

Electronic Supplementary Information

**First-Principles Studies of Oxide Ion Migration Behavior for Different
Valence B-site Ions Doped SrFeO_{3-δ} Ceramic Membrane[†]**

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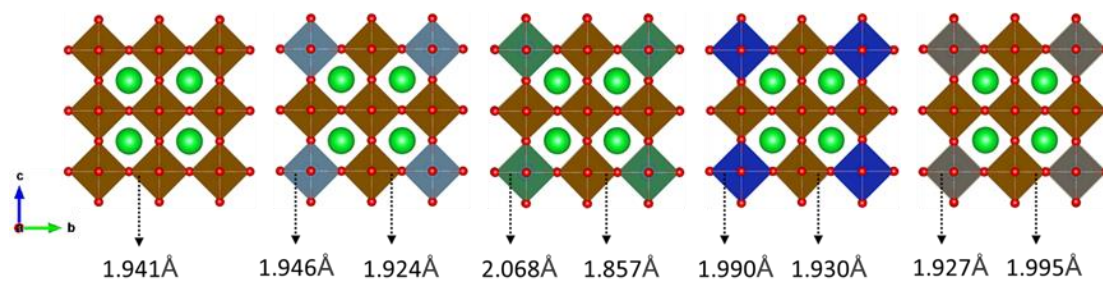


Figure S1. DFT-calculated Fe-O and M-O (M= Al, Zr, Nb, W) bond lengths for (a) $\text{Sr}_8\text{Fe}_8\text{O}_{24}$, (b) $\text{Sr}_8\text{Fe}_7\text{Al}_1\text{O}_{24}$, (c) $\text{Sr}_8\text{Fe}_7\text{Zr}_1\text{O}_{24}$, (d) $\text{Sr}_8\text{Fe}_7\text{Nb}_1\text{O}_{24}$ and (e) $\text{Sr}_8\text{Fe}_7\text{W}_1\text{O}_{24}$.

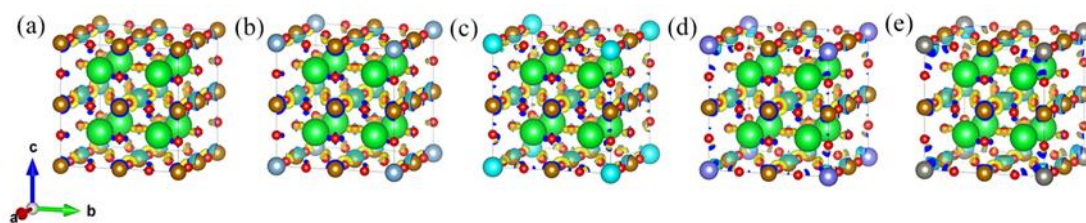


Figure S2. Charge density difference (CDD) configurations for (a) $\text{Sr}_8\text{Fe}_8\text{O}_{24}$, (b) $\text{Sr}_8\text{Fe}_7\text{Al}_1\text{O}_{24}$, (c) $\text{Sr}_8\text{Fe}_7\text{Zr}_1\text{O}_{24}$, (d) $\text{Sr}_8\text{Fe}_7\text{Nb}_1\text{O}_{24}$ and (e) $\text{Sr}_8\text{Fe}_7\text{W}_1\text{O}_{24}$. The yellow region represents electron accumulation and the blue region represents electron depletion.

