Supporting Information for "Combined Density Functional Theory and Molecular Dynamics Study of $Sm_{0.75}A_{0.25}Co_{1-x}Mn_xO_{2.88}$ (A=Ca, Sr; x=0.125, 0.25) Cathode Materials for Next Generation Solid Oxide Fuel Cells"

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The supporting information contains the interatomic potential set used for the molecular dynamics simulations, the oxygen vacancy compensation scheme equation, dopant configuration selection and Boltzmann distributions, and a graphic description of the cobalt spin state.

INTERATOMIC POTENTIALS

Table S1. Interatomic potential parameters used for simulation of $Sm_{0.75}A_{0.25}Co_{1-x}Mn_xO_{2.88}$ (A=Ca, or Sr). Potential cutoff is 12 Å.

	Short range interactions				Shell Model		
Interaction	A (eV)	ρ (Å)	C (eVÅ^6)		Y (e)	k (eVÅ^{-2})	ref
Sm^{3+}-O^{2-}	1252.94	0.3590	0.00	**Sm^{3+}**	-0.250	173.90	1
Ca^{2+}-O^{2-}	1090.40	0.3437	0.00	**Ca^{2+}**	3.135	110.20	2
Sr^{2+}-O^{2-}	959.10	0.3721	0.00	**Sr^{2+}**	3.251	71.70	2
Co^{3+}-O^{2-}	1329.82	0.3087	0.00	**Co^{3+}**	2.040	196.30	3
Mn^{3+}-O^{2-}	1267.50	0.3214	0.00	**Mn^{3+}**	3.00	95.0	3
O^{2-}-O^{2-}	22764.30	0.1490	43.00	**O^{2-}**	-2.389	42.00	3

OXYGEN VACANCY COMPENSATION SCHEME

Upon doping $SmCoO_3$ with A^{2+} (A=Ca, or Sr), to conserve charge neutrality, an oxygen vacancy compensation takes place, according to equation S1 below in Kröger-Vink notation.[4]

$$2AO \xrightarrow{SmCoO_3} 2A'_{Sm} + 2O_O^x + V_O^{\cdot\cdot} \qquad \text{(S1)}$$

DOPANT CONFIGURATION

Table S2. All possible configurations and their relative energy to the lowest energy configuration. Numbering refers to geometries presented in figure S1-2.

	Ca		Sr	
Conf No	x=0.125	x=0.25	x=0.125	x=0.25
1	**0.00**	**0.00**	**0.00**	2.05
2	0.51	0.36	1.29	0.25
3	0.63	0.37	0.20	0.34
4		0.40		0.29
5		0.77		0.88
6		0.79		0.54
7		0.82		0.71
8		0.95		1.23
9		0.98		**0.00**
10		1.04		0.50
11		1.14		2.83
12		1.20		0.32
13		1.28		1.81
14		1.50		2.28
15		1.57		1.88
16		1.62		1.63
17		1.66		1.36
18		1.67		2.45
19		1.71		2.24
20		1.84		1.92
21		2.64		0.51
22		3.06		0.69
23		4.00		2.79

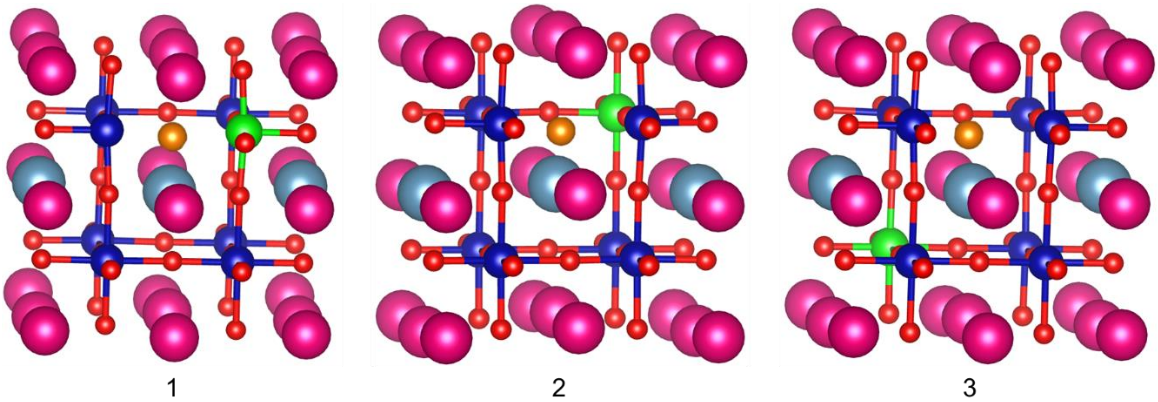
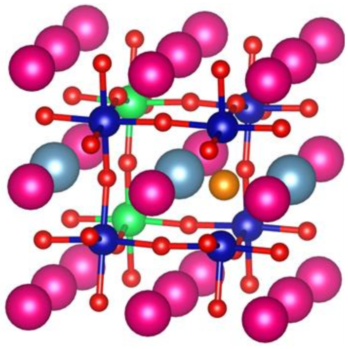


