Table S1. Comparison of Buckingham pair potentials for Co^{3+}–O^{2-} in BSC.

Interaction	A_{ij}/ eV	ρ_{ij}/ Å	C_{ij}/ eV Å^6	Pseudo cubic lattice parameter a_p/ Å	MD stability	Reference
Co^{3+}–O^{2-}	1329.82	0.3087	0	3.766	Stable	[1-3]
Co^{3+}–O^{2-}	1007.11	0.3069	0	3.586	-	[4]
Co^{3+}–O^{2-}	1226.31	0.3087	0	3.712	-	[5]
Co^{3+}–O^{2-}	1371.71	0.3087	0	3.780	-	[5]
Co^{3+}–O^{2-}	1156.61	0.3087	0	3.679	-	[5]
Co^{3+}–O^{2-}	1006.61	0.3087	0	3.601	-	[5]
Co^{3+}–O^{2-}	1226.31	0.3087	0	3.915	Unstable	[5]
Sr^{2+}–O^{2-}	682.172	0.3945	0			[6]
Ba^{2+}–O^{2-}	905.7	0.3976	0			[7]
O^{2-}–O^{2-}	9597.96	0.2192	32.00			[5]

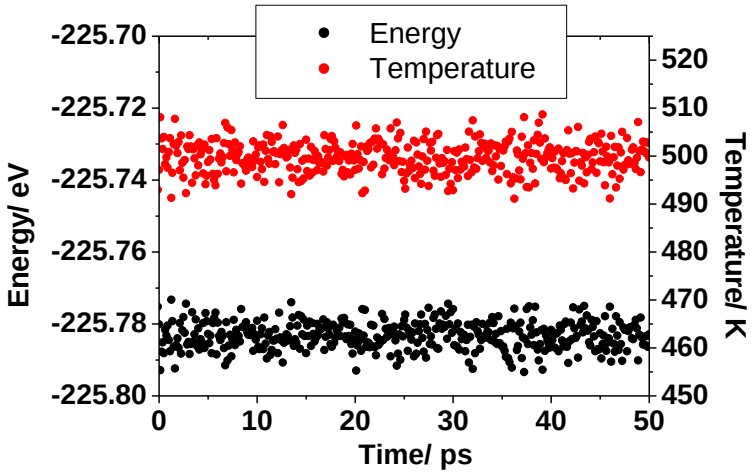

Fig. S1. Configurational energy and temperature for BSCF (d = 0.5) at 500 K as a function of time after 50 ps equilibration by MD simulation.

