000	0.0000000000000000	21.3780994415000016

Al	O	H
16	26	4

Selective dynamics

Direct

0.3434458427110548	0.0935056721817244	0.3283863976620587	T	T	T
0.6137099860000035	0.9423900250000017	0.2445400060000011	F	F	F
0.6137099860000035	0.5931699870000031	0.2445400060000011	F	F	F
0.3534809858245285	0.4411712455966519	0.3301269670281202	T	T	T
0.8528441356807979	0.5825350967216980	0.3859566216602294	T	T	T
0.8684200049999973	0.4392499920000006	0.1509100050000001	F	F	F
0.8684200049999973	0.0963099969999988	0.1509100050000001	F	F	F
0.1453251828135620	0.9146077247227599	0.4352153511427490	T	T	T
0.3634800020000029	0.7677800060000024	0.1464899930000030	F	F	F
0.5884647101758750	0.2556399097391876	0.4419300078612842	T	T	T
0.8610699769999997	0.7677800060000024	0.1462700069999983	F	F	F
0.0682550775944710	0.2527609047730069	0.4200733297220069	T	T	T
0.6803223640078411	0.9109677366347623	0.4050926163585751	T	T	T
0.3675299880000011	0.2677800060000024	0.1946299969999998	F	F	F
0.8476700189999988	0.2677800060000024	0.2866699989999972	F	F	F
0.1107200009999971	0.7677800060000024	0.2873199880000001	F	F	F
0.8435703716017307	0.4048556023576814	0.4331377449195937	T	T	T
0.0989900009999971	0.6112400290000011	0.1378200050000018	F	F	F
0.0989900009999971	0.9243199829999966	0.1378200050000018	F	F	F
0.8359479430432922	0.0924123912667872	0.4311779656973955	T	T	T
0.5929352315789812	0.9441633793152512	0.3290682999897923	T	T	T
0.3739300069999985	0.0993399990000015	0.2440800070000009	F	F	F
0.3739300069999985	0.4362199899999979	0.2440800070000009	F	F	F
0.6052632191336452	0.5879146105664308	0.3327040843066015	T	T	T
0.3302962756801929	0.4108859810005469	0.4239099502386588	T	T	T
0.6267600059999978	0.6110600230000003	0.1536699979999980	F	F	F
0.6267600059999978	0.9244999889999974	0.1536699979999980	F	F	F
0.3255450626732598	0.1110613899057062	0.4197041235464075	T	T	T
0.1274421392203594	0.9263668241514504	0.3427636675266777	T	T	T
0.8471900219999995	0.1002499980000024	0.2357999979999974	F	F	F
0.8471900219999995	0.4353100060000017	0.2357999979999974	F	F	F
0.1090387142145000	0.5920128671107181	0.3351178607121407	T	T	T

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0.00000000E+00 0.00000000E+00 0.00000000E+00

The coordinates of s3a(100) model

1.0000000000000000
5.5376000404000001 0.0000000000000000 0.0000000000000000
0.0000000000000000 8.3437995910999998 0.0000000000000000
0.0000000000000000 0.0000000000000000 21.3780994415000016
Al O H
16 27 6

Selective dynamics

Direct

0.3375388470151111 0.0957241217547260 0.3301677291447319 T T T
0.6144000290000022 0.9425100090000029 0.2470500020000017 F F F
0.6144000290000022 0.5932899709999973 0.2470500020000017 F F F
0.3427186098531904 0.4451035255537183 0.3319440920424899 T T T
0.0747168677340617 0.6133766307811737 0.4268891206021351 T T T
0.8691099879999982 0.4393700059999972 0.1534200010000006 F F F
0.8691099879999982 0.0964300039999983 0.1534200010000006 F F F
0.0788481766275680 0.9296174738062337 0.4188024442675917 T T T
0.3641700149999991 0.7678999899999965 0.1490000040000012 F F F
0.6199729918026764 0.1990220602842145 0.4299532199554973 T T T
0.8617600199999984 0.7678999899999965 0.1487800029999988 F F F
0.1041978552352234 0.2637071266112161 0.4390853625429315 T T T
0.5784812893060487 0.7699651261262529 0.3846221536471359 T T T
0.3682200009999974 0.2678999899999965 0.1971399930000004 F F F
0.8483600019999997 0.2678999899999965 0.2891800109999991 F F F
0.1114099990000028 0.7678999899999965 0.2898299989999984 F F F