Figure S1. Different dopant configurations for $Sm_{0.75}A_{0.25}Co_{0.875}Mn_{0.125}O_{2.88}$ (A=Ca, or Sr). Orange sphere indicate vacancy position, and number refers to configuration number in Table S2. Sm is pink spheres, A grey, O red, Co blue, and Mn green, respectively.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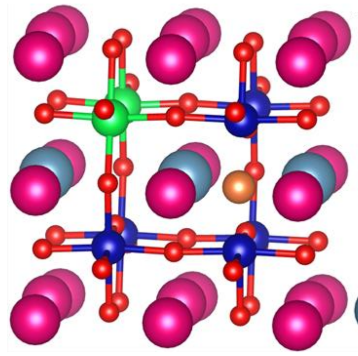
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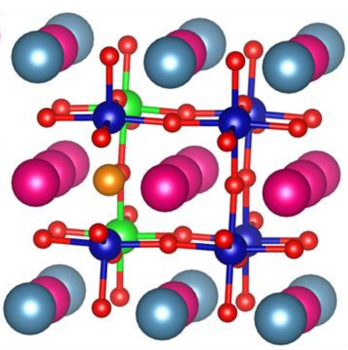
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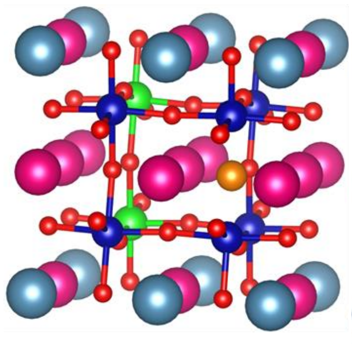
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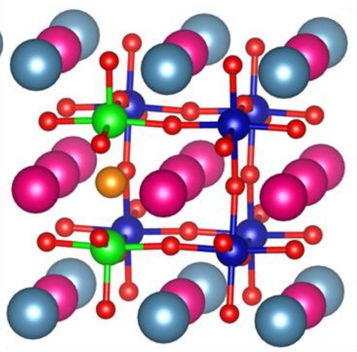
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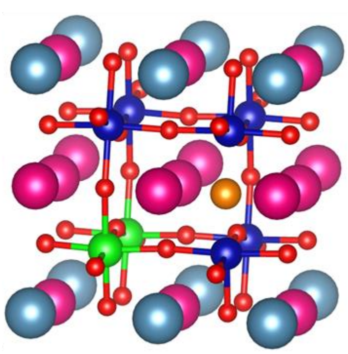