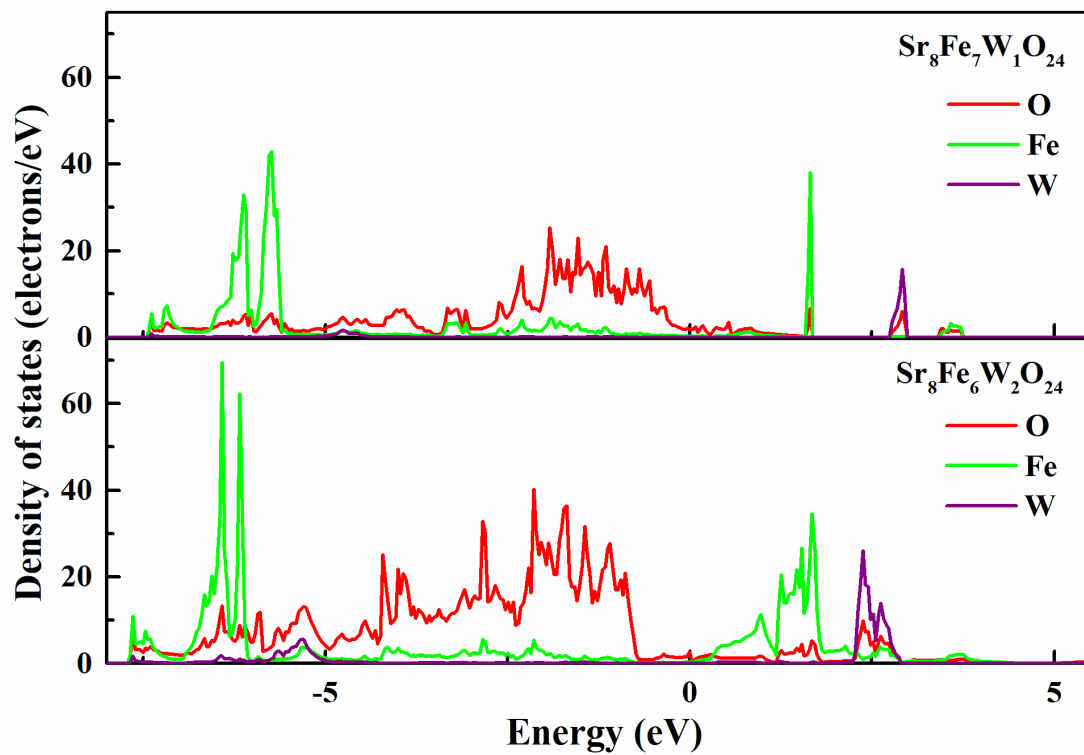


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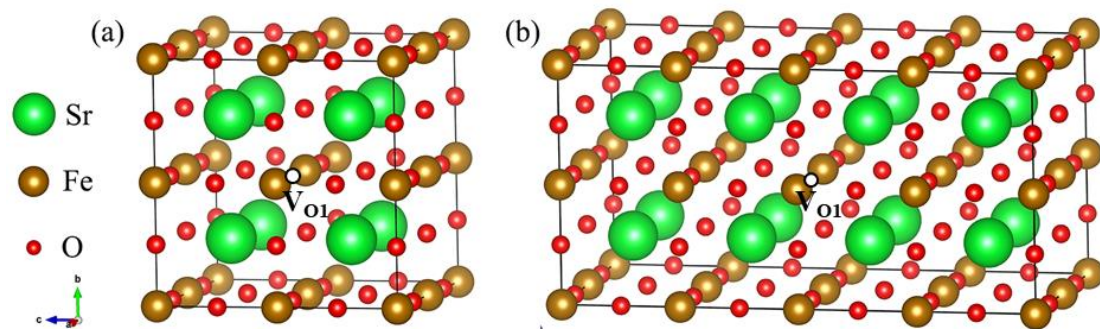


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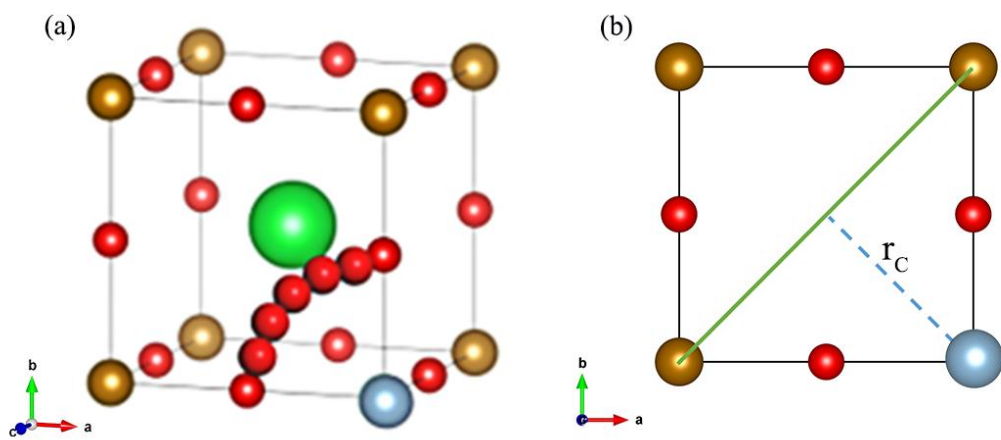


Figure S5. Schematic diagrams of (a) the oxygen migration path in $\text{SrFe}_{0.875}\text{Mo}_{0.125}\text{O}_3$ through the (b) bottleneck of triangle composed by B-site (Al^{3+} , Zr^{4+} , Nb^{5+} and W^{6+}) and two Fe cations.

