

Supporting Information

Mechanistic Study of Structural Regulation and Enhanced Oxygen Reduction Performance in $\text{La}_{0.5}\text{Sr}_{1.5}\text{FeO}_{4+\delta}$ Cathodes via Mg Doping

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Table S1. shows the ASR values of LSFM_x ($x=0.000, 0.025, 0.050, 0.075, 0.100$) within the range of 600-800 °C

T (°C)	ASR ($\Omega\cdot\text{cm}^2$)				
	LSF	$\text{LSFM}_{0.025}$	$\text{LSFM}_{0.050}$	$\text{LSFM}_{0.075}$	$\text{LSFM}_{0.100}$
800	0.201	0.180	0.086	0.121	0.129
750	0.330	0.277	0.118	0.209	0.250
700	0.541	0.481	0.195	0.479	0.383
650	1.116	0.897	0.411	0.689	0.774
600	2.823	2.033	0.747	1.257	1.520

Table S2. Migration barrier of O atom on Sr exposed $\text{La}_9\text{Sr}_{27}\text{Fe}_{18}\text{O}_{63}(100)$ and $\text{La}_9\text{Sr}_{27}\text{Fe}_{17}\text{Mg}_1\text{O}_{63}(100)$.

Srexposed-O-migration path	Relative energy (eV)	
	$\text{La}_9\text{Sr}_{27}\text{Fe}_{18}\text{O}_{63}(100)$	$\text{La}_9\text{Sr}_{27}\text{Fe}_{17}\text{Mg}_1\text{O}_{63}(100)$
00-IS	0.000000	0.000000
01	-0.580100	0.257300
02-TS	-0.508500	0.587400
03	-0.851400	0.191900
04	-1.626100	-0.137400
05-FS	-1.945900	-0.223600

Table S3. Formation energy of oxygen vacancy on Sr exposed $\text{La}_9\text{Sr}_{27}\text{Fe}_{18}\text{O}_{63}(100)$ and $\text{La}_9\text{Sr}_{27}\text{Fe}_{17}\text{Mg}_1\text{O}_{63}(100)$.

System	Energy (eV)	Formation energy of oxygen vacancy	Average formation energy of O_v
$\text{La}_9\text{Sr}_{27}\text{Fe}_{18}\text{O}_{63}(100)$ -Srexposed	-771.6892		
$\text{La}_9\text{Sr}_{27}\text{Fe}_{18}\text{O}_{63}(100)$ -Srexposed-O-IS	-764.5586	2.2024	1.2295
$\text{La}_9\text{Sr}_{27}\text{Fe}_{18}\text{O}_{63}(100)$ -Srexposed-O-FS	-766.5045	0.2565	
$\text{La}_9\text{Sr}_{27}\text{Fe}_{17}\text{Mg}_1\text{O}_{63}(100)$ -Srexposed	-770.3266		
$\text{La}_9\text{Sr}_{27}\text{Fe}_{17}\text{Mg}_1\text{O}_{63}(100)$ -Srexposed-O-IS	-761.0130	4.3854	4.2736
$\text{La}_9\text{Sr}_{27}\text{Fe}_{17}\text{Mg}_1\text{O}_{63}(100)$ -Srexposed-O-FS	-761.2366	4.1618	
$\text{O}_2(\text{g})$	-9.8563		