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Supplementary information

Ab initio study of changing the oxygen reduction activity of Co – Fe-based perovskites by tuning the B-site composition

Ismail A. M. Ibrahim[a,b] and Chan-Yeup Chung[a]

[a]Division of Carbon Neutrality & Materials Digitalization, Korea Institute of Ceramic Engineering & Technology, Jinju 52851, South Korea.

[b]Department of Chemistry, Faculty of Science, Helwan University, 11795 Cairo, Egypt.

E-mail:

ibrahim@kicet.re.kr, ismail.ibrahim@science.helwan.edu.eg (Ismail Ibrahim)

chanyeup@kicet.re.kr (Chan-Yeup Chung)

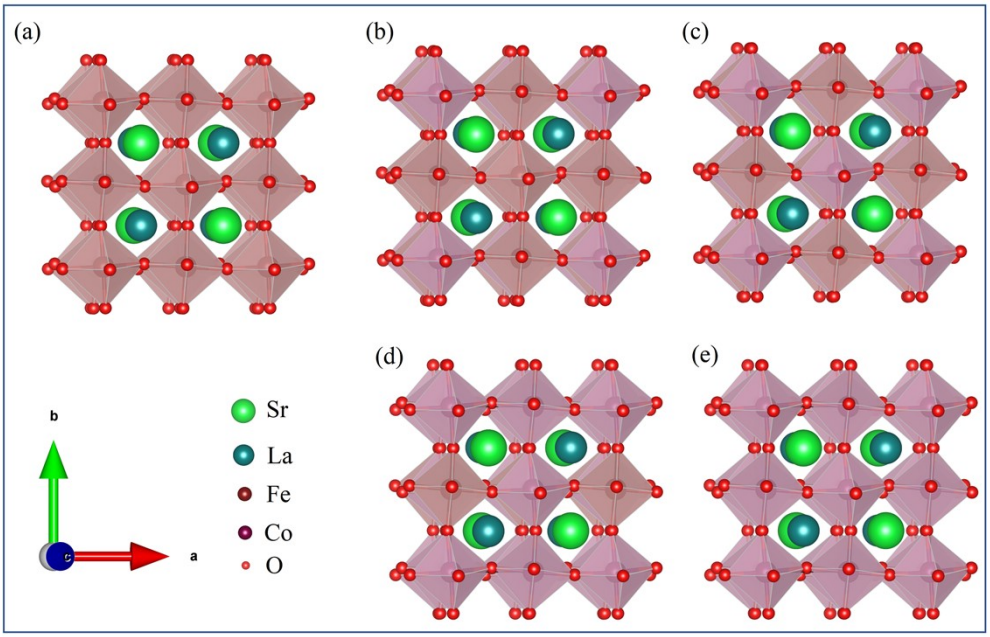

Figure S1: Optimized bulk structures of (a) LSF, (b) LSCF25, (c) LSCF50, (d) LSCF75, and (e) LSC.