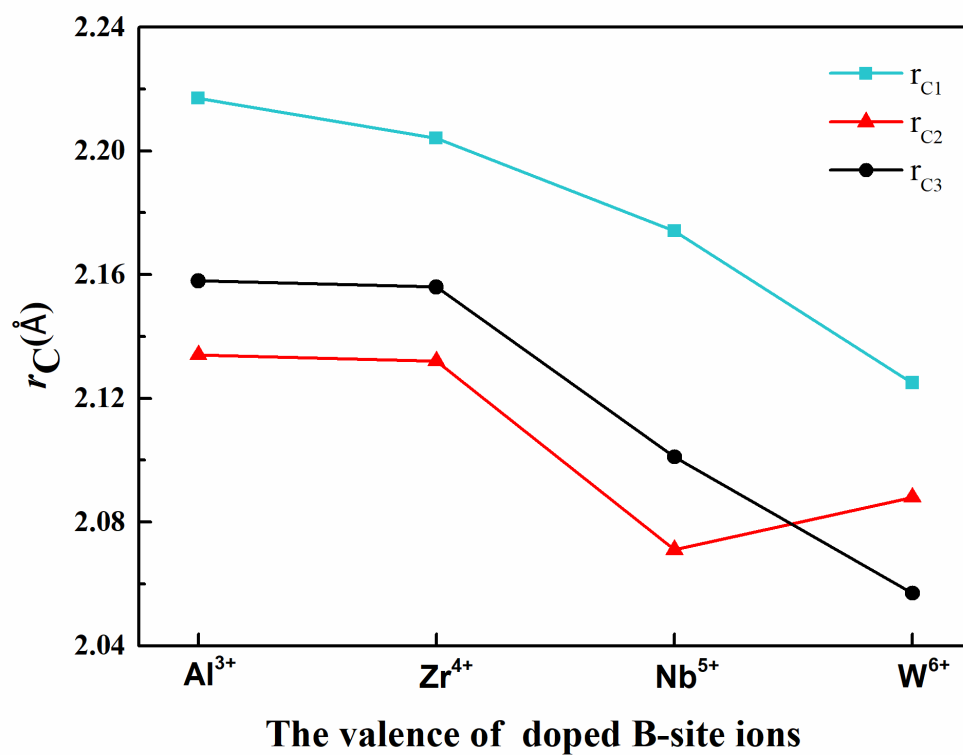


Figure S6. Variations of critical radii r_C in Figure S3 (b) with different B-site ions.

Table S1. Oxygen ion migration energy barriers for different paths in Sr₈Fe₇Al₁O₂₃.

	Migration barrier energy[eV]		
	V _{O1}	V _{O2}	V _{O3}
V _{O1}	0.56	0.87	
V _{O2}	0.86	0.66	0.59
V _{O3}		0.64	1.59

Table S2. Oxygen ion migration energy barriers for different paths in Sr₈Fe₇Zr₁O₂₃.

	Migration barrier energy[eV]		
	V _{O1}	V _{O2}	V _{O3}
V _{O1}	1.67		
V _{O2}	0.34	0.49	
V _{O3}		0.70	0.64

Table S3. Oxygen ion migration energy barriers for different paths in $\text{Sr}_8\text{Fe}_7\text{Nb}_1\text{O}_{23}$.

	Migration barrier energy[eV]		
	V_{O1}	V_{O2}	V_{O3}
V_{O1}	1.02		
V_{O2}	0.21	0.59	
V_{O3}		0.58	0.38

Table S4. Oxygen ion migration energy barriers for different paths in $\text{Sr}_8\text{Fe}_7\text{W}_1\text{O}_{23}$.