0.8703537253265314	0.4297732964660402	0.4343953004878898	T	T	T
0.0996799990000028	0.6113600130000023	0.1403300019999989	F	F	F
0.0996799990000028	0.9244400259999992	0.1403300019999989	F	F	F
0.8906198750177925	0.0972972243367053	0.4402335738184341	T	T	T
0.5781606011249908	0.9371697430308906	0.3330057364577623	T	T	T
0.3746199910000030	0.0994599980000004	0.2465900030000014	F	F	F
0.3746199910000030	0.4363400040000016	0.2465900030000014	F	F	F
0.5798857398062460	0.6013315386544420	0.3330652857464028	T	T	T
0.3186695396419489	0.4400588808313030	0.4247021357058058	T	T	T
0.6274499889999987	0.6111800070000015	0.1561799939999986	F	F	F
0.6274499889999987	0.9246199729999987	0.1561799939999986	F	F	F
0.3321396914058376	0.1022873195436418	0.4237624822572527	T	T	T
0.1030438050677782	0.9417549949406648	0.3357256701172835	T	T	T
0.8478800059999969	0.1003699970000014	0.2383099939999980	F	F	F
0.8478800059999969	0.4354299900000029	0.2383099939999980	F	F	F
0.1078648256701602	0.6010043524237363	0.3405315424775516	T	T	T
0.8492662713174243	0.7727416460233520	0.4294987014792467	T	T	T
0.1041899989999990	0.2678999899999965	0.1482400000000013	F	F	F
0.3124053388897380	0.7756796981085092	0.4343137462148240	T	T	T
0.6239399910000003	0.2678999899999965	0.1433500050000021	F	F	F
0.5928283592804935	0.2626443762532409	0.3454177355253387	T	T	T
0.3694800139999970	0.7678999899999965	0.2369000019999987	F	F	F
0.1153644773221578	0.2714626000128345	0.3393204851664328	T	T	T
0.8484500049999966	0.7678999899999965	0.2414699939999991	F	F	F
0.5922284555525118	0.2975259796719031	0.5053413127094215	T	T	T
0.1330559402682239	0.2903323107551518	0.5259383024890957	T	T	T
0.0982199104893591	0.5943595014034925	0.5214826820970209	T	T	T
0.4417938507362173	0.2760193426801832	0.5288853726624307	T	T	T
0.7891812523046788	0.4313088746336438	0.4757860503384620	T	T	T
0.9962001530441761	0.2417330758365837	0.5472879604923461	T	T	T
0.4454011439225525	0.4387723036176123	0.4578460173329226	T	T	T
0.1202493209280533	0.4737385103336780	0.5327050708752675	T	T	T
0.2379520530154006	0.6554074785052691	0.5355153119283134	T	T	T

0.00000000E+00	0.00000000E+00	0.00000000E+00
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0.00000000E+00	0.00000000E+00	0.00000000E+00
0.00000000E+00	0.00000000E+00	0.00000000E+00
0.00000000E+00	0.00000000E+00	0.00000000E+00
0.00000000E+00	0.00000000E+00	0.00000000E+00

