Supporting Information

Motif for B/O-sites modulation in $LaFeO_3$ towards boosted oxygen evolution

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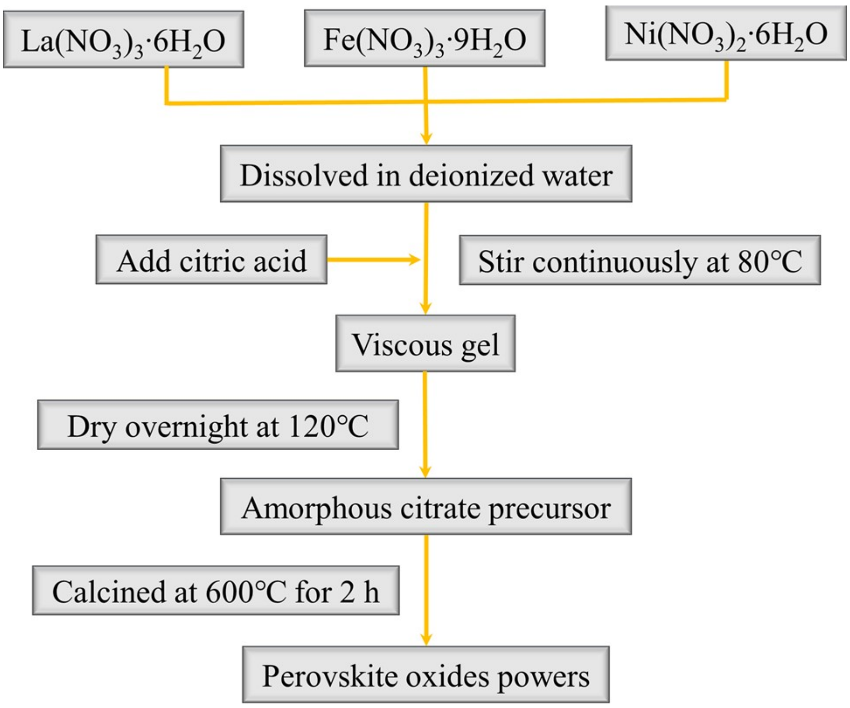

Fig. S1. Detail experiment procedures for fabrication of $LaFe_{1-x}Ni_xO_{3-\delta}$ electrocatalysts with different Ni-concentration synthesized at 600°C.