	Migration barrier energy[eV]		
	V_{O1}	V_{O2}	V_{O3}
V_{O1}	0.73		
V_{O2}	0.27	0.52	
V_{O3}		0.61	0.24

Table S5. The distances of M–O (Fe–O) and O–Fe in the M–O–Fe (Fe–O–Fe) chains.

Distances	Before Doping	After Doping			
	Relaxed	M=Al	M=Zr	M=Nb	M=W
M-O1	-	1.946	2.068	1.990	1.927
O1-Fe1	1.941	1.924	1.857	1.930	1.995
Fe1-O2	1.941	1.947	1.993	1.999	1.989
O2-Fe2	1.941	1.923	1.932	1.921	1.933
Fe2-O3	1.941	1.930	1.975	1.977	2.011
O3-Fe3	1.941	1.940	1.949	1.942	1.911

Table S6. Fractional coordinates of the relaxed Sr₈Fe₈O₂₄.

O Fe Sr

1.0000000000000000		
7.7625010644869574	-0.0000000000000000	0.0000000000000000
0.0000000000000000	7.7625010644869574	-0.0000000000000000
0.0000000000000000	0.0000000000000000	7.7625010644869574

O	Fe	Sr
24	8	8

Direct

-0.0000000000000000	-0.0000000000000000	0.2500000000000000
0.2500000000000000	-0.0000000000000000	-0.0000000000000000
0.0000000000000000	0.2500000000000000	0.0000000000000000
0.5000000000000000	0.0000000000000000	0.2500000000000000
0.7500000000000000	0.0000000000000000	-0.0000000000000000
0.5000000000000000	0.2500000000000000	0.0000000000000000
-0.0000000000000000	0.5000000000000000	0.2500000000000000
0.2500000000000000	0.5000000000000000	-0.0000000000000000
0.0000000000000000	0.7500000000000000	-0.0000000000000000
0.5000000000000000	0.5000000000000000	0.2500000000000000
0.7500000000000000	0.5000000000000000	0.0000000000000000
0.5000000000000000	0.7500000000000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	0.7500000000000000
0.2500000000000000	-0.0000000000000000	0.5000000000000000
-0.0000000000000000	0.2500000000000000	0.5000000000000000
0.5000000000000000	-0.0000000000000000	0.7500000000000000
0.7500000000000000	-0.0000000000000000	0.5000000000000000
0.5000000000000000	0.2500000000000000	0.5000000000000000
-0.0000000000000000	0.5000000000000000	0.7500000000000000
0.2500000000000000	0.5000000000000000	0.5000000000000000
-0.0000000000000000	0.7500000000000000	0.5000000000000000
0.5000000000000000	0.5000000000000000	0.7500000000000000
0.7500000000000000	0.5000000000000000	0.5000000000000000
0.5000000000000000	0.7500000000000000	0.5000000000000000
-0.0000000000000000	-0.0000000000000000	0.0000000000000000
0.5000000000000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	0.5000000000000000	-0.0000000000000000

0.5000000000000000	0.5000000000000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	0.5000000000000000
0.5000000000000000	-0.0000000000000000	0.5000000000000000
0.0000000000000000	0.5000000000000000	0.5000000000000000
0.5000000000000000	0.5000000000000000	0.5000000000000000
0.2500000000000000	0.2500000000000000	0.2500000000000000
0.7500000000000000	0.2500000000000000	0.2500000000000000
0.2500000000000000	0.7500000000000000	0.2500000000000000
0.7500000000000000	0.7500000000000000	0.2500000000000000
0.2500000000000000	0.2500000000000000	0.7500000000000000
0.7500000000000000	0.2500000000000000	0.7500000000000000
0.2500000000000000	0.7500000000000000	0.7500000000000000
0.7500000000000000	0.7500000000000000	0.7500000000000000

Table S7. Fractional coordinates of the relaxed Sr₈Fe₇Al₁O₂₄.

