

Electronic Supplementary Information

**Water Interaction with B-site (B = Al, Zr, Nb, and W) Doped SrFeO_{3-δ}-
Based Perovskite Surfaces for Thermochemical Water Splitting
Applications[†]**

Sha Chen,^a Hongwei Cheng,^{a,*} Yanbo Liu,^a Xiaolu Xiong,^a Qiangchao Sun,^a Qian Xu,^a
Xionggang Lu,^{a,b,*} Shenggang Li,^{c,*}

^a *State Key Laboratory of Advanced Special Steel & Shanghai Key Laboratory of
Advances Ferrometallurgy & School of Materials Science and Engineering, Shanghai
University, 99 Shangda Road, Shanghai 200444, P. R. China*

^b *School of Materials Science, Shanghai Dianji University, 300 Shuihua Road, Shanghai
200240, P. R. China*

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

* Corresponding authors: Tel. & fax: +86-21-66136561. E-mail addresses: hwcheng@shu.edu.cn (H.

Cheng); luxg@shu.edu.cn (X. Lu); lisg@sari.ac.cn (S. Li)

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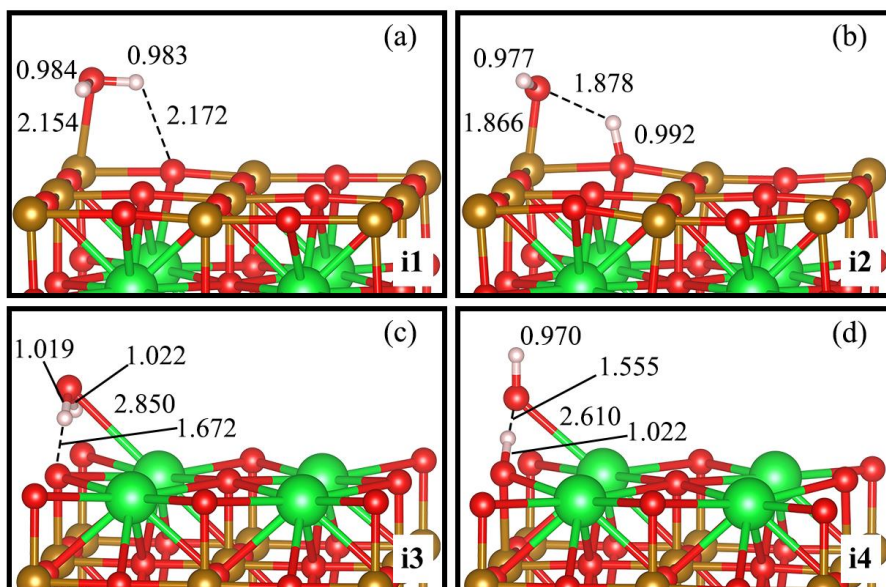


Fig. S1 Side views of stable i1 (a), i2 (b), i3 (c), and i4 (d) types of pure SrFeO_3 . Atom colors: Sr – green, Fe – brown, O – red, H – white. All distances are given in Å.

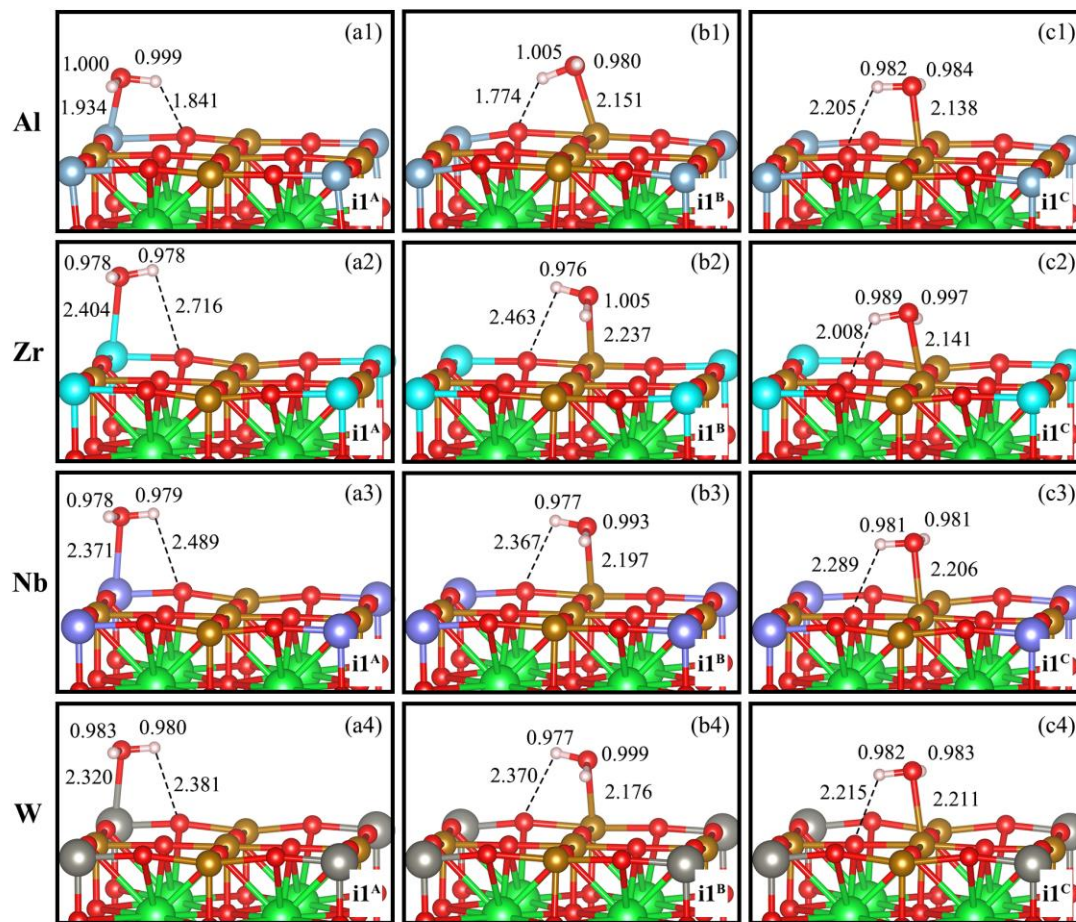


Fig. S2 Side views of stable i1 type of doped structures – brown, Al – silver, Zr – blue, Nb – purple, W – gray, O – red, H – white. All distances are given in Å.

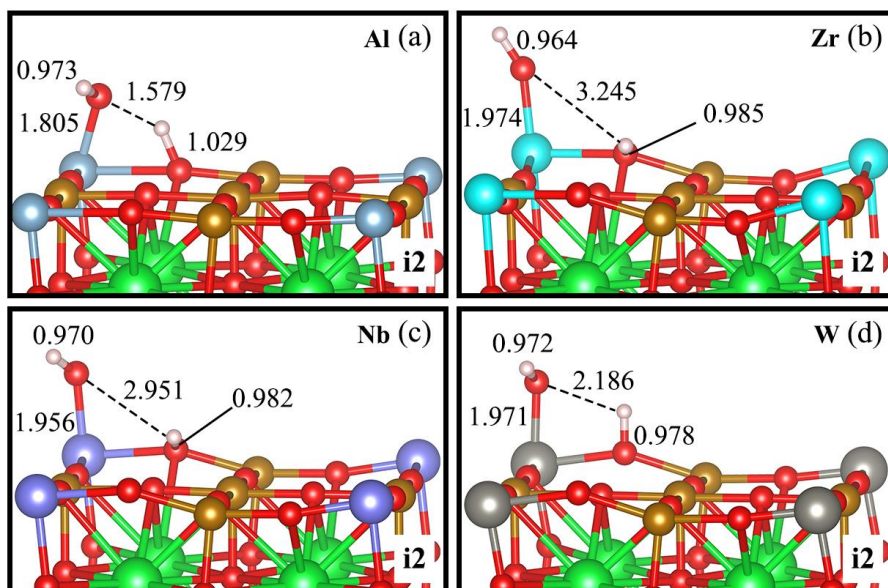


Fig. S3 Side views of stable i2 type of doped structures. Atom colors: Sr – green, Fe – brown, Al – silver, Zr – blue, Nb – purple, W – gray, O – red, H – white. All distances are given in Å.

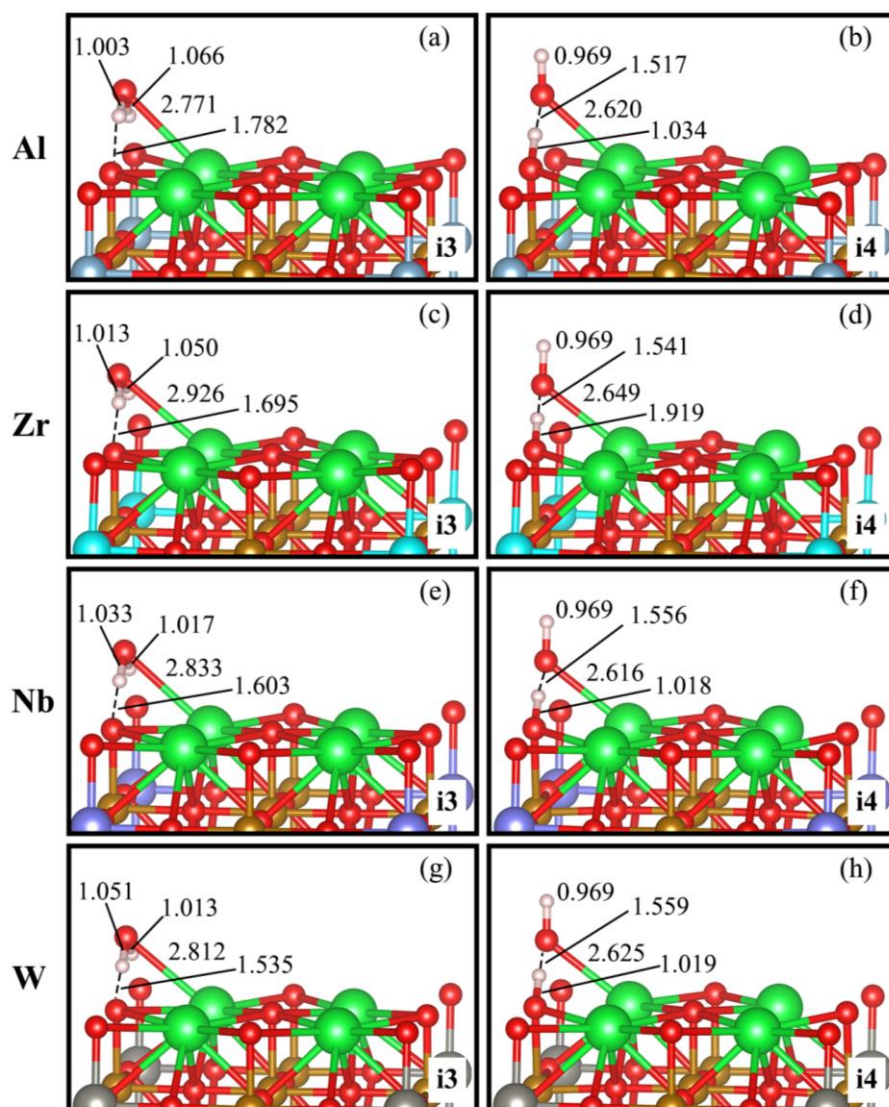


Fig. S4 Side views of stable i3 and i4 type of doped structures. Atom colors: Sr – green, Fe – brown, Al – silver, Zr – blue, Nb – purple, W – gray, O – red, H – white. All distances are given in Å.

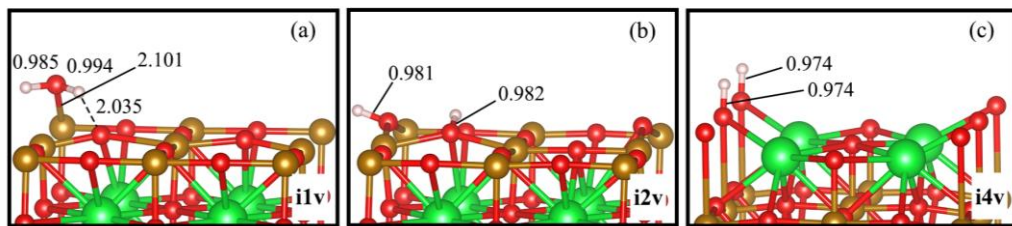


Fig. S5 Side views of stable i1v (a), i2v (b) and i4v (c) types of pure SrFeO₃. Atom colors: Sr – green, Fe – brown, O – red, H – white. All distances are given in Å.