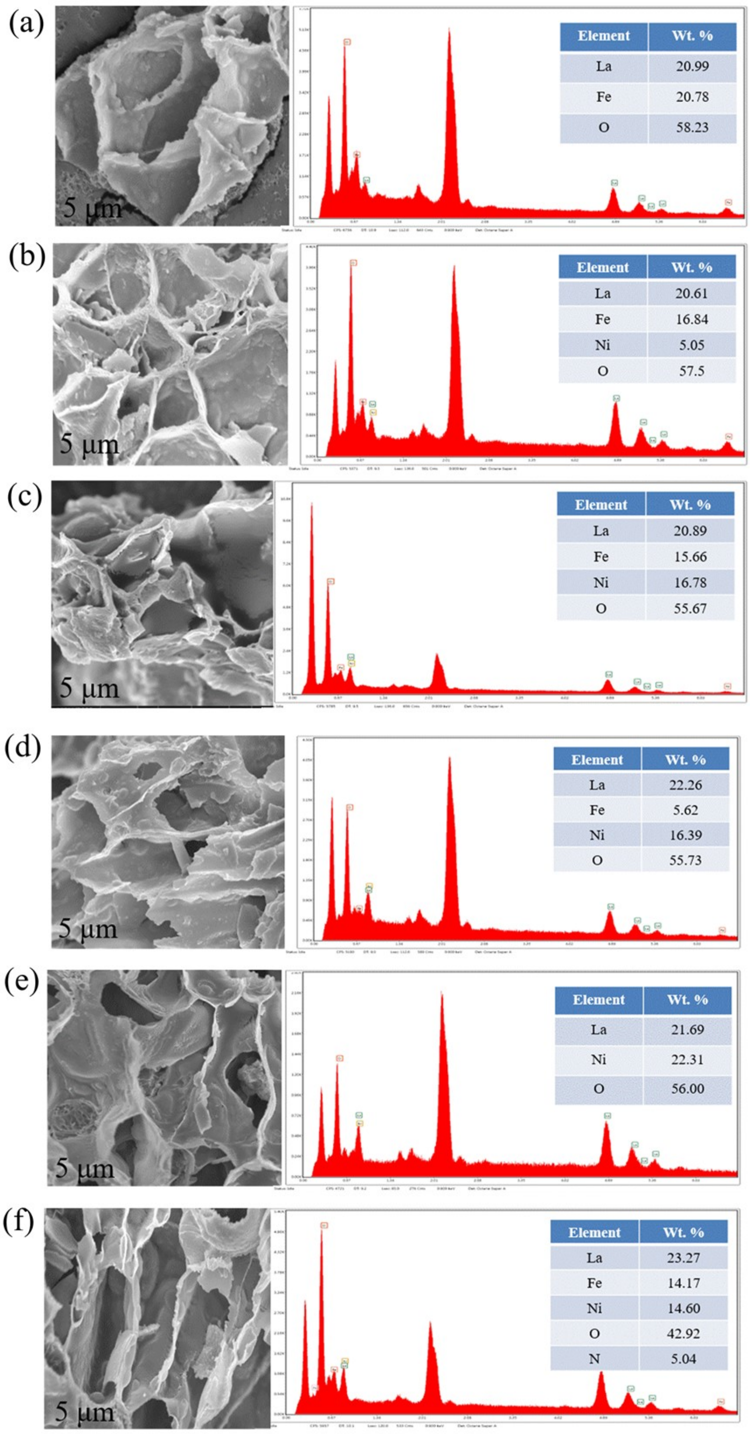

Fig. S2. SEM and EDS of (a) $LaFeO_{3-\delta}$, (b) $LaFe_{0.75}Ni_{0.25}O_{3-\delta}$, (c) $LaFe_{0.5}Ni_{0.5}O_{3-\delta}$, (d) $LaFe_{0.25}Ni_{0.75}O_{3-\delta}$, (e) $LaNiO_{3-\delta}$, and (f) $LaFe_{0.5}Ni_{0.5}O_{3-\delta}$/N catalysts (Inset is the corresponding element atoms percentage).

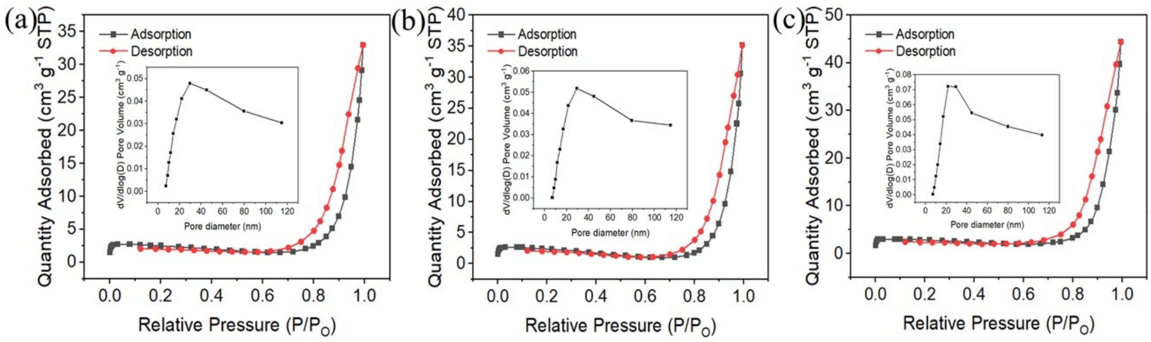

Fig. S3. Nitrogen adsorption-desorption hysteresis curve of (a) $LaFeO_{3-\delta}$, (b) $LaFe_{0.5}Ni_{0.5}O_{3-\delta}$, (c) $LaFe_{0.5}Ni_{0.5}O_{3-\delta}$/N catalysts (inset is the corresponding BJH pore size distribution curves).

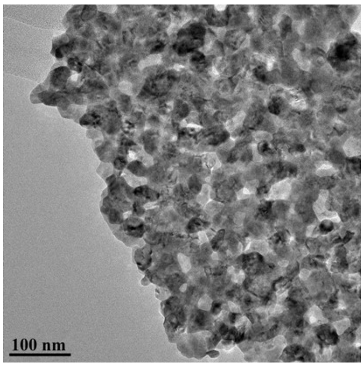

Fig. S4. TEM image of $LaFe_{0.5}Ni_{0.5}O_{3-\delta}$.