0.0000000000000000	8.3437995910999998	0.0000000000000000			
0.0000000000000000	0.0000000000000000	21.3780994415000016			
Al	O	H			
16	27	6			
Selective dynamics					
Direct					
0.3310708107026491	0.0943702148551907	0.3304571236111583	T	T	T
0.6144000290000022	0.9425100090000029	0.2470500020000017	F	F	F
0.6144000290000022	0.5932899709999973	0.2470500020000017	F	F	F
0.3325341996564771	0.4408844832871700	0.3310711843872702	T	T	T
0.0275395681951424	0.6018901161116921	0.4293437554882057	T	T	T
0.8691099879999982	0.4393700059999972	0.1534200010000006	F	F	F
0.8691099879999982	0.0964300039999983	0.1534200010000006	F	F	F
0.0296912671485049	0.9349849093076098	0.4308661934234647	T	T	T
0.3641700149999991	0.7678999899999965	0.1490000040000012	F	F	F
0.6445012458035907	0.2683516571086938	0.4230917044523681	T	T	T
0.8617600199999984	0.7678999899999965	0.1487800029999988	F	F	F
0.1089631742544645	0.2680426616435627	0.4592908606229889	T	T	T
0.5794702312486454	0.7687875474255398	0.3786033955727895	T	T	T
0.3682200009999974	0.2678999899999965	0.1971399930000004	F	F	F
0.8483600019999997	0.2678999899999965	0.2891800109999991	F	F	F
0.1114099990000028	0.7678999899999965	0.2898299989999984	F	F	F
0.8718599227411948	0.4165928338790002	0.4399514686869310	T	T	T
0.0996799990000028	0.6113600130000023	0.1403300019999989	F	F	F
0.0996799990000028	0.9244400259999992	0.1403300019999989	F	F	F
0.8737093378960489	0.1219136157587132	0.4389370377363991	T	T	T
0.5771595735692455	0.9397871708882084	0.3319124718973176	T	T	T
0.3746199910000030	0.0994599980000004	0.2465900030000014	F	F	F
0.3746199910000030	0.4363400040000016	0.2465900030000014	F	F	F
0.5775639797502581	0.5969402296494168	0.3320248027269359	T	T	T
0.3717761034273780	0.4118400031646017	0.4309827534557423	T	T	T
0.6274499889999987	0.6111800070000015	0.1561799939999986	F	F	F
0.6274499889999987	0.9246199729999987	0.1561799939999986	F	F	F
0.3718987306346092	0.1217082718910809	0.4340630830279674	T	T	T
0.1057669909628293	0.9358038769349000	0.3441517455897160	T	T	T
0.8478800059999969	0.1003699970000014	0.2383099939999980	F	F	F
0.8478800059999969	0.4354299900000029	0.2383099939999980	F	F	F
0.1051240072294656	0.5995339954518921	0.3437803787047806	T	T	T
0.8244713519266222	0.7682764689431125	0.4306509852478714	T	T	T
0.1041899989999990	0.2678999899999965	0.1482400000000013	F	F	F
0.3217579999287068	0.7703659685163956	0.4289622039984970	T	T	T
0.6239399910000003	0.2678999899999965	0.1433500050000021	F	F	F
0.5868241602743308	0.2670879709297463	0.3402109926354487	T	T	T
0.3694800139999970	0.7678999899999965	0.2369000019999987	F	F	F


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0.00000000E+00 0.00000000E+00 0.00000000E+00
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0.00000000E+00 0.00000000E+00 0.00000000E+00

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The coordinates of s4a(100) model

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  0.0000000000000000  8.3437995910999998  0.0000000000000000
  0.0000000000000000  0.0000000000000000  21.3780994415000016

```

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Al   O   H
 16  28   8

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Selective dynamics

Direct