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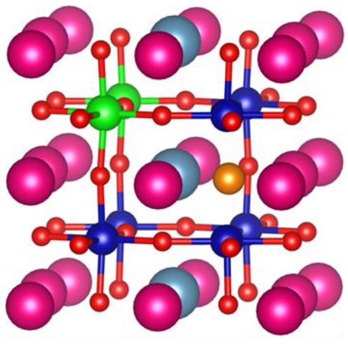
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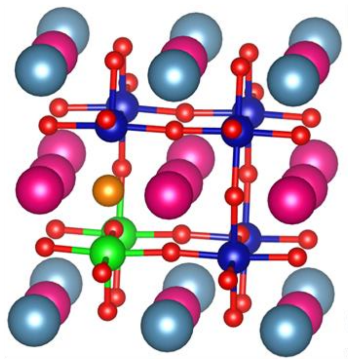
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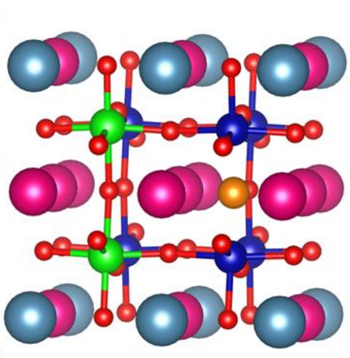
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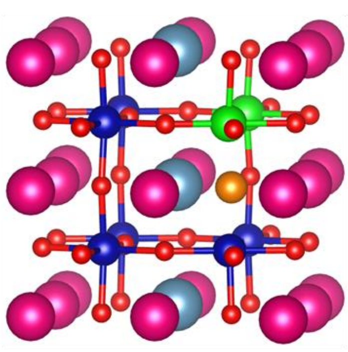
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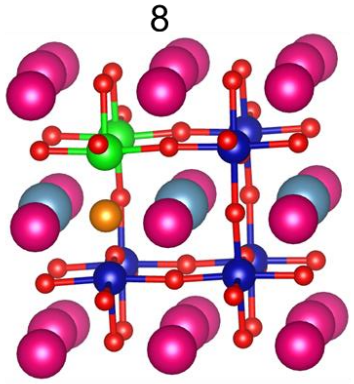
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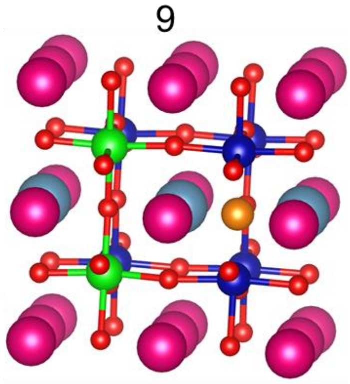
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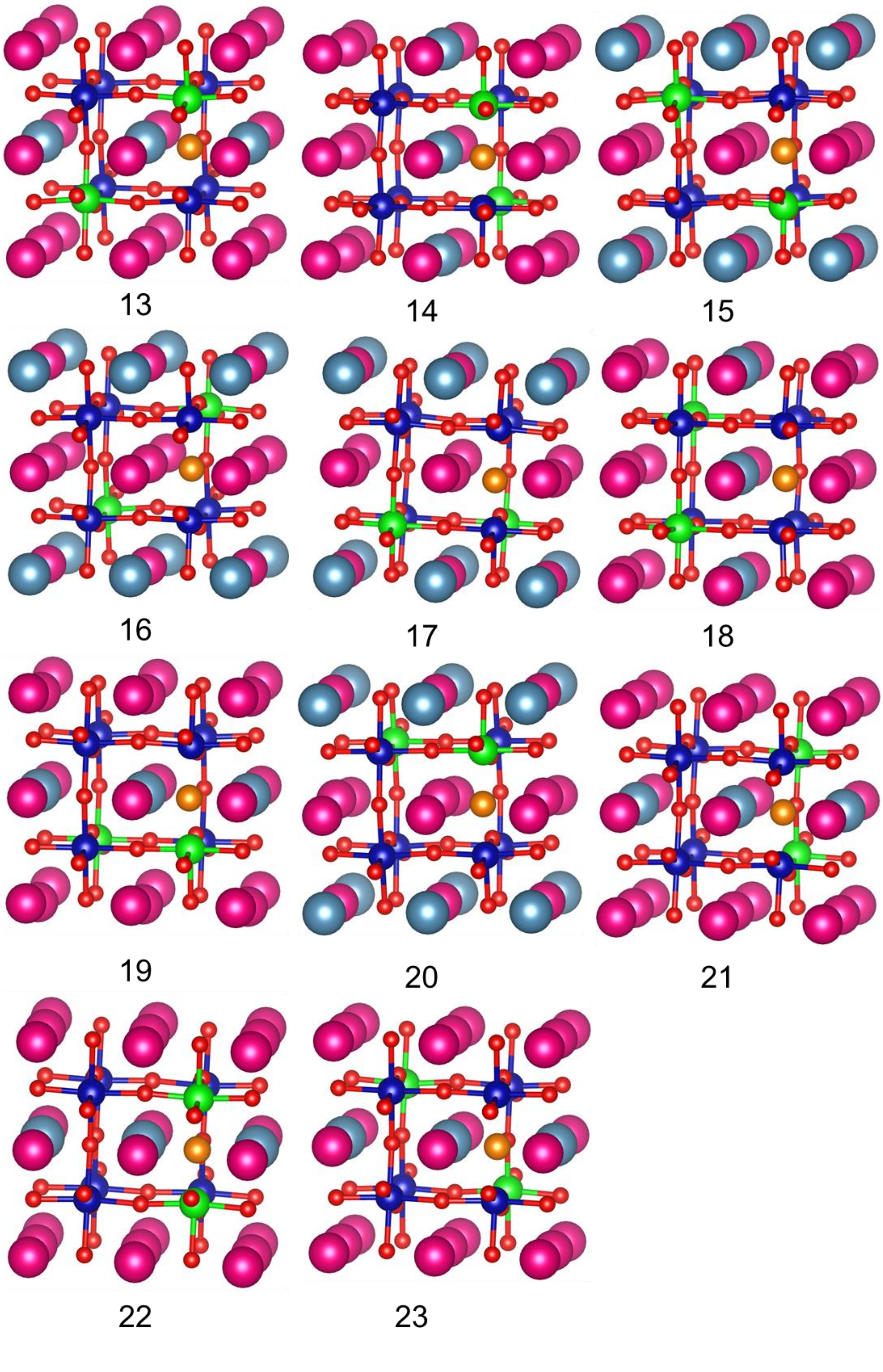