O Al Fe Sr

1.0000000000000000			
7.7388319306714317	0.0000000000000000	-0.0000000000000000	
0.0000000000000000	7.7388319306714317	-0.0000000000000000	
0.0000000000000000	0.0000000000000000	7.7388319306714317	

O	Al	Fe	Sr
24	1	7	8

Direct

0.0000000000000000	-0.0000000000000000	0.2513995560054657
0.2513995560054657	-0.0000000000000000	0.0000000000000000
0.0000000000000000	0.2513995560054657	0.0000000000000000
0.5000000000000000	-0.0000000000000000	0.2515380734888915
0.7486004439945345	-0.0000000000000000	0.0000000000000000
0.5000000000000000	0.2515380734888915	0.0000000000000000
0.0000000000000000	0.5000000000000000	0.2515380734888915
0.2515380734888915	0.5000000000000000	0.0000000000000000
0.0000000000000000	0.7486004439945345	0.0000000000000000
0.5000000000000000	0.5000000000000000	0.2493686298125531
0.7484619265111085	0.5000000000000000	0.0000000000000000
0.5000000000000000	0.7484619265111085	0.0000000000000000
0.0000000000000000	-0.0000000000000000	0.7486004439945345
0.2515380734888915	-0.0000000000000000	0.5000000000000000
0.0000000000000000	0.2515380734888915	0.5000000000000000
0.5000000000000000	-0.0000000000000000	0.7484619265111085
0.7484619265111085	-0.0000000000000000	0.5000000000000000
0.5000000000000000	0.2493686298125531	0.5000000000000000
0.0000000000000000	0.5000000000000000	0.7484619265111085
0.2493686298125531	0.5000000000000000	0.5000000000000000
0.0000000000000000	0.7484619265111085	0.5000000000000000

0.5000000000000000	0.5000000000000000	0.7506313701874469
0.7506313701874469	0.5000000000000000	0.5000000000000000
0.5000000000000000	0.7506313701874469	0.5000000000000000
0.0000000000000000	-0.0000000000000000	0.0000000000000000
0.5000000000000000	-0.0000000000000000	0.0000000000000000
0.0000000000000000	0.5000000000000000	0.0000000000000000
0.5000000000000000	0.5000000000000000	0.0000000000000000
0.0000000000000000	-0.0000000000000000	0.5000000000000000
0.5000000000000000	-0.0000000000000000	0.5000000000000000
0.0000000000000000	0.5000000000000000	0.5000000000000000
0.5000000000000000	0.5000000000000000	0.5000000000000000
0.2492270125558686	0.2492270125558686	0.2492270125558686
0.7507729874441313	0.2492270125558686	0.2492270125558686
0.2492270125558686	0.7507729874441313	0.2492270125558686
0.7507729874441313	0.7507729874441313	0.2492270125558686
0.2492270125558686	0.2492270125558686	0.7507729874441313
0.7507729874441313	0.2492270125558686	0.7507729874441313
0.2492270125558686	0.7507729874441313	0.7507729874441313
0.7507729874441313	0.7507729874441313	0.7507729874441313

Table S8. Fractional coordinates of the relaxed Sr₈Fe₇Zr₁O₂₄.

O Zr Fe Sr

1.0000000000000000			
7.8491345594602393	0.0000000000000000	0.0000000000000000	
-0.0000000000000000	7.8491345594602393	0.0000000000000000	
0.0000000000000000	-0.0000000000000000	7.8491345594602393	

O	Zr	Fe	Sr
24	1	7	8

Direct

-0.0000000000000000	-0.0000000000000000	0.2634298396077951	
0.2634298396077951	-0.0000000000000000	0.0000000000000000	
-0.0000000000000000	0.2634298396077951	0.0000000000000000	
0.5000000000000000	-0.0000000000000000	0.2538558604298679	
0.7365701603922046	-0.0000000000000000	0.0000000000000000	
0.5000000000000000	0.2538558604298679	0.0000000000000000	
-0.0000000000000000	0.5000000000000000	0.2538558604298679	
0.2538558604298679	0.5000000000000000	0.0000000000000000	
-0.0000000000000000	0.7365701603922046	0.0000000000000000	
0.5000000000000000	0.5000000000000000	0.2516575356663439	
0.7461441395701319	0.5000000000000000	0.0000000000000000	
0.5000000000000000	0.7461441395701319	0.0000000000000000	
-0.0000000000000000	-0.0000000000000000	0.7365701603922046	
0.2538558604298679	-0.0000000000000000	0.5000000000000000	
-0.0000000000000000	0.2538558604298679	0.5000000000000000	
0.5000000000000000	-0.0000000000000000	0.7461441395701319	
0.7461441395701319	-0.0000000000000000	0.5000000000000000	
0.5000000000000000	0.2516575356663439	0.5000000000000000	
-0.0000000000000000	0.5000000000000000	0.7461441395701319	
0.2516575356663439	0.5000000000000000	0.5000000000000000	
-0.0000000000000000	0.7461441395701319	0.5000000000000000	
0.5000000000000000	0.5000000000000000	0.7483424643336563	
0.7483424643336563	0.5000000000000000	0.5000000000000000	
0.5000000000000000	0.7483424643336563	0.5000000000000000	
-0.0000000000000000	-0.0000000000000000	0.0000000000000000	
0.5000000000000000	-0.0000000000000000	0.0000000000000000	
-0.0000000000000000	0.5000000000000000	0.0000000000000000	