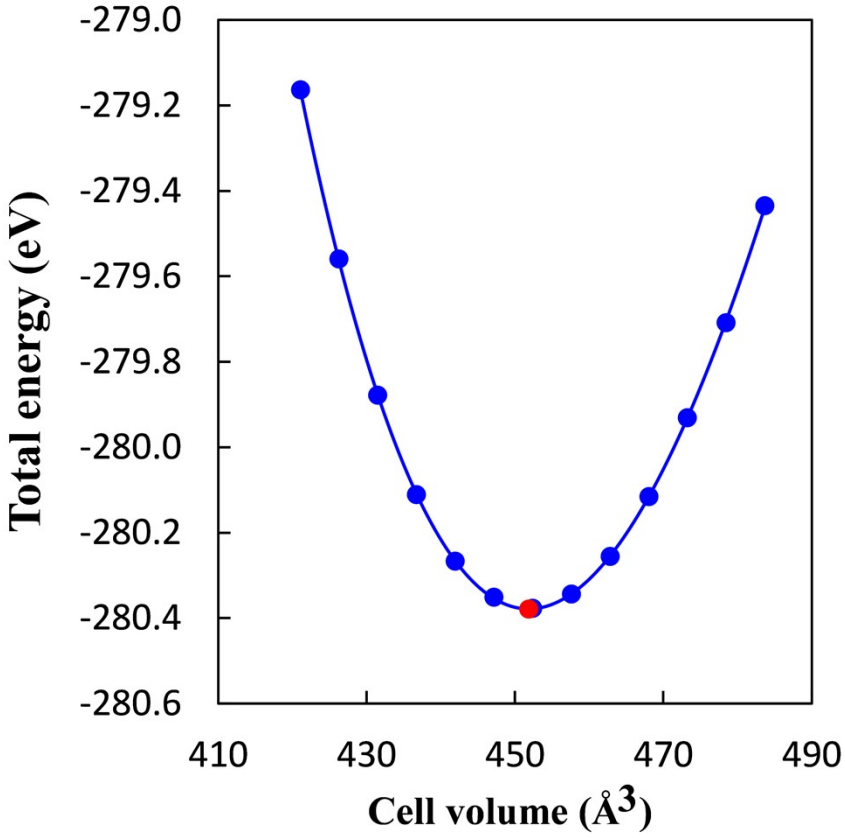

Figure S2: Total energy–Volume curve of LSC. The red ball represents the equilibrium volume obtained by the third-order Birch-Murnaghan equation of states.

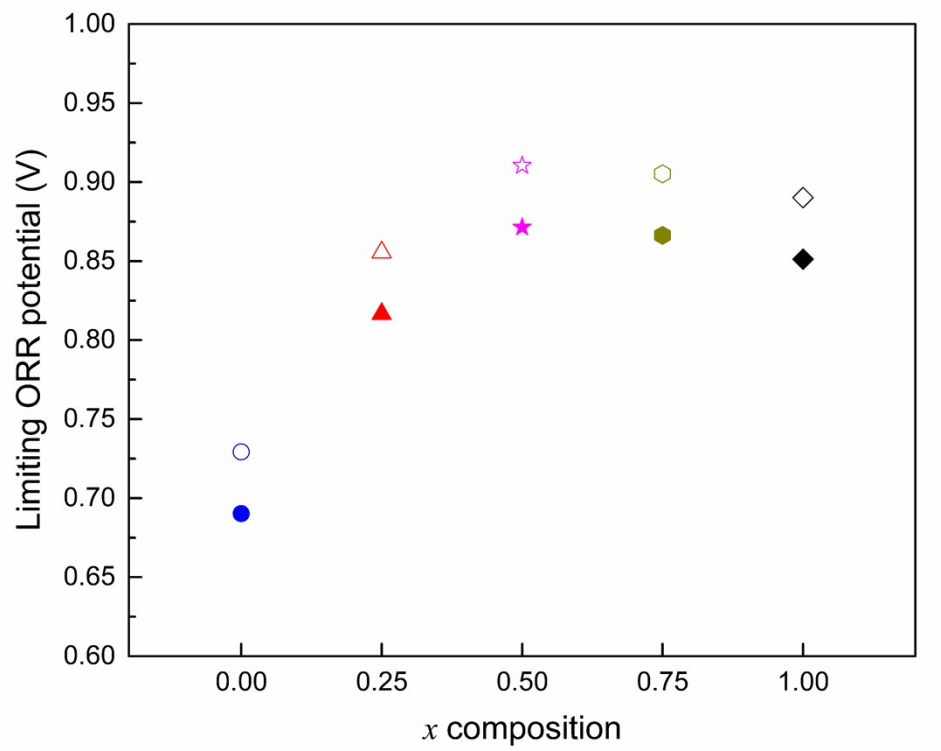

Figure S3: The limiting ORR potential as a function of the Co/Fe composition. The limiting potentials without[23] and with[45] including entropy corrections for the adsorbates are shown as full and empty symbols, respectively.