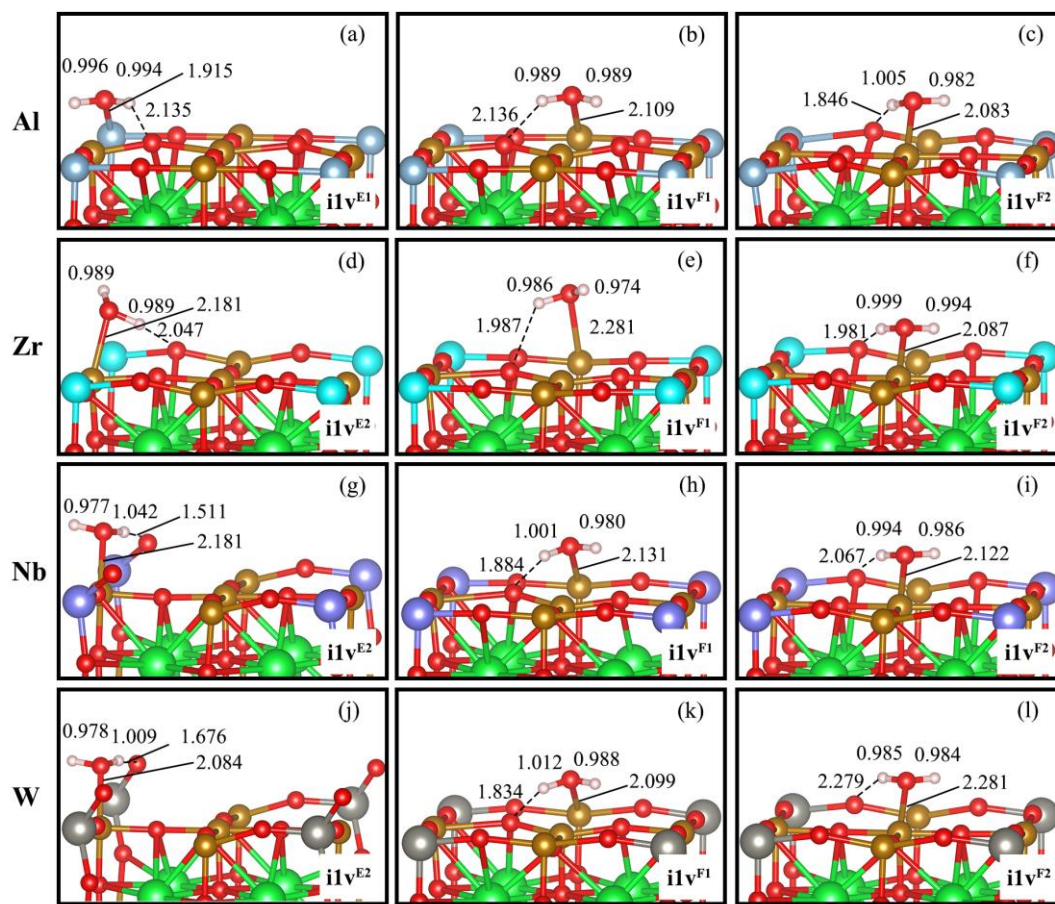


Fig. S6 Side views of stable *i1v* type of doped structures. Atom colors: Sr – green, Fe – brown, Al – silver, Zr – blue, Nb – purple, W – gray, O – red, H – white. All distances are given in Å.

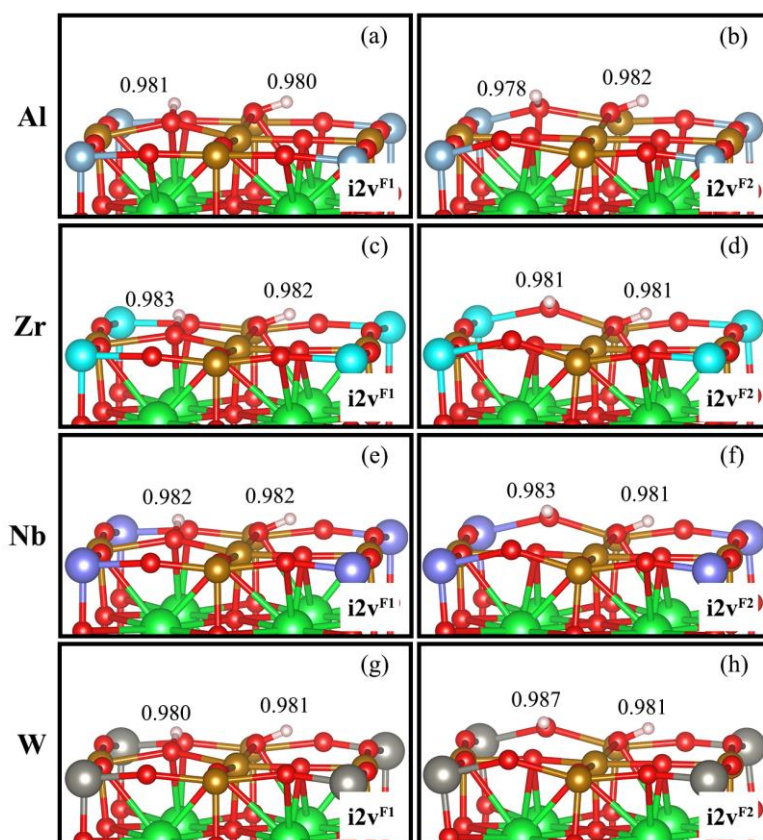


Fig. S7 Side views of stable $i2v^F$ type of doped structures. Atom colors: Sr – green, Fe – brown, Al – silver, Zr – blue, Nb – purple, W – gray, O – red, H – white. All distances are given in Å.

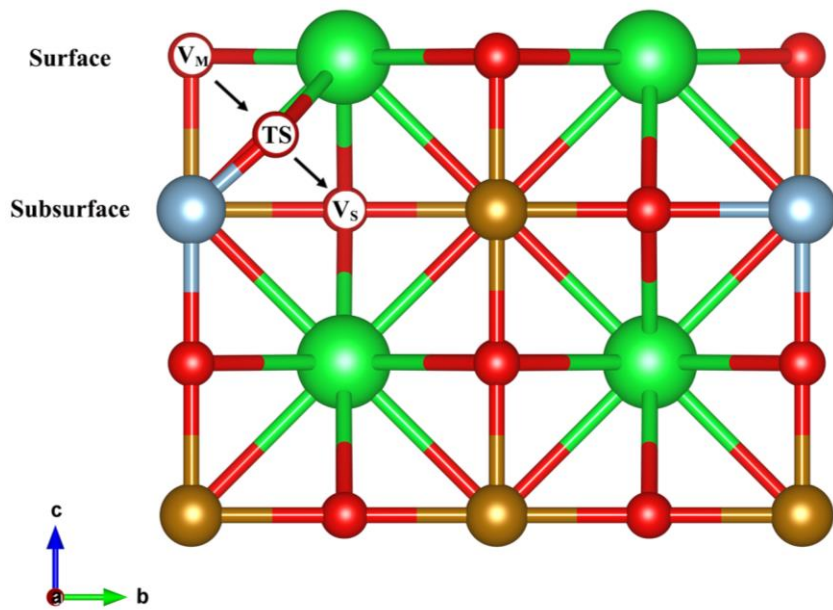


Fig. S8 Side views of the oxygen migration from surface V_M site on the SrO termination to subsurface V_S site in doped structures. Atom colors: Sr – green, Fe – brown, M (Al, Zr, Nb or W) – silver, O – red.

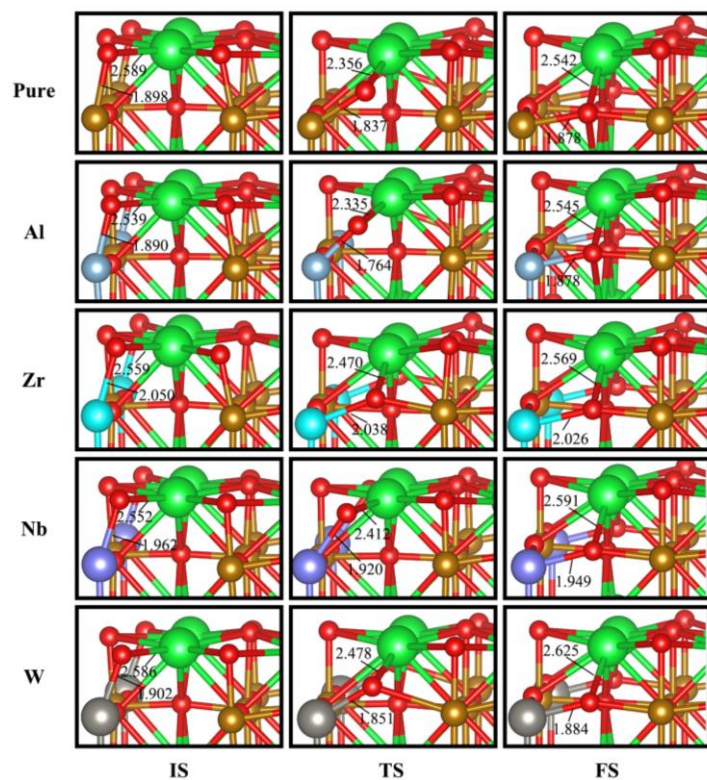


Fig. S9 The optimized initial and final structures of all structures, and the calculated transition states for oxygen migration. Atom colors: Sr – green, Fe – brown, Al – silver, Zr – blue, Nb – purple, W – gray, O – red. All distances are given in Å.

Table S1 Adsorption energies (eV) and structural parameters (Å) for water adsorption on pure, Al, Zr, Nb, and W-doped structures. Surface atoms are indicated by the s subscript, while atoms in the water molecule are denoted by the w subscript.

Type		Pure	Al	Zr	Nb	W
i1 ^A	E _{ads}	-0.71	-0.93	-0.86	-0.75	-0.99
	d(M _s -O _w)	2.154	1.934	2.404	2.371	2.320
	d(O _s -H _w)	2.172	1.841	2.716	2.489	2.381
i1 ^B	E _{ads}	-0.71	-0.65	-0.47	-0.56	-0.77
	d(M _s -O _w)	2.154	2.151	2.237	2.197	2.196
	d(O _s -H _w)	2.172	1.774	2.463	2.367	2.370
i1 ^C	E _{ads}	-0.71	-0.67	-0.74	-0.49	-0.66
	d(M _s -O _w)	2.154	2.138	2.141	2.206	2.211
	d(O _s -H _w)	2.172	2.205	2.008	2.289	2.215
i2	E _{ads}	-0.61	-0.92	-1.09	-0.93	-1.29
	d(M _s -O _w)	1.866	1.805	1.974	1.956	1.971
	d(O _s -H _w)	0.992	1.029	0.985	0.982	0.978
i3	E _{ads}	-0.74	-0.81	-0.93	-0.85	-1.33
	d(Sr _s -O _w)	2.850	2.771	2.926	2.833	2.812
	d(O _s -H _w)	1.672	1.782	1.695	1.603	1.535
i4	E _{ads}	-0.98	-1.17	-1.04	-1.07	-1.61
	d(Sr _s -O _w)	2.610	2.620	2.649	2.616	2.625
	d(O _s -H _w)	1.022	1.034	1.919	1.018	1.019

Table S2 The formation energies (eV) of O₂ after the desorption of H₂ from the i2 and i4 types of pure, Al, Zr, Nb, and W-doped structures.

Structure	FeO ₂ -terminated (i2) (Relaxed)/eV	SrO-terminated (i4) (Relaxed)/eV
Pure	-1.28	-1.21
M=Al	-1.30	-1.31
M=Zr	-1.25	-1.19
M=Nb	-0.26	-1.10
M=W	0.48	-0.72

Table S3 Fractional coordinates of the relaxed FeO₂ termination of Sr₈Fe₈O₂₄ (001) surface.