0.5000000000000000	0.5000000000000000	0.0000000000000000
-0.0000000000000000	-0.0000000000000000	0.5000000000000000
0.5000000000000000	-0.0000000000000000	0.5000000000000000
-0.0000000000000000	0.5000000000000000	0.5000000000000000
0.5000000000000000	0.5000000000000000	0.5000000000000000
0.2566149719060321	0.2566149719060321	0.2566149719060321
0.7433850280939681	0.2566149719060321	0.2566149719060321
0.2566149719060321	0.7433850280939681	0.2566149719060321
0.7433850280939681	0.7433850280939681	0.2566149719060321
0.2566149719060321	0.2566149719060321	0.7433850280939681
0.7433850280939681	0.2566149719060321	0.7433850280939681
0.2566149719060321	0.7433850280939681	0.7433850280939681
0.7433850280939681	0.7433850280939681	0.7433850280939681

Table S9. Fractional coordinates of the relaxed Sr₈Fe₇Nb₁O₂₄.

O Nb Fe Sr

1.0000000000000000			
7.8395231636874918	0.0000000000000000	-0.0000000000000000	
0.0000000000000000	7.8395231636874918	-0.0000000000000000	
0.0000000000000000	0.0000000000000000	7.8395231636874918	

O	Nb	Fe	Sr
24	1	7	8

Direct

-0.0000000000000000	-0.0000000000000000	0.2537930453324826	
0.2537930453324826	-0.0000000000000000	-0.0000000000000000	
-0.0000000000000000	0.2537930453324826	-0.0000000000000000	
0.5000000000000000	-0.0000000000000000	0.2549284135125895	
0.7462069546675173	-0.0000000000000000	-0.0000000000000000	
0.5000000000000000	0.2549284135125895	-0.0000000000000000	
-0.0000000000000000	0.5000000000000000	0.2549284135125895	
0.2549284135125895	0.5000000000000000	-0.0000000000000000	
-0.0000000000000000	0.7462069546675173	-0.0000000000000000	
0.5000000000000000	0.5000000000000000	0.2522424467565099	
0.7450715864874107	0.5000000000000000	-0.0000000000000000	
0.5000000000000000	0.7450715864874107	-0.0000000000000000	
-0.0000000000000000	-0.0000000000000000	0.7462069546675173	
0.2549284135125895	-0.0000000000000000	0.5000000000000000	
-0.0000000000000000	0.2549284135125895	0.5000000000000000	
0.5000000000000000	-0.0000000000000000	0.7450715864874107	
0.7450715864874107	-0.0000000000000000	0.5000000000000000	
0.5000000000000000	0.2522424467565099	0.5000000000000000	
-0.0000000000000000	0.5000000000000000	0.7450715864874107	
0.2522424467565099	0.5000000000000000	0.5000000000000000	
-0.0000000000000000	0.7450715864874107	0.5000000000000000	
0.5000000000000000	0.5000000000000000	0.7477575532434901	
0.7477575532434901	0.5000000000000000	0.5000000000000000	
0.5000000000000000	0.7477575532434901	0.5000000000000000	
-0.0000000000000000	-0.0000000000000000	-0.0000000000000000	
0.5000000000000000	-0.0000000000000000	-0.0000000000000000	
-0.0000000000000000	0.5000000000000000	-0.0000000000000000	