Figure S2. Different dopant configurations for $Sm_{0.75}A_{0.25}Co_{0.75}Mn_{0.25}O_{2.88}$ (A=Ca, or Sr). Orange sphere indicates vacancy position, and number refers to configuration number in Table S2. Sm are pink spheres, A grey, O red, Co blue, and Mn green, respectively.

BOLTZMANN DISTRIBUTION

Under thermodynamic equilibrium, the occurrence probability (P) of the different configurations (n) can be calculated, at each temperature T, as[5]

$$P_n = \frac{1}{Z}\exp(-E_n/k_B T)$$

$$Z = \sum_{n=1}^{N} P_n E_n$$

where Z is the partition function, k_B is Boltzmann's constant, and E_n the energy of configuration n.

COBALT SPIN STATE

Co^{3+} can exist in three different spin states; low spin state (LS, $t_{2g}^6 e_g^0$) with S = 0, intermediate spin state (IS, $t_{2g}^5 e_g^1$) with S = 1, and high spin state (HS, $t_{2g}^4 e_g^2$) with S = 2. These are shown schematically below.

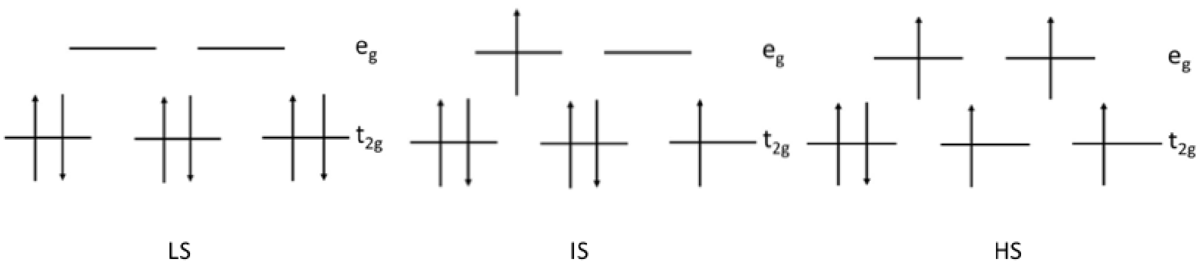

Figure S4. The different spin states of cobalt.

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