```

0.3419133660431449 0.0955445747438356 0.3270950039232732  T  T  T
0.6124699710000030 0.9440600280000027 0.2428800019999997  F  F  F
0.6124699710000030 0.5948399899999970 0.2428800019999997  F  F  F
0.3420485917049098 0.4427096064029322 0.3272741716114508  T  T  T
0.0253998553686031 0.6049122720803193 0.4225260485378099  T  T  T
0.8671799899999968 0.4409199950000016 0.1492500009999986  F  F  F
0.8671799899999968 0.0979799999999997 0.1492500009999986  F  F  F
0.0226276950971983 0.9373000895247817 0.4232626688124413  T  T  T
0.3622399870000024 0.7694500090000034 0.1448300030000027  F  F  F
0.6280965717909274 0.2726226074726745 0.4292506117659004  T  T  T
0.8598300219999970 0.7694500090000034 0.1446100029999968  F  F  F
0.0931418135982663 0.2697719038405154 0.4320541757788480  T  T  T
0.5750808482584941 0.7697185145628899 0.3740741476558320  T  T  T
0.3662900030000031 0.2694500090000034 0.1929699929999984  F  F  F
0.8464300039999983 0.2694500090000034 0.2850100100000006  F  F  F
0.1094800010000014 0.7694500090000034 0.2856599990000035  F  F  F

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0.8656333340578671	0.4232712196182862	0.4294506200837213	T	T	T
0.0977500010000014	0.6129099730000007	0.1361600010000004	F	F	F
0.0977500010000014	0.9259899850000011	0.1361600010000004	F	F	F
0.8621958197369846	0.1196378090163521	0.4265533535151865	T	T	T
0.5805481874911367	0.9394700930762634	0.3271701904602142	T	T	T
0.3726899919999980	0.1010100020000024	0.2424200029999994	F	F	F
0.3726899919999980	0.4378899929999989	0.2424200029999994	F	F	F
0.5802523293128048	0.5994340157936875	0.3274384386681779	T	T	T
0.3534479904885892	0.4191326496992697	0.4231444912166398	T	T	T
0.6255199909999973	0.6127300260000013	0.1520099939999966	F	F	F
0.6255199909999973	0.9261699910000019	0.1520099939999966	F	F	F
0.3529167643479336	0.1158634284962240	0.4220598383126121	T	T	T
0.1097346969758784	0.9362399115380936	0.3383606590085929	T	T	T
0.8459500069999990	0.1019200010000034	0.2341399940000031	F	F	F
0.8459500069999990	0.4369800090000027	0.2341399940000031	F	F	F
0.1099847036266418	0.6020997258174781	0.3383178257413789	T	T	T
0.8215510579559226	0.7698024549103633	0.4253444602783211	T	T	T
0.1022600009999977	0.2694500090000034	0.1440699990000027	F	F	F
0.3191428500804682	0.7727874022057242	0.4258587121815931	T	T	T
0.6220099929999989	0.2694500090000034	0.1391800050000001	F	F	F
0.5847918035480979	0.2706252742144193	0.3379089188540607	T	T	T
0.3675499860000002	0.7694500090000034	0.2327300010000002	F	F	F
0.1196923652447705	0.2694188291233617	0.3349167393727596	T	T	T
0.8465200070000023	0.7694500090000034	0.2372999939999971	F	F	F
0.1304091201616205	0.2538132708778311	0.5224314339764932	T	T	T
0.1179568694235974	0.9525630076301266	0.5066113378519101	T	T	T
0.1583651359614675	0.5979712097022402	0.5032778524063587	T	T	T
0.5699884181762950	0.2687384829696748	0.5145213077519737	T	T	T
0.1020499652708489	0.1337567712557323	0.5290724787425644	T	T	T
0.3410723740376769	0.4903526302150443	0.4626439752074227	T	T	T
0.3603592247693331	0.7599839974624705	0.4702317761106818	T	T	T
0.1103705006041823	0.8526061805102204	0.5301249977730396	T	T	T
0.0843586020594162	0.5198455043782241	0.5311043125313697	T	T	T
0.3743561815777710	0.0454170979500380	0.4591064228087071	T	T	T
0.7082007138034468	0.2742059755052720	0.5421926168387965	T	T	T
0.3209836793531718	0.2651490585099750	0.5299831495563924	T	T	T

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