O Fe Sr

1.0000000000000000		
7.7625000000000002	0.0000000000000000	0.0000000000000000
0.0000000000000005	7.7625000000000002	0.0000000000000000
0.0000000000000013	0.0000000000000013	20.8218999999999994

O	Fe	Sr
24	8	8

Selective dynamics

Direct

0.0000000000000000	0.0000000000000000	0.0480299999999971	F	F	F
0.2500000000000000	0.0000000000000000	0.3285649487842169	T	T	T
-0.0000000000000000	0.2500000000000000	0.3285649487842169	T	T	T
0.5000000000000000	0.0000000000000000	0.0480299999999971	F	F	F
0.7500000000000000	-0.0000000000000000	0.3285649487842169	T	T	T
0.5000000000000000	0.2500000000000000	0.3285649487842169	T	T	T
0.0000000000000000	0.5000000000000000	0.0480299999999971	F	F	F
0.2500000000000000	0.5000000000000000	0.3285649487842169	T	T	T
-0.0000000000000000	0.7500000000000000	0.3285649487842169	T	T	T
0.5000000000000000	0.5000000000000000	0.0480299999999971	F	F	F
0.7500000000000000	0.5000000000000000	0.3285649487842169	T	T	T
0.5000000000000000	0.7500000000000000	0.3285649487842169	T	T	T
0.0000000000000000	0.0000000000000000	0.2323327875146111	T	T	T
0.2500000000000000	0.0000000000000000	0.1412300000000002	F	F	F
0.0000000000000000	0.2500000000000000	0.1412300000000002	F	F	F
0.5000000000000000	0.0000000000000000	0.2323327875146111	T	T	T

0.7500000000000000	0.0000000000000000	0.1412300000000002	F	F	F
0.5000000000000000	0.2500000000000000	0.1412300000000002	F	F	F
0.0000000000000000	0.5000000000000000	0.2323327875146111	T	T	T
0.2500000000000000	0.5000000000000000	0.1412300000000002	F	F	F
0.0000000000000000	0.7500000000000000	0.1412300000000002	F	F	F
0.5000000000000000	0.5000000000000000	0.2323327875146111	T	T	T
0.7500000000000000	0.5000000000000000	0.1412300000000002	F	F	F
0.5000000000000000	0.7500000000000000	0.1412300000000002	F	F	F
-0.0000000000000000	-0.0000000000000000	0.3259439481075966	T	T	T
0.5000000000000000	-0.0000000000000000	0.3259439481075966	T	T	T
-0.0000000000000000	0.5000000000000000	0.3259439481075966	T	T	T
0.5000000000000000	0.5000000000000000	0.3259439481075966	T	T	T
0.0000000000000000	0.0000000000000000	0.1412300000000002	F	F	F
0.5000000000000000	0.0000000000000000	0.1412300000000002	F	F	F
0.0000000000000000	0.5000000000000000	0.1412300000000002	F	F	F
0.5000000000000000	0.5000000000000000	0.1412300000000002	F	F	F
0.2500000000000000	0.2500000000000000	0.0480299999999971	F	F	F
0.7500000000000000	0.2500000000000000	0.0480299999999971	F	F	F
0.2500000000000000	0.7500000000000000	0.0480299999999971	F	F	F
0.7500000000000000	0.7500000000000000	0.0480299999999971	F	F	F
0.2500000000000000	0.2500000000000000	0.2379210977077245	T	T	T
0.7500000000000000	0.2500000000000000	0.2379210977077245	T	T	T
0.2500000000000000	0.7500000000000000	0.2379210977077245	T	T	T
0.7500000000000000	0.7500000000000000	0.2379210977077245	T	T	T

Table S4 Fractional coordinates of the relaxed SrO termination of Sr₈Fe₈O₂₄ (001) surface.

O Fe Sr

1.0000000000000000		
7.7625000000000002	0.0000000000000000	0.0000000000000000
0.0000000000000005	7.7625000000000002	0.0000000000000000
0.0000000000000013	0.0000000000000013	20.8218999999999994

O	Fe	Sr
24	8	8

Selective dynamics

Direct

-0.0000000000000000	-0.0000000000000000	0.3275716266218510	T	T	T
0.2500000000000000	-0.0000000000000000	0.2346614162522072	T	T	T
-0.0000000000000000	0.2500000000000000	0.2346614162522072	T	T	T
0.5000000000000000	-0.0000000000000000	0.3275716266218510	T	T	T
0.7500000000000000	-0.0000000000000000	0.2346614162522072	T	T	T
0.5000000000000000	0.2500000000000000	0.2346614162522072	T	T	T
-0.0000000000000000	0.5000000000000000	0.3275716266218510	T	T	T
0.2500000000000000	0.5000000000000000	0.2346614162522072	T	T	T
0.0000000000000000	0.7500000000000000	0.2346614162522072	T	T	T
0.5000000000000000	0.5000000000000000	0.3275716266218510	T	T	T
0.7500000000000000	0.5000000000000000	0.2346614162522072	T	T	T
0.5000000000000000	0.7500000000000000	0.2346614162522072	T	T	T
0.0000000000000000	0.0000000000000000	0.1412300000000002	F	F	F
0.2500000000000000	0.0000000000000000	0.0480299999999971	F	F	F
0.0000000000000000	0.2500000000000000	0.0480299999999971	F	F	F
0.5000000000000000	0.0000000000000000	0.1412300000000002	F	F	F

0.7500000000000000	0.0000000000000000	0.0480299999999971	F	F	F
0.5000000000000000	0.2500000000000000	0.0480299999999971	F	F	F
0.0000000000000000	0.5000000000000000	0.1412300000000002	F	F	F
0.2500000000000000	0.5000000000000000	0.0480299999999971	F	F	F
0.0000000000000000	0.7500000000000000	0.0480299999999971	F	F	F
0.5000000000000000	0.5000000000000000	0.1412300000000002	F	F	F
0.7500000000000000	0.5000000000000000	0.0480299999999971	F	F	F
0.5000000000000000	0.7500000000000000	0.0480299999999971	F	F	F
-0.0000000000000000	-0.0000000000000000	0.2355196718804249	T	T	T
0.5000000000000000	-0.0000000000000000	0.2355196718804249	T	T	T
-0.0000000000000000	0.5000000000000000	0.2355196718804249	T	T	T
0.5000000000000000	0.5000000000000000	0.2355196718804249	T	T	T
0.0000000000000000	0.0000000000000000	0.0480299999999971	F	F	F
0.5000000000000000	0.0000000000000000	0.0480299999999971	F	F	F
0.0000000000000000	0.5000000000000000	0.0480299999999971	F	F	F
0.5000000000000000	0.5000000000000000	0.0480299999999971	F	F	F
0.2500000000000000	0.2500000000000000	0.3170095512422101	T	T	T
0.7500000000000000	0.2500000000000000	0.3170095512422101	T	T	T
0.2500000000000000	0.7500000000000000	0.3170095512422101	T	T	T
0.7500000000000000	0.7500000000000000	0.3170095512422101	T	T	T
0.2500000000000000	0.2500000000000000	0.1412300000000002	F	F	F
0.7500000000000000	0.2500000000000000	0.1412300000000002	F	F	F
0.2500000000000000	0.7500000000000000	0.1412300000000002	F	F	F
0.7500000000000000	0.7500000000000000	0.1412300000000002	F	F	F

Table S5 Fractional coordinates of the relaxed FeO₂ termination of Sr₈Fe₇AlO₂₄ (001) surface.

O Al Fe Sr

1.0000000000000000			
7.7388000000000003	0.0000000000000000	0.0000000000000000	
0.0000000000000005	7.7388000000000003	0.0000000000000000	
0.0000000000000013	0.0000000000000013	20.810099999999985	

O	Al	Fe	Sr
24	1	7	8

Selective dynamics

Direct

0.0000000000000000	0.0000000000000000	0.0488599999999977	F	F	F
0.2482084284687987	0.0000000000000000	0.3286194275237309	T	T	T
-0.0000000000000000	0.2482084284687987	0.3286194275237309	T	T	T
0.5000000000000000	0.0000000000000000	0.0489099999999993	F	F	F
0.7517915715312014	0.0000000000000000	0.3286194275237309	T	T	T
0.5000000000000000	0.2511040258169404	0.3287143885567403	T	T	T
0.0000000000000000	0.5000000000000000	0.0489099999999993	F	F	F
0.2511040258169404	0.5000000000000000	0.3287143885567403	T	T	T
-0.0000000000000000	0.7517915715312014	0.3286194275237309	T	T	T
0.5000000000000000	0.5000000000000000	0.0481100000000012	F	F	F
0.7488959741830595	0.5000000000000000	0.3287143885567403	T	T	T
0.5000000000000000	0.7488959741830595	0.3287143885567403	T	T	T
-0.0000000000000000	0.0000000000000000	0.2324606979873331	T	T	T
0.2515399999999985	0.0000000000000000	0.1413099999999972	F	F	F
0.0000000000000000	0.2515399999999985	0.1413099999999972	F	F	F

0.5000000000000000	0.0000000000000000	0.2317380547325398	T	T	T
0.7484600000000015	0.0000000000000000	0.1413099999999972	F	F	F
0.5000000000000000	0.2493699999999990	0.1413099999999972	F	F	F
-0.0000000000000000	0.5000000000000000	0.2317380547325398	T	T	T
0.2493699999999990	0.5000000000000000	0.1413099999999972	F	F	F
0.0000000000000000	0.7484600000000015	0.1413099999999972	F	F	F
0.5000000000000000	0.5000000000000000	0.2322176298063957	T	T	T
0.7506300000000010	0.5000000000000000	0.1413099999999972	F	F	F
0.5000000000000000	0.7506300000000010	0.1413099999999972	F	F	F
-0.0000000000000000	0.0000000000000000	0.3220988726831671	T	T	T
0.5000000000000000	0.0000000000000000	0.3265018272163130	T	T	T
-0.0000000000000000	0.5000000000000000	0.3265018272163130	T	T	T
0.5000000000000000	0.5000000000000000	0.3259105704242679	T	T	T
0.0000000000000000	0.0000000000000000	0.1413099999999972	F	F	F
0.5000000000000000	0.0000000000000000	0.1413099999999972	F	F	F
0.0000000000000000	0.5000000000000000	0.1413099999999972	F	F	F
0.5000000000000000	0.5000000000000000	0.1413099999999972	F	F	F
0.2492299999999972	0.2492299999999972	0.0480500000000035	F	F	F
0.7507700000000028	0.2492299999999972	0.0480500000000035	F	F	F
0.2492299999999972	0.7507700000000028	0.0480500000000035	F	F	F
0.7507700000000028	0.7507700000000028	0.0480500000000035	F	F	F
0.2497829222929857	0.2497829222929857	0.2378023711332429	T	T	T
0.7502170777070142	0.2497829222929857	0.2378023711332429	T	T	T
0.2497829222929857	0.7502170777070142	0.2378023711332429	T	T	T
0.7502170777070142	0.7502170777070142	0.2378023711332429	T	T	T

Table S6 Fractional coordinates of the relaxed SrO termination of Sr₈Fe₇AlO₂₄ (001) surface.

O Al Fe Sr

1.0000000000000000			
7.7388000000000003	0.0000000000000000	0.0000000000000000	
0.0000000000000005	7.7388000000000003	0.0000000000000000	
0.0000000000000013	0.0000000000000013	20.815999999999989	

O	Al	Fe	Sr
24	1	7	8

Selective dynamics

Direct

-0.0000000000000000	-0.0000000000000000	0.3245831096852920	T	T	T
0.2535097219226664	-0.0000000000000000	0.2329159171216238	T	T	T
-0.0000000000000000	0.2535097219226664	0.2329159171216238	T	T	T
0.5000000000000000	-0.0000000000000000	0.3266753829923117	T	T	T
0.7464902780773337	-0.0000000000000000	0.2329159171216238	T	T	T
0.5000000000000000	0.2523316174593678	0.2347019938060292	T	T	T
-0.0000000000000000	0.5000000000000000	0.3266753829923117	T	T	T
0.2523316174593678	0.5000000000000000	0.2347019938060292	T	T	T
-0.0000000000000000	0.7464902780773337	0.2329159171216238	T	T	T
0.5000000000000000	0.5000000000000000	0.3275002648050378	T	T	T
0.7476683825406323	0.5000000000000000	0.2347019938060292	T	T	T
0.5000000000000000	0.7476683825406323	0.2347019938060292	T	T	T
0.0000000000000000	0.0000000000000000	0.1404599999999974	F	F	F
0.2515399999999985	0.0000000000000000	0.0480400000000003	F	F	F
0.0000000000000000	0.2515399999999985	0.0480400000000003	F	F	F

0.5000000000000000	0.0000000000000000	0.1404100000000028	F	F	F
0.7484600000000015	0.0000000000000000	0.0480400000000003	F	F	F
0.5000000000000000	0.2493699999999990	0.0480400000000003	F	F	F
0.0000000000000000	0.5000000000000000	0.1404100000000028	F	F	F
0.2493699999999990	0.5000000000000000	0.0480400000000003	F	F	F
0.0000000000000000	0.7484600000000015	0.0480400000000003	F	F	F
0.5000000000000000	0.5000000000000000	0.1412199999999970	F	F	F
0.7506300000000010	0.5000000000000000	0.0480400000000003	F	F	F
0.5000000000000000	0.7506300000000010	0.0480400000000003	F	F	F
-0.0000000000000000	-0.0000000000000000	0.2330792752767148	T	T	T
0.5000000000000000	-0.0000000000000000	0.2353092466779780	T	T	T
-0.0000000000000000	0.5000000000000000	0.2353092466779780	T	T	T
0.5000000000000000	0.5000000000000000	0.2370313518721872	T	T	T
0.0000000000000000	0.0000000000000000	0.0480400000000003	F	F	F
0.5000000000000000	0.0000000000000000	0.0480400000000003	F	F	F
0.0000000000000000	0.5000000000000000	0.0480400000000003	F	F	F
0.5000000000000000	0.5000000000000000	0.0480400000000003	F	F	F
0.2454668751097228	0.2454668751097228	0.3167234416745895	T	T	T
0.7545331248902771	0.2454668751097228	0.3167234416745895	T	T	T
0.2454668751097228	0.7545331248902771	0.3167234416745895	T	T	T
0.7545331248902771	0.7545331248902771	0.3167234416745895	T	T	T
0.2492299999999972	0.2492299999999972	0.1412699999999987	F	F	F
0.7507700000000028	0.2492299999999972	0.1412699999999987	F	F	F
0.2492299999999972	0.7507700000000028	0.1412699999999987	F	F	F
0.7507700000000028	0.7507700000000028	0.1412699999999987	F	F	F

Table S7 Fractional coordinates of the relaxed FeO₂ termination of Sr₈Fe₇ZrO₂₄ (001) surface.