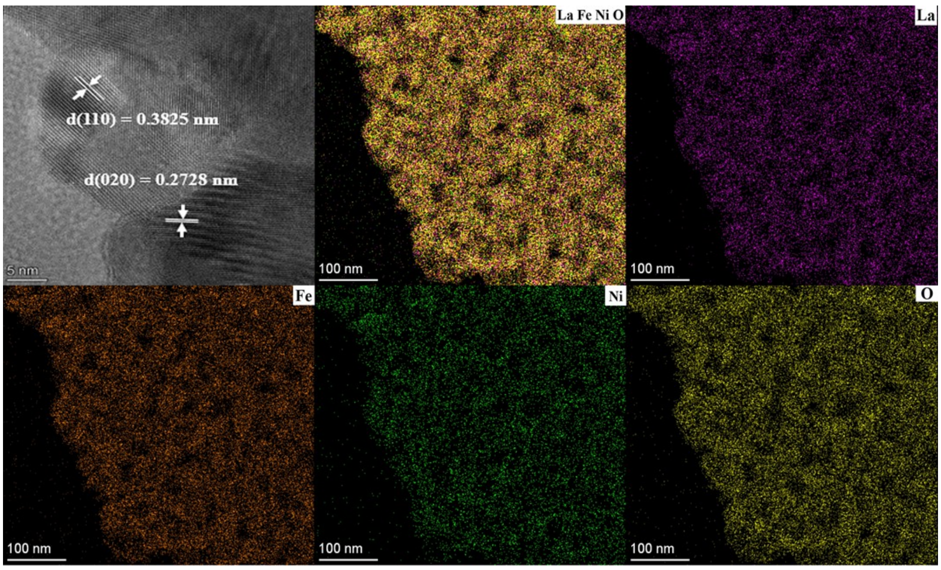

Fig. S5. HRTEM image of $LaFe_{0.5}Ni_{0.5}O_{3-\delta}$ and the corresponding elemental mapping images of La, Fe, Ni, O.

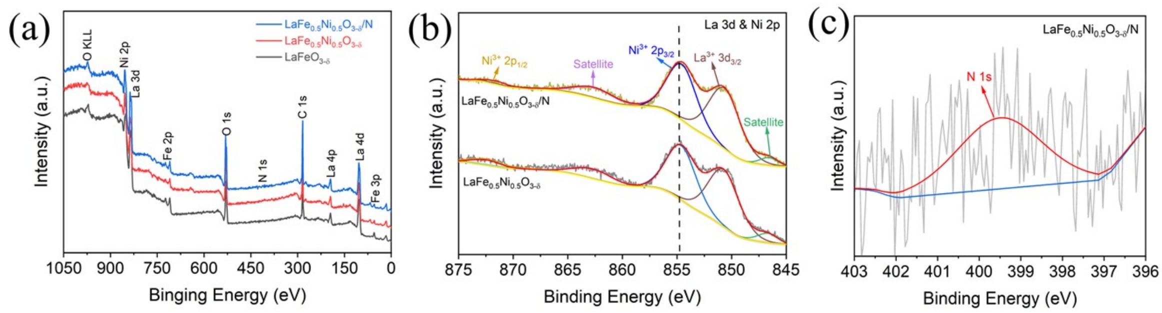

Fig. S6. (a) X-ray photoemission survey spectra of $LaFeO_{3-\delta}$, $LaFe_{0.5}Ni_{0.5}O_{3-\delta}$ and $LaFe_{0.5}Ni_{0.5}O_{3-\delta}/N$. (b-c) X-ray photoemission spectra of $LaFe_{0.5}Ni_{0.5}O_{3-\delta}$ and $LaFe_{0.5}Ni_{0.5}O_{3-\delta}/N$. Each panel are corresponding binding energy range to (b) La3d & Ni2p and (c) N1s.

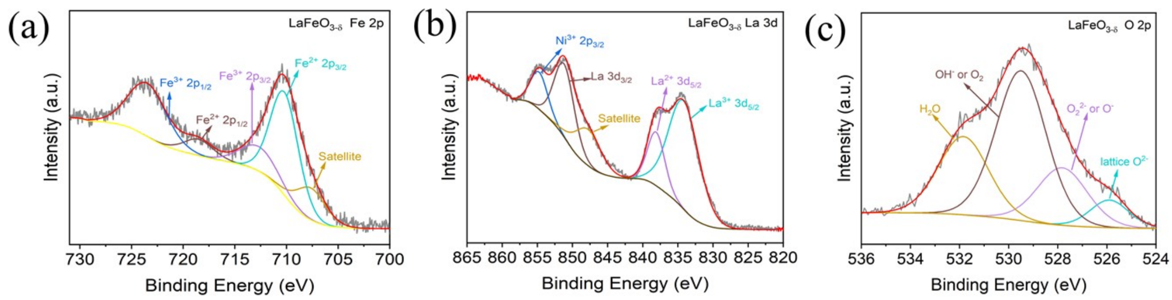

Fig. S7. (a-c) X-ray photoemission spectra of $LaFeO_{3-\delta}$. Each panel are corresponding binding energy range to (a) Fe 2p, (b) La 3d and (c) O 2p.