0.5000000000000000	0.5000000000000000	-0.0000000000000000
-0.0000000000000000	-0.0000000000000000	0.5000000000000000
0.5000000000000000	-0.0000000000000000	0.5000000000000000
-0.0000000000000000	0.5000000000000000	0.5000000000000000
0.5000000000000000	0.5000000000000000	0.5000000000000000
0.2562037181380474	0.2562037181380474	0.2562037181380474
0.7437962818619525	0.2562037181380474	0.2562037181380474
0.2562037181380474	0.7437962818619525	0.2562037181380474
0.7437962818619525	0.7437962818619525	0.2562037181380474
0.2562037181380474	0.2562037181380474	0.7437962818619525
0.7437962818619525	0.2562037181380474	0.7437962818619525
0.2562037181380474	0.7437962818619525	0.7437962818619525
0.7437962818619525	0.7437962818619525	0.7437962818619525

Table S10. Fractional coordinates of the relaxed Sr₈Fe₇W₁O₂₄.

O W Fe Sr

1.0000000000000000			
7.8438174341545617	0.0000000000000000	-0.0000000000000000	
0.0000000000000000	7.8438174341545617	-0.0000000000000000	
0.0000000000000000	0.0000000000000000	7.8438174341545617	

O	W	Fe	Sr
24	1	7	8

Direct

-0.0000000000000000	0.0000000000000000	0.2457004434036427	
0.2457004434036427	0.0000000000000000	0.0000000000000000	
-0.0000000000000000	0.2457004434036427	0.0000000000000000	
0.5000000000000000	0.0000000000000000	0.2535573355128342	
0.7542995565963573	0.0000000000000000	0.0000000000000000	
0.5000000000000000	0.2535573355128342	0.0000000000000000	
-0.0000000000000000	0.5000000000000000	0.2535573355128342	
0.2535573355128342	0.5000000000000000	0.0000000000000000	
-0.0000000000000000	0.7542995565963573	0.0000000000000000	
0.5000000000000000	0.5000000000000000	0.2563959370863749	
0.7464426644871659	0.5000000000000000	0.0000000000000000	
0.5000000000000000	0.7464426644871659	0.0000000000000000	
-0.0000000000000000	0.0000000000000000	0.7542995565963573	
0.2535573355128342	0.0000000000000000	0.5000000000000000	
-0.0000000000000000	0.2535573355128342	0.5000000000000000	
0.5000000000000000	0.0000000000000000	0.7464426644871659	
0.7464426644871659	0.0000000000000000	0.5000000000000000	
0.5000000000000000	0.2563959370863749	0.5000000000000000	
-0.0000000000000000	0.5000000000000000	0.7464426644871659	
0.2563959370863749	0.5000000000000000	0.5000000000000000	
-0.0000000000000000	0.7464426644871659	0.5000000000000000	
0.5000000000000000	0.5000000000000000	0.7436040629136250	
0.7436040629136250	0.5000000000000000	0.5000000000000000	
0.5000000000000000	0.7436040629136250	0.5000000000000000	
-0.0000000000000000	0.0000000000000000	0.0000000000000000	
0.5000000000000000	0.0000000000000000	0.0000000000000000	
-0.0000000000000000	0.5000000000000000	0.0000000000000000	

0.5000000000000000	0.5000000000000000	0.0000000000000000
-0.0000000000000000	0.0000000000000000	0.5000000000000000
0.5000000000000000	0.0000000000000000	0.5000000000000000
-0.0000000000000000	0.5000000000000000	0.5000000000000000
0.5000000000000000	0.5000000000000000	0.5000000000000000
0.2583571702964959	0.2583571702964959	0.2583571702964959
0.7416428297035039	0.2583571702964959	0.2583571702964959
0.2583571702964959	0.7416428297035039	0.2583571702964959
0.7416428297035039	0.7416428297035039	0.2583571702964959
0.2583571702964959	0.2583571702964959	0.7416428297035039
0.7416428297035039	0.2583571702964959	0.7416428297035039
0.2583571702964959	0.7416428297035039	0.7416428297035039
0.7416428297035039	0.7416428297035039	0.7416428297035039