O Zr Fe Sr

1.0000000000000000		
7.8491000000000000	0.0000000000000000	0.0000000000000000
0.0000000000000005	7.8491000000000000	0.0000000000000000
0.0000000000000013	0.0000000000000013	20.873799999999992

O	Zr	Fe	Sr
24	1	7	8

Selective dynamics

Direct

0.0000000000000000	0.0000000000000000	0.0523299999999978	F	F	F
0.2664157004546704	0.0000004503413632	0.3347639971740875	T	T	T
0.0000004503413632	0.2664157004546704	0.3347639971740875	T	T	T
0.5000000000000000	0.0000000000000000	0.0487299999999991	F	F	F
0.7335847376521258	0.0000004241321372	0.3347640251937642	T	T	T
0.5000001808013962	0.2548194767150235	0.3255484455689323	T	T	T
0.0000000000000000	0.5000000000000000	0.0487299999999991	F	F	F
0.2548194767150235	0.5000001808013962	0.3255484455689323	T	T	T
0.0000004241321372	0.7335847376521258	0.3347640251937642	T	T	T
0.5000000000000000	0.5000000000000000	0.0479100000000017	F	F	F
0.7451803685356863	0.5000001940552861	0.3255486605359175	T	T	T
0.5000001940552861	0.7451803685356863	0.3255486605359175	T	T	T
0.0000002854872062	0.0000002854872062	0.2374361510243113	T	T	T
0.2538600000000031	0.0000000000000000	0.1412899999999979	F	F	F
0.0000000000000000	0.2538600000000031	0.1412899999999979	F	F	F

0.5000003004999968	-0.0000000126920939	0.2324177079212518	T	T	T
0.7461399999999969	0.0000000000000000	0.1412899999999979	F	F	F
0.5000000000000000	0.2516600000000011	0.1412899999999979	F	F	F
-0.0000000126920939	0.5000003004999968	0.2324177079212518	T	T	T
0.2516600000000011	0.5000000000000000	0.1412899999999979	F	F	F
0.0000000000000000	0.7461399999999969	0.1412899999999979	F	F	F
0.4999999526131603	0.4999999526131603	0.2309220082376367	T	T	T
0.7483399999999989	0.5000000000000000	0.1412899999999979	F	F	F
0.5000000000000000	0.7483399999999989	0.1412899999999979	F	F	F
0.0000002041681919	0.0000002041681919	0.3339042418366789	T	T	T
0.5000002034798791	0.0000013835019578	0.3253954301309051	T	T	T
0.0000013835019578	0.5000002034798791	0.3253954301309051	T	T	T
0.5000010028645370	0.5000010028645370	0.3244277116600488	T	T	T
0.0000000000000000	0.0000000000000000	0.1412899999999979	F	F	F
0.5000000000000000	0.0000000000000000	0.1412899999999979	F	F	F
0.0000000000000000	0.5000000000000000	0.1412899999999979	F	F	F
0.5000000000000000	0.5000000000000000	0.1412899999999979	F	F	F
0.2566199999999981	0.2566199999999981	0.0497700000000023	F	F	F
0.7433899999999980	0.2566199999999981	0.0497700000000023	F	F	F
0.2566199999999981	0.7433899999999980	0.0497700000000023	F	F	F
0.7433899999999980	0.7433899999999980	0.0497700000000023	F	F	F
0.2544161427545483	0.2544161427545483	0.2360468761955581	T	T	T
0.7455842623233171	0.2544162149326799	0.2360469378031209	T	T	T
0.2544162149326799	0.7455842623233171	0.2360469378031209	T	T	T
0.7455841581429451	0.7455841581429451	0.2360470534225733	T	T	T

Table S8 Fractional coordinates of the relaxed SrO termination of Sr₈Fe₇ZrO₂₄ (001) surface.

O Zr Fe Sr

1.0000000000000000		
7.8491000000000000	0.0000000000000000	0.0000000000000000
0.0000000000000005	7.8491000000000000	0.0000000000000000
0.0000000000000013	0.0000000000000013	20.9923000000000002

O	Zr	Fe	Sr
24	1	7	8

Selective dynamics

Direct

0.0000011630189592	0.0000011630189592	0.3350241514060680	T	T	T
0.2635662585423476	0.0000021939458488	0.2342519549413796	T	T	T
0.0000021939458488	0.2635662585423476	0.2342519549413796	T	T	T
0.5000022371503696	0.0000022455265600	0.3257593503799768	T	T	T
0.7364366150521610	0.0000021774125417	0.2342514843255195	T	T	T
0.5000017782558406	0.2587023340489511	0.2347977173649752	T	T	T
0.0000022455265600	0.5000022371503696	0.3257593503799768	T	T	T
0.2587023340489511	0.5000017782558406	0.2347977173649752	T	T	T
0.0000021774125417	0.7364366150521610	0.2342514843255195	T	T	T
0.5000019141749890	0.5000019141749890	0.3297303113487141	T	T	T
0.7413011847333774	0.5000017860327419	0.2347976016084111	T	T	T
0.5000017860327419	0.7413011847333774	0.2347976016084111	T	T	T
0.0000000000000000	0.0000000000000000	0.1360900000000029	F	F	F
0.2538600000000031	0.0000000000000000	0.0476400000000012	F	F	F
0.0000000000000000	0.2538600000000031	0.0476400000000012	F	F	F

0.5000000000000000	0.0000000000000000	0.1396700000000024	F	F	F
0.7461399999999969	0.0000000000000000	0.0476400000000012	F	F	F
0.5000000000000000	0.2516600000000011	0.0476400000000012	F	F	F
0.0000000000000000	0.5000000000000000	0.1396700000000024	F	F	F
0.2516600000000011	0.5000000000000000	0.0476400000000012	F	F	F
0.0000000000000000	0.7461399999999969	0.0476400000000012	F	F	F
0.5000000000000000	0.5000000000000000	0.1404899999999998	F	F	F
0.7483399999999989	0.5000000000000000	0.0476400000000012	F	F	F
0.5000000000000000	0.7483399999999989	0.0476400000000012	F	F	F
0.0000013906220145	0.0000013906220145	0.2359398105299555	T	T	T
0.5000027388885890	0.0000016615388373	0.2346997203792637	T	T	T
0.0000016615388373	0.5000027388885890	0.2346997203792637	T	T	T
0.5000018014285038	0.5000018014285038	0.2352082533936198	T	T	T
0.0000000000000000	0.0000000000000000	0.0476400000000012	F	F	F
0.5000000000000000	0.0000000000000000	0.0476400000000012	F	F	F
0.0000000000000000	0.5000000000000000	0.0476400000000012	F	F	F
0.5000000000000000	0.5000000000000000	0.0476400000000012	F	F	F
0.2573982497409782	0.2573982497409782	0.3179012639015322	T	T	T
0.7426034434320181	0.2573973969402762	0.3179012578642323	T	T	T
0.2573973969402762	0.7426034434320181	0.3179012578642323	T	T	T
0.7426042325681159	0.7426042325681159	0.3179012210409718	T	T	T
0.2566199999999981	0.2566199999999981	0.1386400000000023	F	F	F
0.7433899999999980	0.2566199999999981	0.1386400000000023	F	F	F
0.2566199999999981	0.7433899999999980	0.1386400000000023	F	F	F
0.7433899999999980	0.7433899999999980	0.1386400000000023	F	F	F

Table S9 Fractional coordinates of the relaxed FeO₂ termination of Sr₈Fe₇NbO₂₄ (001) surface.

O Nb Fe Sr

1.0000000000000000			
7.8395000000000001	0.0000000000000000	0.0000000000000000	
0.0000000000000005	7.8395000000000001	0.0000000000000000	
0.0000000000000013	0.0000000000000013	20.8621000000000016	

O	Nb	Fe	Sr
24	1	7	8

Selective dynamics

Direct

0.0000000000000000	0.0000000000000000	0.0485200000000034	F	F	F
0.2536999847699140	0.0000000000000000	0.3358692562867452	T	T	T
0.0000000000000000	0.2536999847699140	0.3358692562867452	T	T	T
0.5000000000000000	0.0000000000000000	0.0489400000000018	F	F	F
0.7463000152300860	0.0000000000000000	0.3358692562867452	T	T	T
0.5000000000000000	0.2607633121649536	0.3266477818572792	T	T	T
0.0000000000000000	0.5000000000000000	0.0489400000000018	F	F	F
0.2607633121649536	0.5000000000000000	0.3266477818572792	T	T	T
0.0000000000000000	0.7463000152300860	0.3358692562867452	T	T	T
0.5000000000000000	0.5000000000000000	0.0479300000000009	F	F	F
0.7392366878350467	0.5000000000000000	0.3266477818572792	T	T	T
0.5000000000000000	0.7392366878350467	0.3266477818572792	T	T	T
0.0000000000000000	0.0000000000000000	0.2386851112339327	T	T	T
0.2549300000000017	0.0000000000000000	0.1410399999999967	F	F	F
0.0000000000000000	0.2549300000000017	0.1410399999999967	F	F	F

0.5000000000000000	0.0000000000000000	0.2339602969755552	T	T	T
0.7450699999999983	0.0000000000000000	0.1410399999999967	F	F	F
0.5000000000000000	0.2522400000000005	0.1410399999999967	F	F	F
0.0000000000000000	0.5000000000000000	0.2339602969755552	T	T	T
0.2522400000000005	0.5000000000000000	0.1410399999999967	F	F	F
0.0000000000000000	0.7450699999999983	0.1410399999999967	F	F	F
0.5000000000000000	0.5000000000000000	0.2295375970787996	T	T	T
0.7477599999999995	0.5000000000000000	0.1410399999999967	F	F	F
0.5000000000000000	0.7477599999999995	0.1410399999999967	F	F	F
0.0000000000000000	0.0000000000000000	0.3296020196336100	T	T	T
0.5000000000000000	0.0000000000000000	0.3259560886326792	T	T	T
0.0000000000000000	0.5000000000000000	0.3259560886326792	T	T	T
0.5000000000000000	0.5000000000000000	0.3260792382175727	T	T	T
0.0000000000000000	0.0000000000000000	0.1410399999999967	F	F	F
0.5000000000000000	0.0000000000000000	0.1410399999999967	F	F	F
0.0000000000000000	0.5000000000000000	0.1410399999999967	F	F	F
0.5000000000000000	0.5000000000000000	0.1410399999999967	F	F	F
0.2561999999999998	0.2561999999999998	0.0494199999999978	F	F	F
0.7438000000000002	0.2561999999999998	0.0494199999999978	F	F	F
0.2561999999999998	0.7438000000000002	0.0494199999999978	F	F	F
0.7438000000000002	0.7438000000000002	0.0494199999999978	F	F	F
0.2573960529024039	0.2573960529024039	0.2364480824194356	T	T	T
0.7426039470975963	0.2573960529024039	0.2364480824194356	T	T	T
0.2573960529024039	0.7426039470975963	0.2364480824194356	T	T	T
0.7426039470975963	0.7426039470975963	0.2364480824194356	T	T	T

Table S10 Fractional coordinates of the relaxed SrO termination of Sr₈Fe₇NbO₂₄ (001) surface.