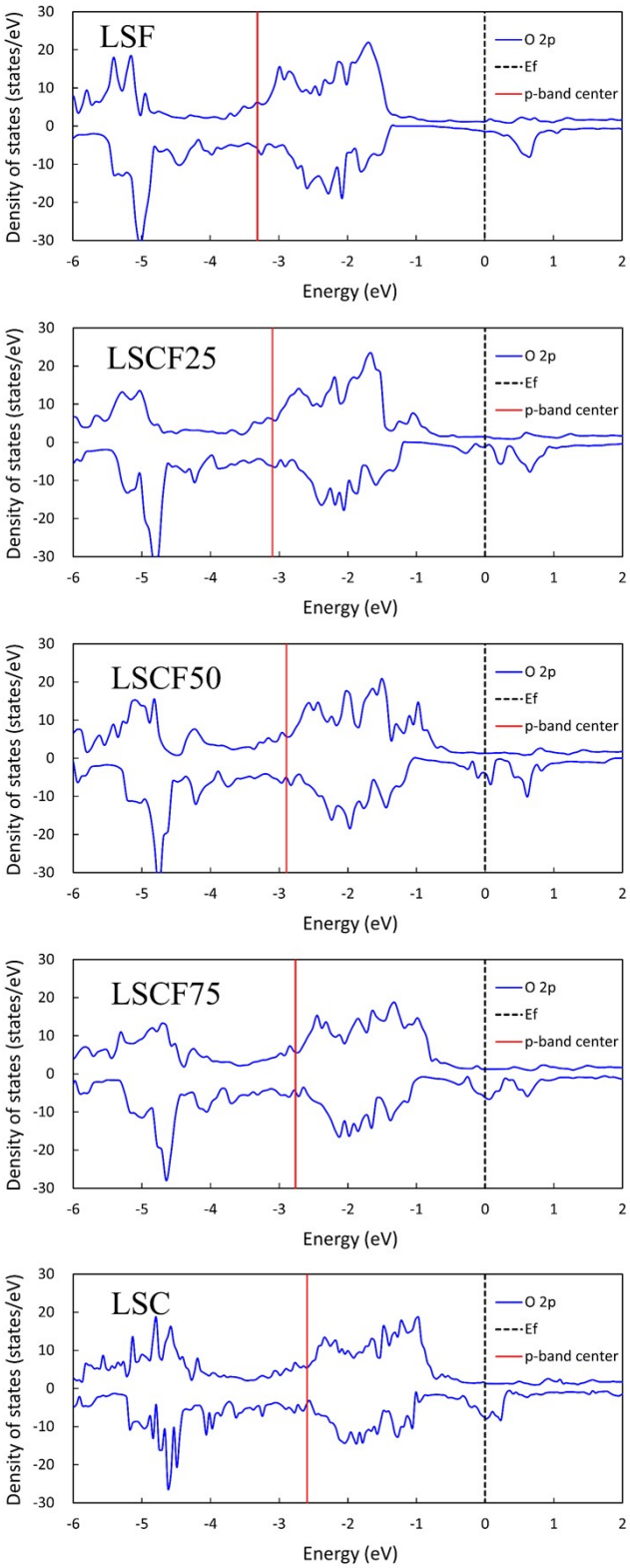

Figure S4: Partial density of states of bulk $La_{0.5}Sr_{0.5}Co_xFe_{1-x}O_3$ structures. Fermi level (E_f) is set at 0 eV.

Table S1: The optimized lattice constant (a) of $La_{0.5}Sr_{0.5}Co_xFe_{1-x}O_3$ perovskite supercells.

Perovskite	Lattice constant a (Å)
LSF	7.723
LSCF25	7.720
LSCF50	7.689
LSCF75	7.683
LSC	7.674

Table S2: Zero-point energy (ZPE) and entropy contribution (TS) of the gas phase and adsorbed species at T = 298 K. The entropy corrections for the adsorbates on the perovskite surface were considered as zero.[23]

Species	ZPE (eV)	TS (eV)
H_2	0.27	0.41
O_2	0.10	0.64
H_2O	0.57	0.67
O*	0.07	
OO*	0.14	
HO*	0.35	
HOO*	0.43	