

Supplementary Information

Nickel-Doped Pyrrhotite Iron Sulfide Nanosheets as Highly Efficient Electrocatalysts for Water Splitting

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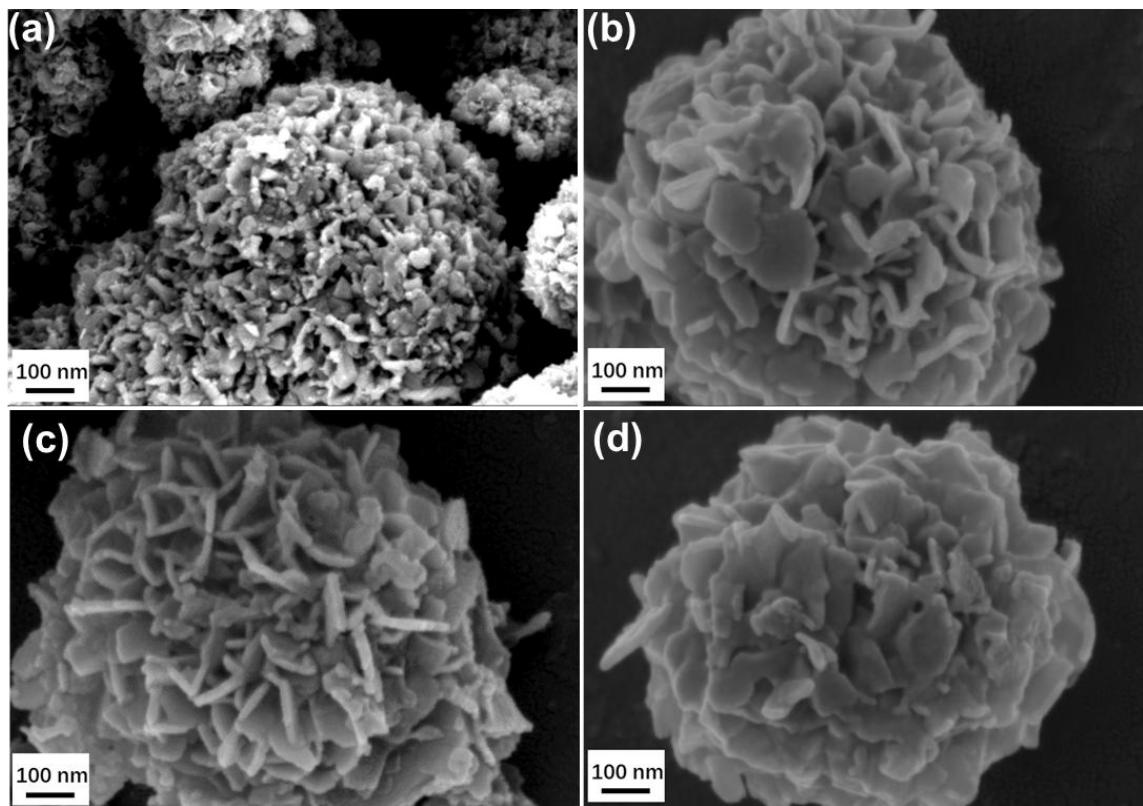
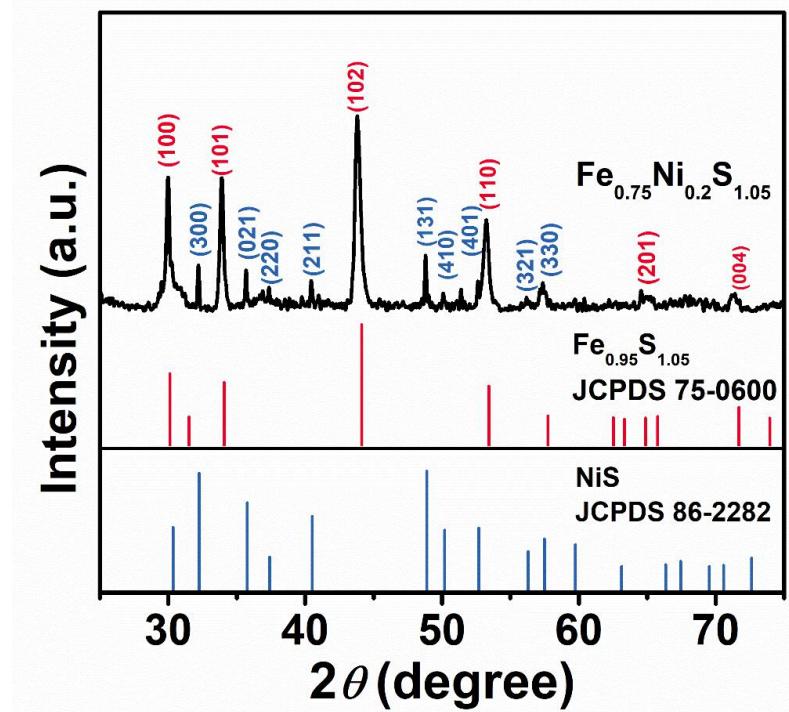


Figure S1 SEM image of (a) $\text{Fe}_{0.95}\text{S}_{1.05}$ (b) $\text{Fe}_{0.9}\text{Ni}_{0.05}\text{S}_{1.05}$ (c) $\text{Fe}_{0.85}\text{Ni}_{0.1}\text{S}_{1.05}$ (d) $\text{Fe}_{0.75}\text{Ni}_{0.2}\text{S}_{1.05}$.