O Nb Fe Sr

1.0000000000000000			
7.8395000000000001	0.0000000000000000	0.0000000000000000	
0.0000000000000005	7.8395000000000001	0.0000000000000000	
0.0000000000000013	0.0000000000000013	20.9283000000000001	

O	Nb	Fe	Sr
24	1	7	8

Selective dynamics

Direct

-0.0000000000000000	-0.0000000000000000	0.3323848078932898	T	T	T
0.2530656541789250	-0.0000000000000000	0.2357862114548918	T	T	T
-0.0000000000000000	0.2530656541789250	0.2357862114548918	T	T	T
0.5000000000000000	-0.0000000000000000	0.3284961789831079	T	T	T
0.7469343458210747	-0.0000000000000000	0.2357862114548918	T	T	T
0.5000000000000000	0.2517844623696381	0.2351505315814085	T	T	T
-0.0000000000000000	0.5000000000000000	0.3284961789831079	T	T	T
0.2517844623696381	0.5000000000000000	0.2351505315814085	T	T	T
-0.0000000000000000	0.7469343458210747	0.2357862114548918	T	T	T
0.5000000000000000	0.5000000000000000	0.3300215926993478	T	T	T
0.7482155376303619	0.5000000000000000	0.2351505315814085	T	T	T
0.5000000000000000	0.7482155376303619	0.2351505315814085	T	T	T
0.0000000000000000	0.0000000000000000	0.1400999999999966	F	F	F
0.2549300000000017	0.0000000000000000	0.0477800000000030	F	F	F
0.0000000000000000	0.2549300000000017	0.0477800000000030	F	F	F

0.5000000000000000	0.0000000000000000	0.1395800000000023	F	F	F
0.7450699999999983	0.0000000000000000	0.0477800000000030	F	F	F
0.5000000000000000	0.2522400000000005	0.0477800000000030	F	F	F
0.0000000000000000	0.5000000000000000	0.1395800000000023	F	F	F
0.2522400000000005	0.5000000000000000	0.0477800000000030	F	F	F
0.0000000000000000	0.7450699999999983	0.0477800000000030	F	F	F
0.5000000000000000	0.5000000000000000	0.1405900000000031	F	F	F
0.7477599999999995	0.5000000000000000	0.0477800000000030	F	F	F
0.5000000000000000	0.7477599999999995	0.0477800000000030	F	F	F
-0.0000000000000000	-0.0000000000000000	0.2369833787428623	T	T	T
0.5000000000000000	-0.0000000000000000	0.2362327776488183	T	T	T
-0.0000000000000000	0.5000000000000000	0.2362327776488183	T	T	T
0.5000000000000000	0.5000000000000000	0.2352319741746561	T	T	T
0.0000000000000000	0.0000000000000000	0.0477800000000030	F	F	F
0.5000000000000000	0.0000000000000000	0.0477800000000030	F	F	F
0.0000000000000000	0.5000000000000000	0.0477800000000030	F	F	F
0.5000000000000000	0.5000000000000000	0.0477800000000030	F	F	F
0.2584250713578896	0.2584250713578896	0.3186502279267652	T	T	T
0.7415749286421105	0.2584250713578896	0.3186502279267652	T	T	T
0.2584250713578896	0.7415749286421105	0.3186502279267652	T	T	T
0.7415749286421105	0.7415749286421105	0.3186502279267652	T	T	T
0.2561999999999998	0.2561999999999998	0.1391100000000023	F	F	F
0.7438000000000002	0.2561999999999998	0.1391100000000023	F	F	F
0.2561999999999998	0.7438000000000002	0.1391100000000023	F	F	F
0.7438000000000002	0.7438000000000002	0.1391100000000023	F	F	F

Table S11 Fractional coordinates of the relaxed FeO₂ termination of Sr₈Fe₇WO₂₄ (001) surface.

O W Fe Sr

1.0000000000000000

7.8437999999999999 0.0000000000000000 0.0000000000000000

0.0000000000000005 7.8437999999999999 0.0000000000000000

0.0000000000000013 0.0000000000000013 20.9165999999999990

O W Fe Sr

24 1 7 8

Selective dynamics

Direct

0.0000000000000000 0.0000000000000000 0.0478099999999984 F F F

0.2426495057893622 0.0000000000000000 0.3385688642729209 T T T

0.0000000000000000 0.2426495057893622 0.3385688642729209 T T T

0.5000000000000000 0.0000000000000000 0.0507599999999968 F F F

0.7573504942106377 0.0000000000000000 0.3385688642729209 T T T

0.5000000000000000 0.2558337880101787 0.3277977380247555 T T T

0.0000000000000000 0.5000000000000000 0.0507599999999968 F F F

0.2558337880101787 0.5000000000000000 0.3277977380247555 T T T

0.0000000000000000 0.7573504942106377 0.3385688642729209 T T T

0.5000000000000000 0.5000000000000000 0.0518199999999993 F F F

0.7441662119898212 0.5000000000000000 0.3277977380247555 T T T

0.5000000000000000 0.7441662119898212 0.3277977380247555 T T T

0.0000000000000000 0.0000000000000000 0.2415235594051936 T T T

0.2535600000000002 0.0000000000000000 0.1431699999999978 F F F

0.0000000000000000 0.2535600000000002 0.1431699999999978 F F F

0.5000000000000000	0.0000000000000000	0.2367934830148447	T	T	T
0.7464399999999998	0.0000000000000000	0.1431699999999978	F	F	F
0.5000000000000000	0.2563999999999993	0.1431699999999978	F	F	F
0.0000000000000000	0.5000000000000000	0.2367934830148447	T	T	T
0.2563999999999993	0.5000000000000000	0.1431699999999978	F	F	F
0.0000000000000000	0.7464399999999998	0.1431699999999978	F	F	F
0.5000000000000000	0.5000000000000000	0.2325607469522956	T	T	T
0.7436000000000007	0.5000000000000000	0.1431699999999978	F	F	F
0.5000000000000000	0.7436000000000007	0.1431699999999978	F	F	F
0.0000000000000000	0.0000000000000000	0.3295511764864695	T	T	T
0.5000000000000000	0.0000000000000000	0.3278869232755739	T	T	T
0.0000000000000000	0.5000000000000000	0.3278869232755739	T	T	T
0.5000000000000000	0.5000000000000000	0.3283043232123281	T	T	T
0.0000000000000000	0.0000000000000000	0.1431699999999978	F	F	F
0.5000000000000000	0.0000000000000000	0.1431699999999978	F	F	F
0.0000000000000000	0.5000000000000000	0.1431699999999978	F	F	F
0.5000000000000000	0.5000000000000000	0.1431699999999978	F	F	F
0.2583600000000033	0.2583600000000033	0.0525599999999997	F	F	F
0.7416399999999967	0.2583600000000033	0.0525599999999997	F	F	F
0.2583600000000033	0.7416399999999967	0.0525599999999997	F	F	F
0.7416399999999967	0.7416399999999967	0.0525599999999997	F	F	F
0.2611895644625509	0.2611895644625509	0.2389168160732051	T	T	T
0.7388104355374492	0.2611895644625509	0.2389168160732051	T	T	T
0.2611895644625509	0.7388104355374492	0.2389168160732051	T	T	T
0.7388104355374492	0.7388104355374492	0.2389168160732051	T	T	T

Table S12 Fractional coordinates of the relaxed SrO termination of Sr₈Fe₇WO₂₄ (001) surface.

O W Fe Sr

1.0000000000000000

7.8437999999999999 0.0000000000000000 0.0000000000000000

0.0000000000000005 7.8437999999999999 0.0000000000000000

0.0000000000000013 0.0000000000000013 20.9483999999999995

O W Fe Sr

24 1 7 8

Selective dynamics

Direct

-0.0000000000000000	-0.0000000000000000	0.3292481193387159	T	T	T
0.2444578881122293	-0.0000000000000000	0.2362368879433157	T	T	T
-0.0000000000000000	0.2444578881122293	0.2362368879433157	T	T	T
0.5000000000000000	-0.0000000000000000	0.3280333178852223	T	T	T
0.7555421118877709	-0.0000000000000000	0.2362368879433157	T	T	T
0.5000000000000000	0.2479012556780917	0.2342401573474084	T	T	T
-0.0000000000000000	0.5000000000000000	0.3280333178852223	T	T	T
0.2479012556780917	0.5000000000000000	0.2342401573474084	T	T	T
-0.0000000000000000	0.7555421118877709	0.2362368879433157	T	T	T
0.5000000000000000	0.5000000000000000	0.3294323536783088	T	T	T
0.7520987443219082	0.5000000000000000	0.2342401573474084	T	T	T
0.5000000000000000	0.7520987443219082	0.2342401573474084	T	T	T
0.0000000000000000	0.0000000000000000	0.1429600000000022	F	F	F
0.2535600000000002	0.0000000000000000	0.0477399999999975	F	F	F
0.0000000000000000	0.2535600000000002	0.0477399999999975	F	F	F

0.5000000000000000	0.0000000000000000	0.1400099999999966	F	F	F
0.7464399999999998	0.0000000000000000	0.0477399999999975	F	F	F
0.5000000000000000	0.2563999999999993	0.0477399999999975	F	F	F
0.0000000000000000	0.5000000000000000	0.1400099999999966	F	F	F
0.2563999999999993	0.5000000000000000	0.0477399999999975	F	F	F
0.0000000000000000	0.7464399999999998	0.0477399999999975	F	F	F
0.5000000000000000	0.5000000000000000	0.1389500000000012	F	F	F
0.7436000000000007	0.5000000000000000	0.0477399999999975	F	F	F
0.5000000000000000	0.7436000000000007	0.0477399999999975	F	F	F
-0.0000000000000000	-0.0000000000000000	0.2359048535266771	T	T	T
0.5000000000000000	-0.0000000000000000	0.2350950700600649	T	T	T
-0.0000000000000000	0.5000000000000000	0.2350950700600649	T	T	T
0.5000000000000000	0.5000000000000000	0.2339597785522029	T	T	T
0.0000000000000000	0.0000000000000000	0.0477399999999975	F	F	F
0.5000000000000000	0.0000000000000000	0.0477399999999975	F	F	F
0.0000000000000000	0.5000000000000000	0.0477399999999975	F	F	F
0.5000000000000000	0.5000000000000000	0.0477399999999975	F	F	F
0.2602152911654706	0.2602152911654706	0.3180832660932583	T	T	T
0.7397847088345295	0.2602152911654706	0.3180832660932583	T	T	T
0.2602152911654706	0.7397847088345295	0.3180832660932583	T	T	T
0.7397847088345295	0.7397847088345295	0.3180832660932583	T	T	T
0.2583600000000033	0.2583600000000033	0.1382199999999969	F	F	F
0.7416399999999967	0.2583600000000033	0.1382199999999969	F	F	F
0.2583600000000033	0.7416399999999967	0.1382199999999969	F	F	F
0.7416399999999967	0.7416399999999967	0.1382199999999969	F	F	F

Table S13 The calculated imaginary frequency and the fractional coordinates of the optimized transition state for H₂O adsorption on the FeO₂ termination of Sr₈Fe₈O₂₄ (001) surface.

9 f/i= 24.111730 THz 151.498468 2PiTHz 804.280718 cm-1 99.718136 meV

O Fe Sr O H

1.0000000000000000

7.7625000000000002 0.0000000000000000 0.0000000000000000

0.0000000000000000 7.7625000000000002 0.0000000000000000

0.0000000000000000 0.0000000000000000 20.8218999999999994

O Fe Sr O H

24 8 8 1 2

Selective dynamics

Direct

0.0000000000000000 0.0000000000000000 0.0480299999999971 F F F

0.2586116010541204 0.0008163930732437 0.3279166697682783 F F F

0.0038468508441341 0.2653658573433191 0.3284333165690398 F F F

0.5000000000000000 0.0000000000000000 0.0480299999999971 F F F

0.7305372739594205 0.0030643598920008 0.3350642410912670 F F F

0.4939490748503630 0.2488173365203821 0.3287077665157057 F F F

0.0000000000000000 0.5000000000000000 0.0480299999999971 F F F

0.2456277675153444 0.5024013642377909 0.3298065420807532 F F F

0.0024411662846973 0.7406164802902069 0.3260798272322631 F F F

0.5000000000000000 0.5000000000000000 0.0480299999999971 F F F

0.7537304906630098 0.5012400708258795 0.3285214288034979 F F F

0.4949916759533721 0.7535145685589058 0.3283777870650155 F F F

0.9976820094068088 0.0016758651554625 0.2360046588424467 F F F

0.2500000000000000 0.0000000000000000 0.1412300000000002 F F F

0.0000000000000000	0.2500000000000000	0.1412300000000002	F	F	F
0.5041486218152897	0.0004581771793681	0.2320161622088577	F	F	F
0.7500000000000000	0.0000000000000000	0.1412300000000002	F	F	F
0.5000000000000000	0.2500000000000000	0.1412300000000002	F	F	F
0.0006877071846816	0.4996706203095727	0.2303864412871306	F	F	F
0.2500000000000000	0.5000000000000000	0.1412300000000002	F	F	F
0.0000000000000000	0.7500000000000000	0.1412300000000002	F	F	F
0.4993296877489044	0.5003267151703099	0.2330877560035844	F	F	F
0.7500000000000000	0.5000000000000000	0.1412300000000002	F	F	F
0.5000000000000000	0.7500000000000000	0.1412300000000002	F	F	F
0.0172403377898362	0.9934596654038685	0.3301536825488895	F	F	F
0.4932194996236348	0.0003887258086692	0.3258180708103282	F	F	F
0.9997223211203945	0.5005619537546764	0.3258838182926027	F	F	F
0.5006185879632881	0.5002314894638005	0.3255994032963301	F	F	F
0.0000000000000000	0.0000000000000000	0.1412300000000002	F	F	F
0.5000000000000000	0.0000000000000000	0.1412300000000002	F	F	F
0.0000000000000000	0.5000000000000000	0.1412300000000002	F	F	F
0.5000000000000000	0.5000000000000000	0.1412300000000002	F	F	F
0.2500000000000000	0.2500000000000000	0.0480299999999971	F	F	F
0.7500000000000000	0.2500000000000000	0.0480299999999971	F	F	F
0.2500000000000000	0.7500000000000000	0.0480299999999971	F	F	F
0.7500000000000000	0.7500000000000000	0.0480299999999971	F	F	F
0.2487588140823647	0.2514658179137115	0.2368062837127596	F	F	F
0.7523570446446399	0.2491779218300820	0.2390447952829717	F	F	F
0.2497478398465347	0.7483115359822037	0.2361503746535050	F	F	F
0.7518000415688633	0.7509136757812911	0.2385394427827521	F	F	F
0.9320602452360163	0.0113393062590461	0.4199347887262022	T	T	T