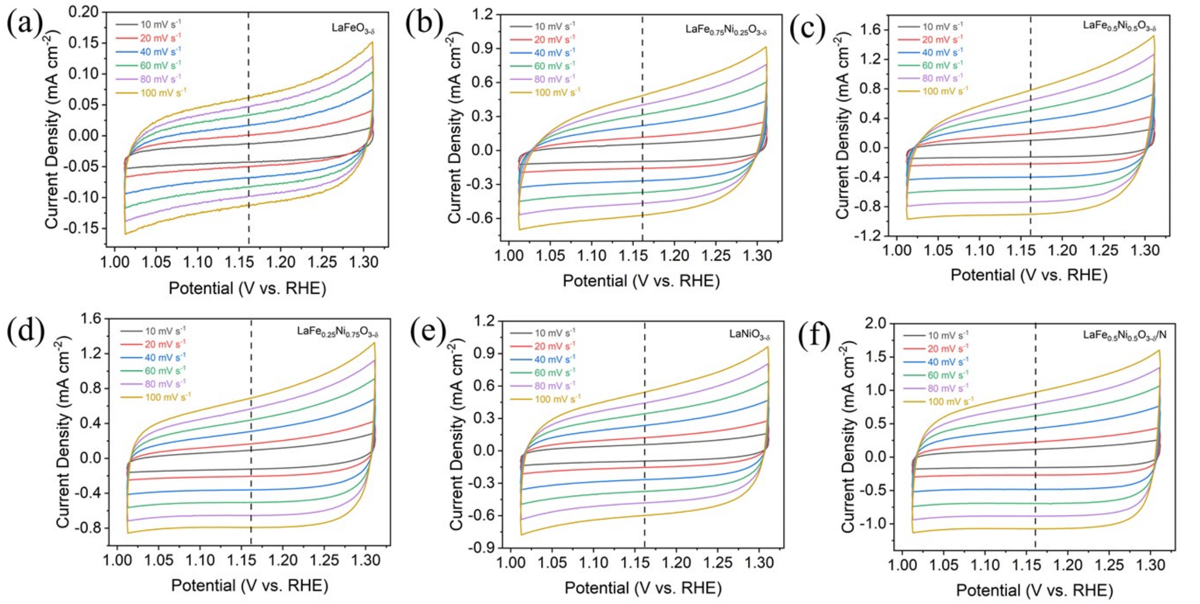

Fig. S8. CV measurements at different scan rates in a non-faradic current region with the scan interval of 100 mV s^{-1} for (a) $LaFeO_{3-\delta}$, (b) $LaFe_{0.75}Ni_{0.25}O_{3-\delta}$, (c) $LaFe_{0.5}Ni_{0.5}O_{3-\delta}$, (d) $LaFe_{0.25}Ni_{0.75}O_{3-\delta}$, (e) $LaNiO_{3-\delta}$, and (f) $LaFe_{0.5}Ni_{0.5}O_{3-\delta}$/N catalysts.

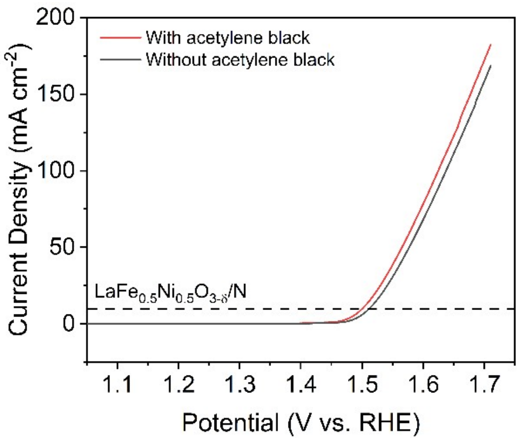

Fig. S9 Comparison of LSV polarization curves of sample $LaFe_{0.5}Ni_{0.5}O_{3-\delta}$/N with and without acetylene black.

