Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

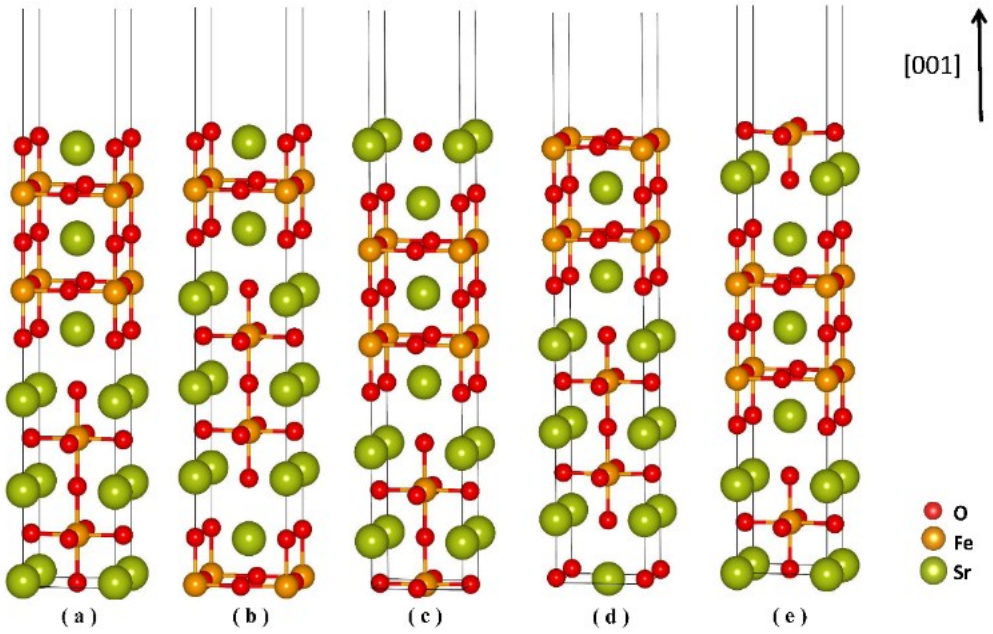

Figure S1 (a)SrO-1, (b)SrO-2, (c)SrO-3, (d) FeO-1 and (e) FeO-2 (001) terminal surfaces of $Sr_3Fe_2O_7$.

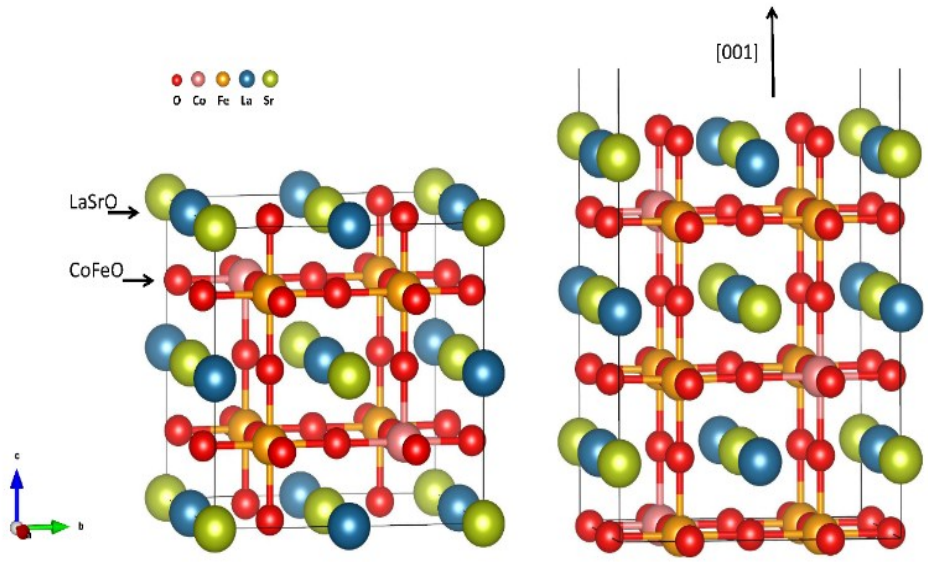

Figure S2 (left) The elementary LSCF crystal structure with 40 atoms. (right) Side views of the perfect LSCF (001) surface.