0.7937481479531812	0.0120008256401647	0.3858994002166867	T	T	T
0.9543898558550765	0.1294246428155361	0.4330914848374490	T	T	T

Table S14 The calculated imaginary frequency and the fractional coordinates of the optimized transition state for H₂O adsorption on the SrO termination of Sr₈Fe₈O₂₄ (001) surface.

9 f/i= 20.480027 THz 128.679804 2PiTHz 683.140143 cm-1 84.698613 meV

O Fe Sr O H

1.0000000000000000

7.7625000000000002 0.0000000000000000 0.0000000000000000

0.0000000000000000 7.7625000000000002 0.0000000000000000

0.0000000000000000 0.0000000000000000 20.8218999999999994

O Fe Sr O H

24 8 8 1 2

Selective dynamics

Direct

0.9999978182876248 0.9859461635559583 0.3265094322373088 F F F

0.2500993465877599 0.0000243901244730 0.2343292429273518 F F F

0.0000528278259324 0.2532856248758861 0.2390060651706918 F F F

0.5001235160530371 0.0017326212091717 0.3262706983143815 F F F

0.7500263309289181 0.9999625960916916 0.2343078228659721 F F F

0.5001687068482568 0.2488937343534303 0.2328394838841774 F F F

0.9999412311559013 0.5215933853501085 0.3303039329108088 F F F

0.2499520002817022 0.4994895680496256 0.2348586783131168 F F F

0.0001100137424217 0.7474423547971085 0.2323810481532149 F F F

0.5001278398557503 0.4979023428667020 0.3257832396022877 F F F

0.7501657694828481 0.4995645497811552 0.2348242240126268 F F F

0.5000246285697472 0.7506859420295697 0.2343103617291504 F F F

0.0000000000000000 0.0000000000000000 0.1412300000000002 F F F

0.2500000000000000 0.0000000000000000 0.0480299999999971 F F F

0.0000000000000000	0.2500000000000000	0.0480299999999971	F	F	F
0.5000000000000000	0.0000000000000000	0.1412300000000002	F	F	F
0.7500000000000000	0.0000000000000000	0.0480299999999971	F	F	F
0.5000000000000000	0.2500000000000000	0.0480299999999971	F	F	F
0.0000000000000000	0.5000000000000000	0.1412300000000002	F	F	F
0.2500000000000000	0.5000000000000000	0.0480299999999971	F	F	F
0.0000000000000000	0.7500000000000000	0.0480299999999971	F	F	F
0.5000000000000000	0.5000000000000000	0.1412300000000002	F	F	F
0.7500000000000000	0.5000000000000000	0.0480299999999971	F	F	F
0.5000000000000000	0.7500000000000000	0.0480299999999971	F	F	F
0.0000531857261450	0.9990597861696742	0.2357327245263718	F	F	F
0.5000760376387703	0.9994357474611064	0.2347714386250175	F	F	F
0.0000517016585917	0.5003581467697487	0.2347713337694302	F	F	F
0.5000731949660846	0.5000819659363174	0.2349163382366442	F	F	F
0.0000000000000000	0.0000000000000000	0.0480299999999971	F	F	F
0.5000000000000000	0.0000000000000000	0.0480299999999971	F	F	F
0.0000000000000000	0.5000000000000000	0.0480299999999971	F	F	F
0.5000000000000000	0.5000000000000000	0.0480299999999971	F	F	F
0.2610680468819950	0.2483880051426226	0.3191453308615877	F	F	F
0.7393886420295246	0.2484310801333862	0.3191464327564759	F	F	F
0.2495885412708745	0.7503589037212564	0.3179340604422762	F	F	F
0.7504822709085559	0.7503699747479828	0.3179368400932816	F	F	F
0.2500000000000000	0.2500000000000000	0.1412300000000002	F	F	F
0.7500000000000000	0.2500000000000000	0.1412300000000002	F	F	F
0.2500000000000000	0.7500000000000000	0.1412300000000002	F	F	F
0.7500000000000000	0.7500000000000000	0.1412300000000002	F	F	F
0.0007476737560310	0.2763040580896075	0.4044275575168399	T	T	T

0.0003156933714337	0.3960268569182475	0.3679628080044068	T	T	T
0.0003648540427861	0.1596554577194524	0.3836678269995147	T	T	T

Table S15 The calculated imaginary frequency and the fractional coordinates of the optimized transition state for H₂O adsorption on the FeO₂ termination of Sr₈Fe₇AlO₂₄ (001) surface.

9 f_i= 20.580208 THz 129.309260 2PiTHz 686.481823 cm-1 85.112929 meV

O Al Fe Sr O H

1.0000000000000000

7.7388000000000003 0.0000000000000000 0.0000000000000000

0.0000000000000000 7.7388000000000003 0.0000000000000000

0.0000000000000000 0.0000000000000000 20.8100999999999985

O Al Fe Sr O H

24 1 7 8 1 2

Selective dynamics

Direct

0.0000000000000000 0.0000000000000000 0.0488599999999977 F F F

0.2574229325730073 0.0026641016563644 0.3280918319055033 F F F

0.0060799939666225 0.2753761533347969 0.3300455553772821 F F F

0.5000000000000000 0.0000000000000000 0.0489099999999993 F F F

0.7221386402280032 0.0014636123640415 0.3343180582296412 F F F

0.4944325342303060 0.2530993702518600 0.3290991879836014 F F F

0.0000000000000000 0.5000000000000000 0.0489099999999993 F F F

0.2492023407944473 0.5046701220182825 0.3310020514222813 F F F

0.0033943748914496 0.7427387809594777 0.3247518515390269 F F F

0.5000000000000000 0.5000000000000000 0.0481100000000012 F F F

0.7514977483267913 0.5032398316236240 0.3288327575090122 F F F

0.4932476568261848 0.7497801451591073 0.3289587767823008 F F F

0.9960572184040331 0.0050786883517304 0.2395523012947294 F F F

0.2515399999999985 0.0000000000000000 0.1413099999999972 F F F

0.0000000000000000	0.2515399999999985	0.1413099999999972	F	F	F
0.5030610732001648	0.9999747336334011	0.2321800058807497	F	F	F
0.7484600000000015	0.0000000000000000	0.1413099999999972	F	F	F
0.5000000000000000	0.2493699999999990	0.1413099999999972	F	F	F
0.0014926646330835	0.4988664752434318	0.2306766418910513	F	F	F
0.2493699999999990	0.5000000000000000	0.1413099999999972	F	F	F
0.0000000000000000	0.7484600000000015	0.1413099999999972	F	F	F
0.4988450158274205	0.5008723788462888	0.2331287446115198	F	F	F
0.7506300000000010	0.5000000000000000	0.1413099999999972	F	F	F
0.5000000000000000	0.7506300000000010	0.1413099999999972	F	F	F
0.0285905545640617	0.9767608789339590	0.3275877893612957	F	F	F
0.4894515027121997	0.9994872131034569	0.3262537094373030	F	F	F
0.0003692200963670	0.5048131816276964	0.3260131652699485	F	F	F
0.5015255554410203	0.4996331131252063	0.3259291484494042	F	F	F
0.0000000000000000	0.0000000000000000	0.1413099999999972	F	F	F
0.5000000000000000	0.0000000000000000	0.1413099999999972	F	F	F
0.0000000000000000	0.5000000000000000	0.1413099999999972	F	F	F
0.5000000000000000	0.5000000000000000	0.1413099999999972	F	F	F
0.2492299999999972	0.2492299999999972	0.0480500000000035	F	F	F
0.7507700000000028	0.2492299999999972	0.0480500000000035	F	F	F
0.2492299999999972	0.7507700000000028	0.0480500000000035	F	F	F
0.7507700000000028	0.7507700000000028	0.0480500000000035	F	F	F
0.2478087387068086	0.2504023330441640	0.2371948048376780	F	F	F
0.7538702357664491	0.2471889392385691	0.2400155323368480	F	F	F
0.2521504801422054	0.7465737049467478	0.2346427305563097	F	F	F
0.7515660465866247	0.7522714312275838	0.2384809249506503	F	F	F
0.9451893494266130	0.0159313412629061	0.4100602801052702	T	T	T

0.8045969195567082	0.0151883301061915	0.3838424139644800	T	T	T
0.9693826626502187	0.1364863983458307	0.4202150940976437	T	T	T

Table S16 The calculated imaginary frequency and the fractional coordinates of the optimized transition state for H₂O adsorption on the SrO termination of Sr₈Fe₇AlO₂₄ (001) surface.

9 f/i= 3.663230 THz 23.016754 2PiTHz 122.192205 cm-1 15.149908 meV

O Al Fe Sr O H

1.0000000000000000

7.7388000000000003 0.0000000000000000 0.0000000000000000

0.0000000000000000 7.7388000000000003 0.0000000000000000

0.0000000000000000 0.0000000000000000 20.8159999999999989

O Al Fe Sr O H

24 1 7 8 1 2

Selective dynamics

Direct

0.0000004076872671 0.9763689582574528 0.3216771451244469 F F F

0.2550712199934466 0.9999733269940378 0.2325321371459026 F F F

0.9999644009418276 0.2517606570954456 0.2393898630317608 F F F

0.4999498057323279 0.0008557668200879 0.3257952996015518 F F F

0.7448863222094957 0.9999747684379443 0.2325411957068013 F F F

0.4999636736390443 0.2528977685688432 0.2329357493379405 F F F

0.0000084256215800 0.5437161522309140 0.3379449688335399 F F F

0.2469117440892461 0.4982878748306021 0.2360819625107808 F F F

0.9999778061729572 0.7459777681451456 0.2335835977744551 F F F

0.4999592985337387 0.4976886127392746 0.3258200582295743 F F F

0.7530402052730096 0.4982948215206378 0.2360869759477282 F F F

0.4999778936687349 0.7457906416792071 0.2337933627150122 F F F

0.0000000000000000 0.0000000000000000 0.1404599999999974 F F F

0.2515399999999985 0.0000000000000000 0.0480400000000003 F F F

0.0000000000000000	0.2515399999999985	0.0480400000000003	F	F	F
0.5000000000000000	0.0000000000000000	0.1404100000000028	F	F	F
0.7484600000000015	0.0000000000000000	0.0480400000000003	F	F	F
0.5000000000000000	0.2493699999999990	0.0480400000000003	F	F	F
0.0000000000000000	0.5000000000000000	0.1404100000000028	F	F	F
0.2493699999999990	0.5000000000000000	0.0480400000000003	F	F	F
0.0000000000000000	0.7484600000000015	0.0480400000000003	F	F	F
0.5000000000000000	0.5000000000000000	0.1412199999999970	F	F	F
0.7506300000000010	0.5000000000000000	0.0480400000000003	F	F	F
0.5000000000000000	0.7506300000000010	0.0480400000000003	F	F	F
0.9999751126497642	0.0011066098364552	0.2320795778041216	F	F	F
0.4999711993474278	0.0009106735720295	0.2346928730096280	F	F	F
0.9999768097038313	0.5000662139120209	0.2327144902828522	F	F	F
0.4999712150877897	0.4979214380744139	0.2368838355458394	F	F	F
0.0000000000000000	0.0000000000000000	0.0480400000000003	F	F	F
0.5000000000000000	0.0000000000000000	0.0480400000000003	F	F	F
0.0000000000000000	0.5000000000000000	0.0480400000000003	F	F	F
0.5000000000000000	0.5000000000000000	0.0480400000000003	F	F	F
0.2477267964231871	0.2403799820813006	0.3218460865676676	F	F	F
0.7521228634403343	0.2404041446219480	0.3218410610721563	F	F	F
0.2493778916709957	0.7548557191102105	0.3178688134340817	F	F	F
0.7505885792022795	0.7548666839812199	0.3178696166359885	F	F	F
0.2492299999999972	0.2492299999999972	0.1412699999999987	F	F	F
0.7507700000000028	0.2492299999999972	0.1412699999999987	F	F	F
0.2492299999999972	0.7507700000000028	0.1412699999999987	F	F	F
0.7507700000000028	0.7507700000000028	0.1412699999999987	F	F	F
0.9998525338216808	0.2571025644659528	0.4049185369880632	T	T	T

0.9999599670346697	0.4482869195581571	0.3698349025803935	T	T	T
0.9998837520245019	0.1338517164074702	0.4135333559526371	T	T	T

Table S17 The calculated imaginary frequency and the fractional coordinates of the optimized transition state for H₂O adsorption on the FeO₂ termination of Sr₈Fe₇ZrO₂₄ (001) surface.