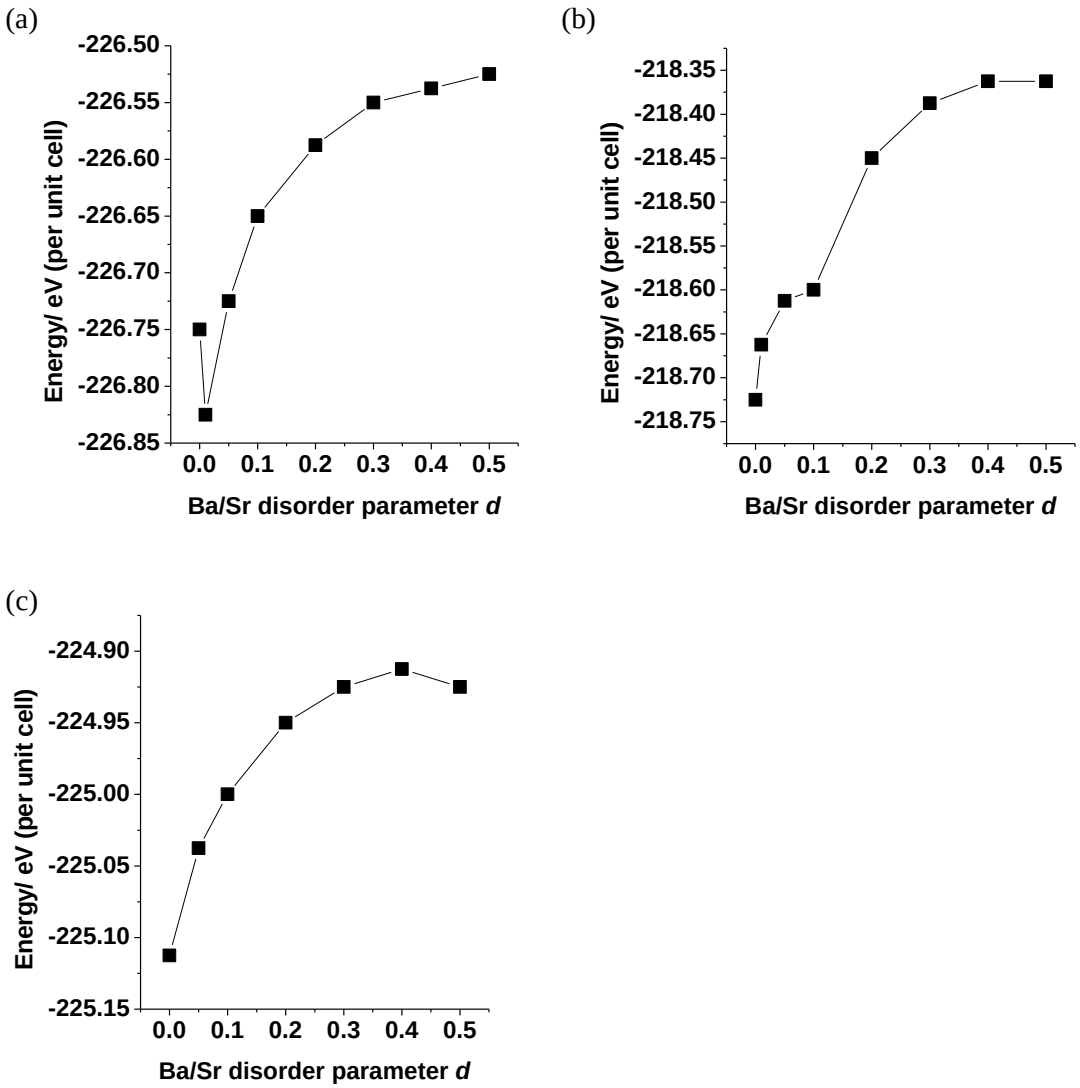

Fig. S2. Configurational energies for (a) BSC, (b) BSF and (c) BSCF as a function of Ba/Sr disorder parameter *d*. Energies were averaged during 50 ps of production run after equilibration at 1200 K by MD simulations.

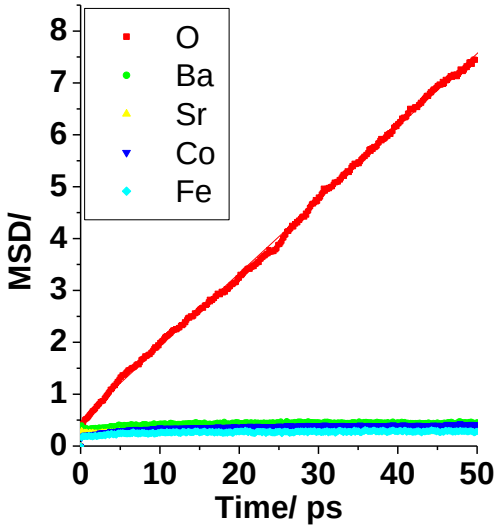

Fig. S3. Mean square displacements (MSDs) of ions in BSCF as a function of time at 2000 K.

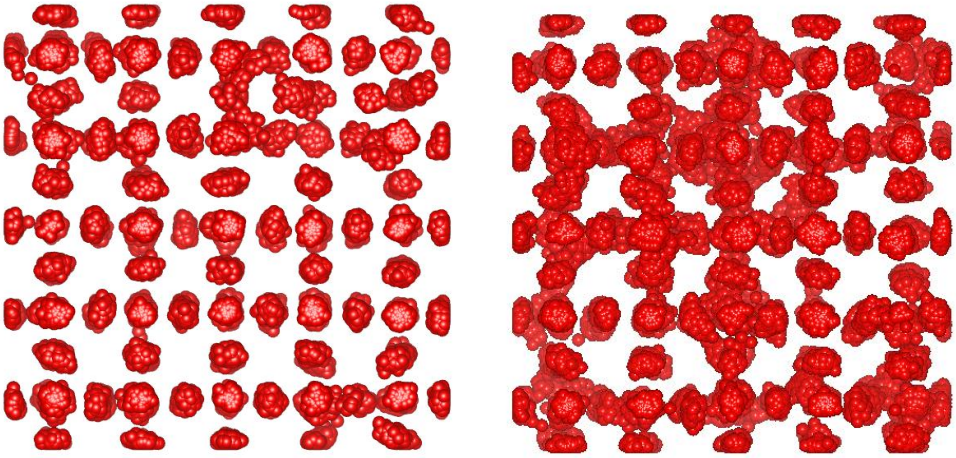

Fig. S4. Trajectories of oxygen atoms (red) in MD simulations for BSCF with ordered (d=0, left panel) and disordered (d=0.5, right panel) Ba/Sr arrangement at 1200 K. Both the figures were viewed along c-axis. Note that three oxygen layers, Ba-O, Sr-O, and TM-O_2 layers, are included. (See figure 1 in main text.)

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