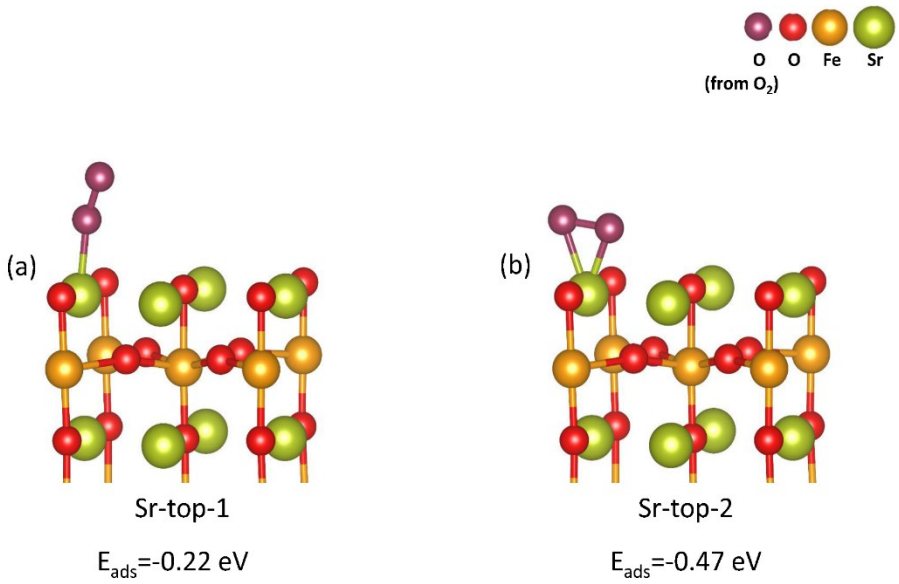

Figure S3 (left) The optimized O_2 adsorption structures on the SrO-terminated $Sr_3Fe_2O_7$ (001) surface.

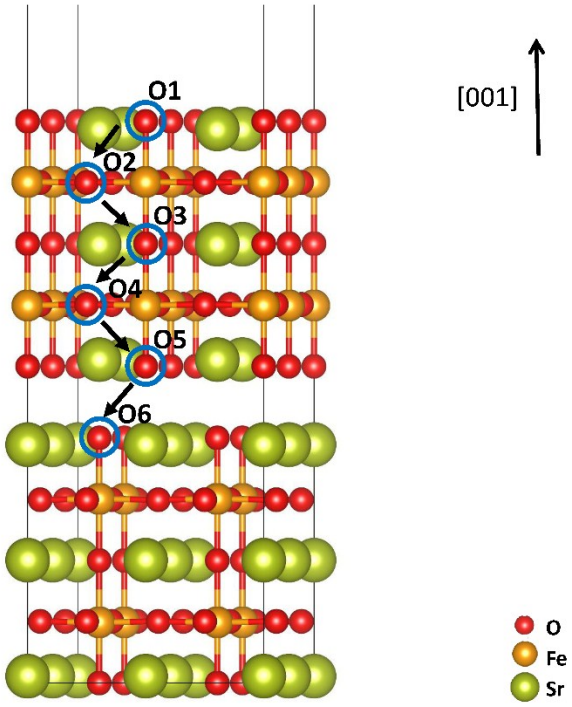

Figure S4 Migration paths of oxygen ions in the surface model of $Sr_3Fe_2O_7$, where O_n (n = 1, 2, 3, 4, 5, 6) denotes the sites of oxygen ions.

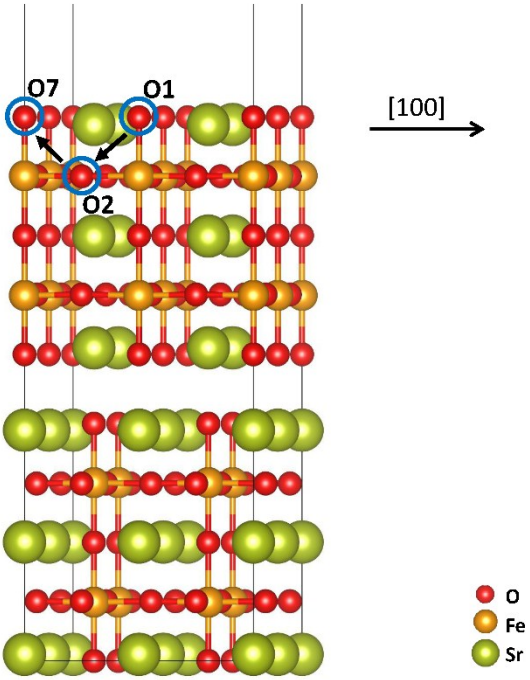

Figure S5 Migration path of oxygen ions along [100] direction in the surface model of $Sr_3Fe_2O_7$, where On (n = 1, 2, 3, 4, 5, 6) denotes the sites of oxygen ions.