9 f/i= 26.095925 THz 163.965533 2PiTHz 870.466335 cm-1 107.924110 meV

O Zr Fe Sr O H

1.0000000000000000

7.8491000000000000 0.0000000000000000 0.0000000000000000

0.0000000000000000 7.8491000000000000 0.0000000000000000

0.0000000000000000 0.0000000000000000 20.8737999999999992

O Zr Fe Sr O H

24 1 7 8 1 2

Selective dynamics

Direct

0.0000000000000000 0.0000000000000000 0.0523299999999978 F F F

0.2662550591089925 0.0022498456273112 0.3346188225063216 F F F

0.0023360362470868 0.2686800750356895 0.3298284024237077 F F F

0.5000000000000000 0.0000000000000000 0.0487299999999991 F F F

0.7281431386405544 0.0053651574595577 0.3425151893680791 F F F

0.4987062448599247 0.2677260268008865 0.3263631449360460 F F F

0.0000000000000000 0.5000000000000000 0.0487299999999991 F F F

0.2492690218976890 0.5025254763156468 0.3249828494088476 F F F

0.0004251896838028 0.7330486011499033 0.3301682757553408 F F F

0.5000000000000000 0.5000000000000000 0.0479100000000017 F F F

0.7501856042446562 0.5010710239092333 0.3250434781893290 F F F

0.4998692051816462 0.7402929645585985 0.3245937273872457 F F F

0.9930229301394391 0.0002857126133904 0.2373525427304060 F F F

0.2538600000000031 0.0000000000000000 0.1412899999999979 F F F

0.0000000000000000	0.2538600000000031	0.1412899999999979	F	F	F
0.5053400993748909	0.0022467844125416	0.2335841162428878	F	F	F
0.7461399999999969	0.0000000000000000	0.1412899999999979	F	F	F
0.5000000000000000	0.2516600000000011	0.1412899999999979	F	F	F
0.0001967747480194	0.5007888523775037	0.2309309166700260	F	F	F
0.2516600000000011	0.5000000000000000	0.1412899999999979	F	F	F
0.0000000000000000	0.7461399999999969	0.1412899999999979	F	F	F
0.4994548913537500	0.5006835007424399	0.2307065248577160	F	F	F
0.7483399999999989	0.5000000000000000	0.1412899999999979	F	F	F
0.5000000000000000	0.7483399999999989	0.1412899999999979	F	F	F
0.0098467817177266	0.9994451383217111	0.3384369068042403	F	F	F
0.4965384584615009	0.9874212699072800	0.3244125755354617	F	F	F
0.0026089795684356	0.5004467635762140	0.3242022030231411	F	F	F
0.5021732873569960	0.4984306571180923	0.3235411009718803	F	F	F
0.0000000000000000	0.0000000000000000	0.1412899999999979	F	F	F
0.5000000000000000	0.0000000000000000	0.1412899999999979	F	F	F
0.0000000000000000	0.5000000000000000	0.1412899999999979	F	F	F
0.5000000000000000	0.5000000000000000	0.1412899999999979	F	F	F
0.2566199999999981	0.2566199999999981	0.0497700000000023	F	F	F
0.7433899999999980	0.2566199999999981	0.0497700000000023	F	F	F
0.2566199999999981	0.7433899999999980	0.0497700000000023	F	F	F
0.7433899999999980	0.7433899999999980	0.0497700000000023	F	F	F
0.2533996655797424	0.2539939131526197	0.2360502040294463	F	F	F
0.7492783406563035	0.2526996676286828	0.2365621276780558	F	F	F
0.2514962017842493	0.7437811004831616	0.2348290161916040	F	F	F
0.7507111175470840	0.7446388591103812	0.2352446234574614	F	F	F
0.8988986070254867	0.0157917370111917	0.4356707663728940	T	T	T

0.7743981322043325	0.0177530388451075	0.3973324560129683	T	T	T
0.9050437204294043	0.1200188439495875	0.4599504320796224	T	T	T

Table S18 The calculated imaginary frequency and the fractional coordinates of the optimized transition state for H₂O adsorption on the SrO termination of Sr₈Fe₇ZrO₂₄ (001) surface.

9 f/i= 6.216789 THz 39.061235 2PiTHz 207.369743 cm-1 25.710581 meV

O Zr Fe Sr O H

1.0000000000000000

7.8491000000000000 0.0000000000000000 0.0000000000000000

0.0000000000000000 7.8491000000000000 0.0000000000000000

0.0000000000000000 0.0000000000000000 20.9923000000000002

O Zr Fe Sr O H

24 1 7 8 1 2

Selective dynamics

Direct

0.9998029193515805 0.9608711822785310 0.3325864379138110 F F F

0.2644116732189232 0.0126749761192215 0.2343527219197057 F F F

0.9904648376792906 0.2655507248503426 0.2449633278463637 F F F

0.5002383501463186 0.0051078056805309 0.3252657362582809 F F F

0.7351518449281826 0.9931604137269829 0.2338655839172148 F F F

0.5094924767984708 0.2630418941207822 0.2330733994779948 F F F

0.9980402456744812 0.5562413195743332 0.3385742112924177 F F F

0.2377532278151335 0.4892437022733631 0.2370935443682001 F F F

0.0118513605005504 0.7367209073612315 0.2294032767145850 F F F

0.5002802243173505 0.4982804855672001 0.3272392593072411 F F F

0.7621433520575351 0.5102157177399604 0.2361905460792570 F F F

0.4910779785438493 0.7385799391564873 0.2344867375101245 F F F

0.0000000000000000 0.0000000000000000 0.1360900000000029 F F F

0.2538600000000031 0.0000000000000000 0.0476400000000012 F F F

0.0000000000000000	0.2538600000000031	0.0476400000000012	F	F	F
0.4999999999999929	0.0000000000000000	0.1396700000000024	F	F	F
0.7461399999999898	0.0000000000000000	0.0476400000000012	F	F	F
0.4999999999999929	0.2516600000000011	0.0476400000000012	F	F	F
0.0000000000000000	0.4999999999999929	0.1396700000000024	F	F	F
0.2516600000000011	0.4999999999999929	0.0476400000000012	F	F	F
0.0000000000000000	0.7461399999999898	0.0476400000000012	F	F	F
0.4999999999999929	0.4999999999999929	0.1404899999999998	F	F	F
0.7483399999999918	0.4999999999999929	0.0476400000000012	F	F	F
0.4999999999999929	0.7483399999999918	0.0476400000000012	F	F	F
0.9996208187781122	0.0006321186632832	0.2368029150396254	F	F	F
0.4998304589907434	0.0040519947483517	0.2351679105164806	F	F	F
0.9999134529276148	0.5027849318437916	0.2329628077891712	F	F	F
0.4998491608084734	0.4999870633779011	0.2362431810588461	F	F	F
0.0000000000000000	0.0000000000000000	0.0476400000000012	F	F	F
0.4999999999999929	0.0000000000000000	0.0476400000000012	F	F	F
0.0000000000000000	0.4999999999999929	0.0476400000000012	F	F	F
0.4999999999999929	0.4999999999999929	0.0476400000000012	F	F	F
0.2544838767559128	0.2547997690139567	0.3249085404453709	F	F	F
0.7435841036144382	0.2580215969223687	0.3252719057545619	F	F	F
0.2531440878910018	0.7476280126018082	0.3202258679170384	F	F	F
0.7433679700862115	0.7500663594208916	0.3207095593398677	F	F	F
0.2566199999999981	0.2566199999999981	0.1386400000000023	F	F	F
0.7433899999999980	0.2566199999999981	0.1386400000000023	F	F	F
0.2566199999999981	0.7433899999999980	0.1386400000000023	F	F	F
0.7433899999999980	0.7433899999999980	0.1386400000000023	F	F	F
0.0008369020004650	0.2767863765091931	0.4021246155832401	T	T	T

0.9991872939931739	0.4622071147424265	0.3704162840201306	T	T	T
0.9997919939622192	0.1614433988049413	0.4183726109584053	T	T	T

Table S19 The calculated imaginary frequency and the fractional coordinates of the optimized transition state for H₂O adsorption on the FeO₂ termination of Sr₈Fe₇NbO₂₄ (001) surface.

9 f/i= 27.610757 THz 173.483500 2PiTHz 920.995676 cm-1 114.188952 meV

O Nb Fe Sr O H

1.0000000000000000

7.8395000000000001 0.0000000000000000 0.0000000000000000

0.0000000000000000 7.8395000000000001 0.0000000000000000

0.0000000000000000 0.0000000000000000 20.8621000000000016

O Nb Fe Sr O H

24 1 7 8 1 2

Selective dynamics

Direct

0.0000000000000000 0.0000000000000000 0.0485200000000034 F F F

0.2590924240049333 0.0021402336154992 0.3396013418100381 F F F

0.0044721507782484 0.2563240993790359 0.3316118647752191 F F F

0.5000000000000000 0.0000000000000000 0.0489400000000018 F F F

0.7354397376931061 0.0056850444267553 0.3401909413021400 F F F

0.4968470154810589 0.2653349574266244 0.3266448980457710 F F F

0.0000000000000000 0.5000000000000000 0.0489400000000018 F F F

0.2607832510143879 0.5026028525051842 0.3264441929954529 F F F

0.0015056802023992 0.7470266885598349 0.3330592893729332 F F F

0.5000000000000000 0.5000000000000000 0.0479300000000009 F F F

0.7403314781059080 0.5005326764951477 0.3262960617273762 F F F

0.4988487255394602 0.7405102983922234 0.3250148770721921 F F F

0.9959392721879752 0.0006564001618159 0.2408165836540590 F F F

0.2549300000000017 0.0000000000000000 0.1410399999999967 F F F

0.0000000000000000	0.254930000000017	0.141039999999967	F	F	F
0.4992163788718358	0.0016619999722494	0.2340563077677942	F	F	F
0.745069999999983	0.0000000000000000	0.141039999999967	F	F	F
0.5000000000000000	0.2522400000000005	0.141039999999967	F	F	F
0.0009164515651392	0.5022317872465223	0.2328770422009399	F	F	F
0.2522400000000005	0.5000000000000000	0.141039999999967	F	F	F
0.0000000000000000	0.745069999999983	0.141039999999967	F	F	F
0.4999091757523928	0.5002484215062921	0.2292454887903048	F	F	F
0.747759999999995	0.5000000000000000	0.141039999999967	F	F	F
0.5000000000000000	0.747759999999995	0.141039999999967	F	F	F
0.0185546049705039	0.9974196044613564	0.3344145854062077	F	F	F
0.5004793700494190	0.9920200002560264	0.3248968776719749	F	F	F
0.0008118426191572	0.4990236481752959	0.3249770136667394	F	F	F
0.5006475856108850	0.4995319529924416	0.3252584324963834	F	F	F
0.0000000000000000	0.0000000000000000	0.141039999999967	F	F	F
0.5000000000000000	0.0000000000000000	0.141039999999967	F	F	F
0.0000000000000000	0.5000000000000000	0.141039999999967	F	F	F
0.5000000000000000	0.5000000000000000	0.141039999999967	F	F	F
0.256199999999998	0.256199999999998	0.049419999999978	F	F	F
0.7438000000000002	0.256199999999998	0.049419999999978	F	F	F
0.256199999999998	0.7438000000000002	0.049419999999978	F	F	F
0.7438000000000002	0.7438000000000002	0.049419999999978	F	F	F
0.2564472998438845	0.2583482545772711	0.2352383947856822	F	F	F
0.7474357221414039	0.2537832171540941	0.2378712497245985	F	F	F
0.2567659381186616	0.7400790578330927	0.2339421704551015	F	F	F
0.7481128502776642	0.7435969877269386	0.2365039334445669	F	F	F
0.9128653008566161	0.0155397834719651	0.4311307406124811	T	T	T

0.7889781070504753	0.0175847827362929	0.3961528608803135	T	T	T
0.9288273765909238	0.1281716406202520	0.4491831283807901	T	T	T

Table S20 The calculated imaginary frequency and the fractional coordinates of the optimized transition state for H₂O adsorption on the SrO termination of Sr₈Fe₇NbO₂₄ (001) surface.