Table S1. Atoms ratios of the $LaFe_{1-x}Ni_xO_{3-\delta}$ (x = 0, 0.25, 0.5, 0.75, 1) and $LaFe_{0.5}Ni_{0.5}O_{3-\delta}$/N derived from EDS analysis.

Element	**La /wt%**	**Fe /wt%**	**Ni /wt%**	**O /wt%**	**N /wt%**
$LaFeO_{3-\delta}$	20.99%	20.78%	\	58.23%	\
$LaFe_{0.75}Ni_{0.25}O_{3-\delta}$	20.61%	16.84%	5.05%	57.50%	\
$LaFe_{0.5}Ni_{0.5}O_{3-\delta}$	20.89%	15.66%	16.78%	55.67%	\
$LaFe_{0.25}Ni_{0.75}O_{3-\delta}$	22.26%	5.62%	16.39%	55.73%	\
$LaNiO_{3-\delta}$	21.69%	\	22.31%	56.00%	\
$LaFe_{0.5}Ni_{0.5}O_{3-\delta}$/N	23.27%	14.17%	14.60%	42.92%	5.04%

Table S2. The details of the standard crystal planes of the reported materials.

Materials	Crystal planes (h k l)	d (Å)	2θ (º)	Intensity (a.u.)
$LaFe_{0.5}Ni_{0.5}O_3$	020	2.7356	32.710	31.7
	110	3.8852	22.871	18.5

Table S3. Atoms ratios of the $LaFeO_{3-\delta}$, $LaFe_{0.5}Ni_{0.5}O_{3-\delta}$, and $LaFe_{0.5}Ni_{0.5}O_{3-\delta}$/N derived from XPS analysis.

Element (Atomic %)	Electrocatalysts		
	$LaFeO_{3-\delta}$	$LaFe_{0.5}Ni_{0.5}O_{3-\delta}$	$LaFe_{0.5}Ni_{0.5}O_{3-\delta}$/N
La 3d	9.15	9.54	8.93
Fe 2p	8.06	5.84	6.11
Ni 2p	\	6.01	6.65
O 1s	37.33	35.04	30.43
N 2s	\	\	2.35
C 1s	45.46	43.57	45.53

Table S4. O 1s XPS deconvolution results of the $LaFeO_{3-\delta}$, $LaFe_{0.5}Ni_{0.5}O_{3-\delta}$, and $LaFe_{0.5}Ni_{0.5}O_{3-\delta}$/N.

Element	H_2O	OH^- or O_2	O_2^{2-} or O^-	Lattice O^{2-}
$LaFeO_{3-\delta}$	25.55%	48.93%	18.69%	6.83%
$LaFe_{0.5}Ni_{0.5}O_{3-\delta}$	18.33%	29.47%	21.16%	31.05%
$LaFe_{0.5}Ni_{0.5}O_{3-\delta}$/N	15.43%	25.59%	28.80%	30.17%

Table S5. OER activities of perovskite oxides.

Catalysts	Overpotential@10 mA cm^{-2} (mV)	Tafel (mV dec^{-1})	References
$LaFe_{0.5}Ni_{0.5}O_{3-\delta}$	**281.4**	**75**	**This work**
$LaFe_{0.5}Ni_{0.5}O_{3-\delta}/N$	**270.6**	**65**	**This work**
$LaFe_{0.2}Ni_{0.8}O_3$	420	89	1
3D microporous $LaFe_{0.8}Co_{0.2}O_3$	410	56	2
$La_{0.5}Sr_{0.5}Ni_{0.4}Fe_{0.6}O_{3-\delta}$	342	85	3
$SrNb_{0.1}Co_{0.7}Fe_{0.2}O_{3-\delta}$	370	48	4
$NdBaMn_2O_{5.5}$	370	75	5
$LaNi_{0.8}Fe_{0.2}O_{3-\delta}$-NR	302	50	6
$PrBaCo_2O_{5.75}$	360	70	7
$LaNi_{0.96}Ir_{0.04}O_3$	280	62	8
$LaCoO_3$/N-rGO	560	65	9
$LaNiO_3$/NiO	346	73	10
$BaCo_{0.4}Fe_{0.4}Zr_{0.1}Y_{0.1}O_{3-\delta}$	324	69	11
La_2NiMnO_6	370	58	12

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