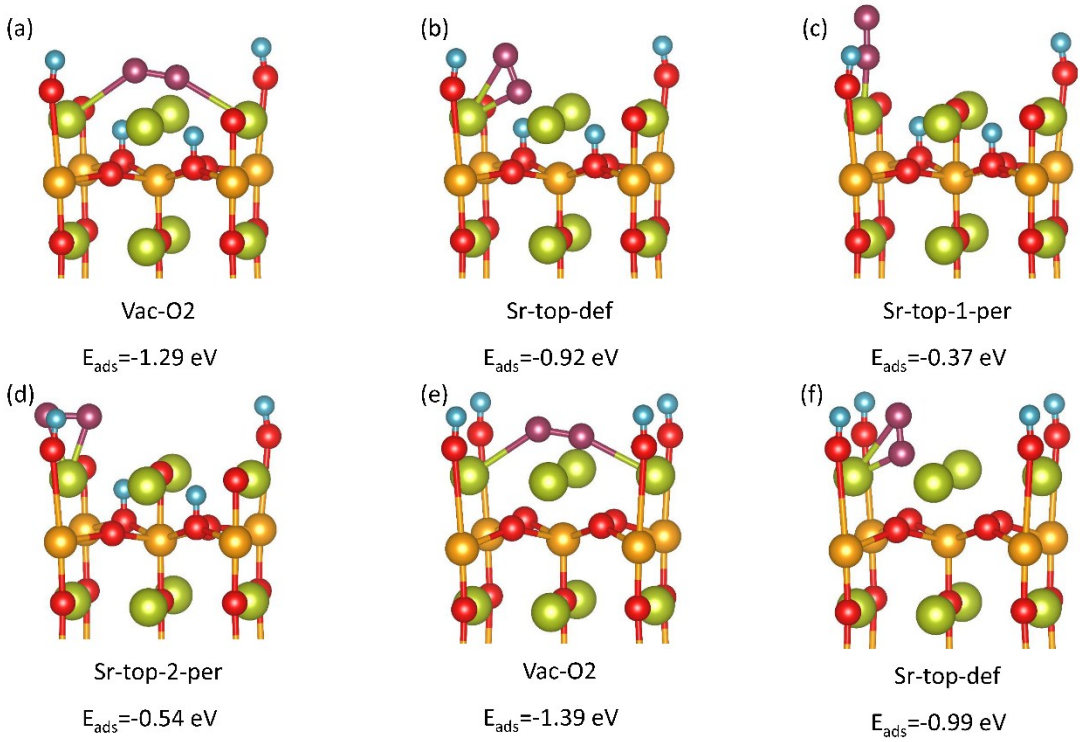

Figure S6 Optimized O_2 adsorption structures on the SrO-terminal $Sr_3Fe_2O_7$ (001) surface. (a) and (b) is on SrO-1-2H with one oxygen vacancy, (c) and (d) is on SrO-1-2H without oxygen vacancy, and (e) and (f) is on SrO-1-4H with one oxygen vacancy.

Table S1 Energy barriers for oxygen ion migration in the surface model and bulk model[1] along the [001] direction.

Barriers/eV	O1→O2	O2→O3	O3→O4	O4→O5	O5→O6
Surface model	0.35	0.22	0.74	0.26	1.04
Bulk model [1]	0.38	0.40	0.97	0.86	1.40

Table S2 Energy barriers of oxygen ion migration in the surface model and bulk model[1] along the [100] direction.

Barriers/eV	O1→O2	O2→O7
Surface model	0.35	0.18
Bulk model[1]	0.97	0.40

Notes and references

1.Huan, D.; Wang, Z.; Wang, Z.; Peng, R.; Xia, C.; Lu, Y., High-Performanced Cathode with a Two-Layered R-P Structure for Intermediate Temperature Solid Oxide Fuel Cells. *ACS applied materials & interfaces* **2016,** *8* (7), 4592-9.