9 f/i= 6.281600 THz 39.468460 2PiTHz 209.531632 cm-1 25.978621 meV

O Nb Fe Sr O H

1.0000000000000000		
7.8395000000000001	0.0000000000000000	0.0000000000000000
0.0000000000000000	7.8395000000000001	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.9283000000000001

O	Nb	Fe	Sr	O	H
24	1	7	8	1	2

Selective dynamics

Direct

0.0000132559696908	0.9775936402287400	0.3323730577060999	F	F	F
0.2531553605814807	0.9998481471301091	0.2356240571966310	F	F	F
0.0000132884438386	0.2524703056503412	0.2422998083521648	F	F	F
0.4999927024810020	0.0037777554049043	0.3274467286401759	F	F	F
0.7468419337703196	0.9998823305412188	0.2356285491294656	F	F	F
0.4999766844309974	0.2525422669962865	0.2332834628028806	F	F	F
0.0000166714983010	0.5233303752914793	0.3302188034480125	F	F	F
0.2528801614011726	0.4983730802508362	0.2353409320791400	F	F	F
0.9999769374959087	0.7465588893679325	0.2322883972735639	F	F	F
0.4999906805649346	0.4972540230060076	0.3285956415971896	F	F	F
0.7471160712323694	0.4983407971902452	0.2353441660477600	F	F	F
0.5000156709544115	0.7465053552238530	0.2352777587511454	F	F	F
0.0000000000000000	0.0000000000000000	0.1400099999999966	F	F	F
0.2549300000000017	0.0000000000000000	0.0477800000000030	F	F	F

0.0000000000000000	0.254930000000017	0.047780000000030	F	F	F
0.5000000000000000	0.0000000000000000	0.139580000000023	F	F	F
0.745069999999983	0.0000000000000000	0.047780000000030	F	F	F
0.5000000000000000	0.252240000000005	0.047780000000030	F	F	F
0.0000000000000000	0.5000000000000000	0.139580000000023	F	F	F
0.252240000000005	0.5000000000000000	0.047780000000030	F	F	F
0.0000000000000000	0.745069999999983	0.047780000000030	F	F	F
0.5000000000000000	0.5000000000000000	0.140590000000031	F	F	F
0.747759999999995	0.5000000000000000	0.047780000000030	F	F	F
0.5000000000000000	0.747759999999995	0.047780000000030	F	F	F
0.999999055130644	0.9992134161083612	0.2371445356803221	F	F	F
0.4999968356748425	0.9988376687649776	0.2354083756345275	F	F	F
0.9999984630725507	0.5004564317758238	0.2353797737174332	F	F	F
0.4999963647739847	0.4998856243565371	0.2349946004217145	F	F	F
0.0000000000000000	0.0000000000000000	0.047780000000030	F	F	F
0.5000000000000000	0.0000000000000000	0.047780000000030	F	F	F
0.0000000000000000	0.5000000000000000	0.047780000000030	F	F	F
0.5000000000000000	0.5000000000000000	0.047780000000030	F	F	F
0.2700898280841670	0.2553448267005933	0.3209258639778980	F	F	F
0.7298646971523297	0.2553273111813326	0.3209252431455809	F	F	F
0.2551403793120386	0.7411436025013955	0.3200925973294275	F	F	F
0.7448728574702983	0.7411373212281518	0.3200913247170050	F	F	F
0.256199999999998	0.256199999999998	0.139110000000023	F	F	F
0.7438000000000002	0.256199999999998	0.139110000000023	F	F	F
0.256199999999998	0.7438000000000002	0.139110000000023	F	F	F
0.7438000000000002	0.7438000000000002	0.139110000000023	F	F	F
0.9999347618268359	0.2740162169083220	0.4026999112550627	T	T	T

0.9999715555669084	0.3870387613609054	0.3692235524876750	T	T	T
0.9999697919599555	0.1584332740955361	0.3813700084452451	T	T	T

Table S21 The calculated imaginary frequency and the fractional coordinates of the optimized transition state for H₂O adsorption on the FeO₂ termination of Sr₈Fe₇WO₂₄ (001) surface.

9 f/i= 10.437139 THz 65.578481 2PiTHz 348.145485 cm-1 43.164554 meV

O W Fe Sr O H

1.0000000000000000

7.8437999999999999 0.0000000000000000 0.0000000000000000

0.0000000000000000 7.8437999999999999 0.0000000000000000

0.0000000000000000 0.0000000000000000 20.9165999999999990

O W Fe Sr O H

24 1 7 8 1 2

Selective dynamics

Direct

0.0000000000000000 0.0000000000000000 0.0478099999999984 F F F

0.2469532072725897 0.0071888928610875 0.3440440076360858 F F F

0.9945138223695551 0.2432728149445893 0.3362432733448841 F F F

0.5000000000000000 0.0000000000000000 0.0507599999999968 F F F

0.7433350450309248 0.9977159270044638 0.3299717014024210 F F F

0.4975714605267569 0.2674041548164752 0.3267950882136716 F F F

0.0000000000000000 0.5000000000000000 0.0507599999999968 F F F

0.2513930777418452 0.4998540543017143 0.3278594223440976 F F F

0.0013672258403403 0.7600415772030118 0.3356013121765855 F F F

0.5000000000000000 0.5000000000000000 0.0518199999999993 F F F

0.7384572719394242 0.5061904949375773 0.3277466040426020 F F F

0.4879461857676191 0.7403143809307480 0.3285774940557715 F F F

0.0083674751169553 0.0027308093178036 0.2432497776584199 F F F

0.2535600000000002 0.0000000000000000 0.1431699999999978 F F F

0.0000000000000000	0.2535600000000002	0.1431699999999978	F	F	F
0.4874154889498783	0.9998489221476419	0.2353185206377262	F	F	F
0.7464400000000069	0.0000000000000000	0.1431699999999978	F	F	F
0.5000000000000000	0.2563999999999993	0.1431699999999978	F	F	F
0.9981221941718204	0.5008526636540580	0.2353813414234693	F	F	F
0.2563999999999993	0.5000000000000000	0.1431699999999978	F	F	F
0.0000000000000000	0.7464400000000069	0.1431699999999978	F	F	F
0.4972698875739425	0.5041090327391728	0.2308892816446004	F	F	F
0.7436000000000007	0.5000000000000000	0.1431699999999978	F	F	F
0.5000000000000000	0.7436000000000007	0.1431699999999978	F	F	F
0.0145544085035922	0.0000032900813167	0.3323309603071962	F	F	F
0.4994974337399043	0.9795808667951249	0.3254147328681967	F	F	F
0.0096249135718054	0.4989331652282232	0.3270895702085213	F	F	F
0.5030085504372579	0.4956439312302336	0.3271811447522808	F	F	F
0.0000000000000000	0.0000000000000000	0.1431699999999978	F	F	F
0.5000000000000000	0.0000000000000000	0.1431699999999978	F	F	F
0.0000000000000000	0.5000000000000000	0.1431699999999978	F	F	F
0.5000000000000000	0.5000000000000000	0.1431699999999978	F	F	F
0.2583600000000033	0.2583600000000033	0.0525599999999997	F	F	F
0.7416400000000039	0.2583600000000033	0.0525599999999997	F	F	F
0.2583600000000033	0.7416400000000039	0.0525599999999997	F	F	F
0.7416400000000039	0.7416400000000039	0.0525599999999997	F	F	F
0.2618798046002553	0.2612239482435825	0.2370922178901793	F	F	F
0.7421152771338555	0.2571875392266421	0.2415113206156505	F	F	F
0.2586207135568230	0.7353115163144253	0.2351959946590370	F	F	F
0.7439582855488709	0.7385484369607340	0.2390377313391099	F	F	F
0.8967287854575900	0.0025445759470983	0.4275638970654114	T	T	T

0.7861890234978972	0.0000638672686648	0.3939739082776512	T	T	T
0.8999632943355423	0.1180569356152432	0.4441550403604034	T	T	T

Table S22 The calculated imaginary frequency and the fractional coordinates of the optimized transition state for H₂O adsorption on the SrO termination of Sr₈Fe₇WO₂₄ (001) surface.

9 f/i= 3.416740 THz 21.468010 2PiTHz 113.970172 cm-1 14.130506 meV

O W Fe Sr O H

1.0000000000000000

7.8437999999999999 0.0000000000000000 0.0000000000000000

0.0000000000000000 7.8437999999999999 0.0000000000000000

0.0000000000000000 0.0000000000000000 20.9483999999999995

O W Fe Sr O H

24 1 7 8 1 2

Selective dynamics

Direct

0.9994063793660715 0.9772112874996566 0.3287807613804574 F F F

0.2436048417153316 0.0004228470635113 0.2359545827299172 F F F

0.9991767577283071 0.2423474801117251 0.2422291231506151 F F F

0.5004346887379896 0.0034259105287049 0.3267733132331756 F F F

0.7565170835599346 0.9983712882920557 0.2356979850999537 F F F

0.5010590014543013 0.2458825780677358 0.2325178506946699 F F F

0.9993321947097016 0.5196576867410698 0.3295673089747808 F F F

0.2502986136272440 0.4968378833671068 0.2345015825552963 F F F

0.0013013490234215 0.7535394418582442 0.2326227286002975 F F F

0.5003101262151262 0.4974910805714003 0.3284030253251018 F F F

0.7498115375212606 0.4984068719854946 0.2342908950591109 F F F

0.4992395483518450 0.7524461662345630 0.2343574937479005 F F F

0.0000000000000000 0.0000000000000000 0.1429600000000022 F F F

0.2535600000000002 0.0000000000000000 0.0477399999999975 F F F

0.0000000000000000	0.2535600000000002	0.0477399999999975	F	F	F
0.5000000000000000	0.0000000000000000	0.1400099999999966	F	F	F
0.7464400000000069	0.0000000000000000	0.0477399999999975	F	F	F
0.5000000000000000	0.2563999999999993	0.0477399999999975	F	F	F
0.0000000000000000	0.5000000000000000	0.1400099999999966	F	F	F
0.2563999999999993	0.5000000000000000	0.0477399999999975	F	F	F
0.0000000000000000	0.7464400000000069	0.0477399999999975	F	F	F
0.5000000000000000	0.5000000000000000	0.1389500000000012	F	F	F
0.7436000000000007	0.5000000000000000	0.0477399999999975	F	F	F
0.5000000000000000	0.7436000000000007	0.0477399999999975	F	F	F
0.0000566457580149	0.9975886671676335	0.2358332665394940	F	F	F
0.5001402666856620	0.9988733650866095	0.2343891764315416	F	F	F
0.0000200619982209	0.4989009996484981	0.2344970272929388	F	F	F
0.5001063498665843	0.4997670324161305	0.2338022247962854	F	F	F
0.0000000000000000	0.0000000000000000	0.0477399999999975	F	F	F
0.5000000000000000	0.0000000000000000	0.0477399999999975	F	F	F
0.0000000000000000	0.5000000000000000	0.0477399999999975	F	F	F
0.5000000000000000	0.5000000000000000	0.0477399999999975	F	F	F
0.2729947436503934	0.2561616007018870	0.3201932696243972	F	F	F
0.7286637919628944	0.2567249949109396	0.3201038162438152	F	F	F
0.2574222327775857	0.7378448148285344	0.3191346184920434	F	F	F
0.7422703106567425	0.7383693746643445	0.3191847239101619	F	F	F
0.2583600000000033	0.2583600000000033	0.1382199999999969	F	F	F
0.7416400000000039	0.2583600000000033	0.1382199999999969	F	F	F
0.2583600000000033	0.7416400000000039	0.1382199999999969	F	F	F
0.7416400000000039	0.7416400000000039	0.1382199999999969	F	F	F
0.0030714256150333	0.2675127984480383	0.4015820186997843	T	T	T

0.0011127098004948	0.3804864326493700	0.3692117138889870	T	T	T
0.0011510168849185	0.1538490202693268	0.3790648457160924	T	T	T