Figures S2 XRD pattern of $\text{Fe}_{0.75}\text{Ni}_{0.2}\text{S}_{1.05}$.

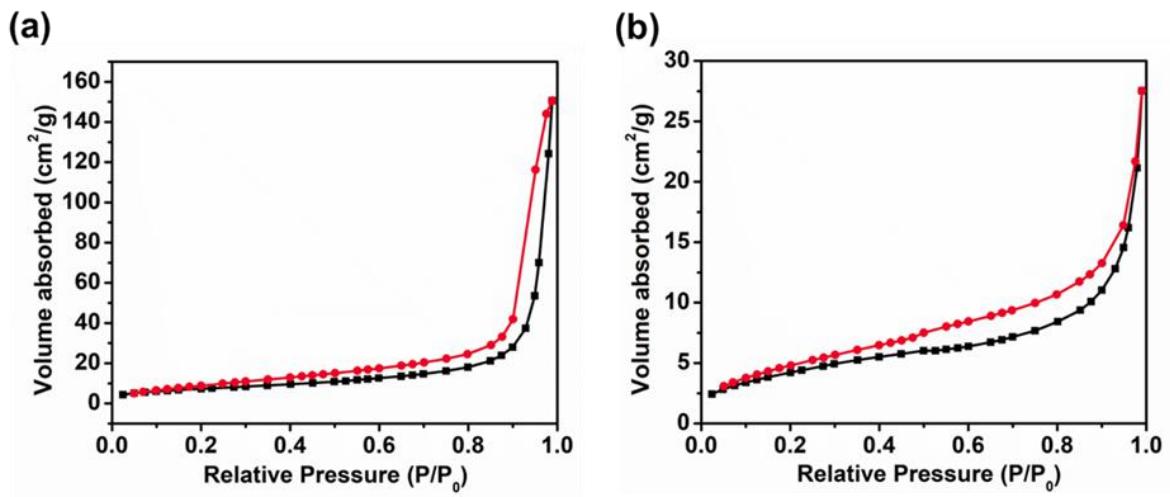


Figure S3 Nitrogen isotherm and pore size distribution of (a) $\text{Fe}_{0.95}\text{S}_{1.05}$ and (b) $\text{Fe}_{0.8}\text{Ni}_{0.15}\text{S}_{1.05}$ catalysts

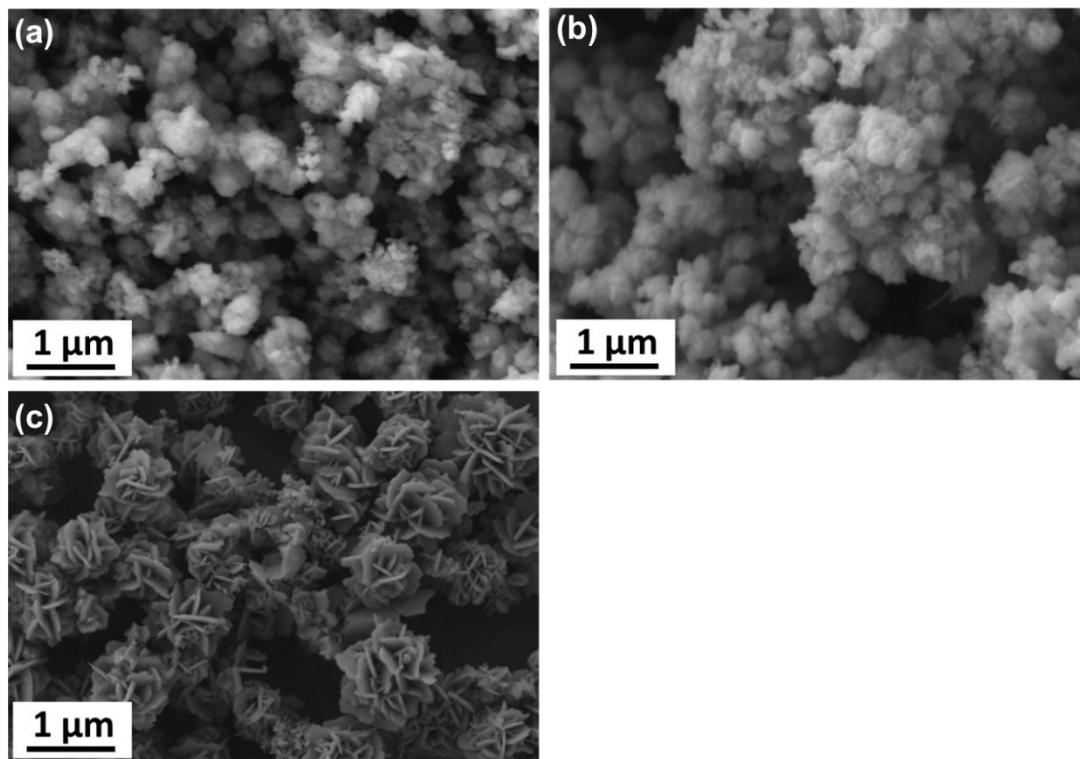


Figure S4 SEM images of the $\text{Fe}_{0.8}\text{Ni}_{0.15}\text{S}_{1.05}$ products synthesized at various reaction temperatures, (a) 150°C , (b) 180°C , (c) 210°C for 16 h.

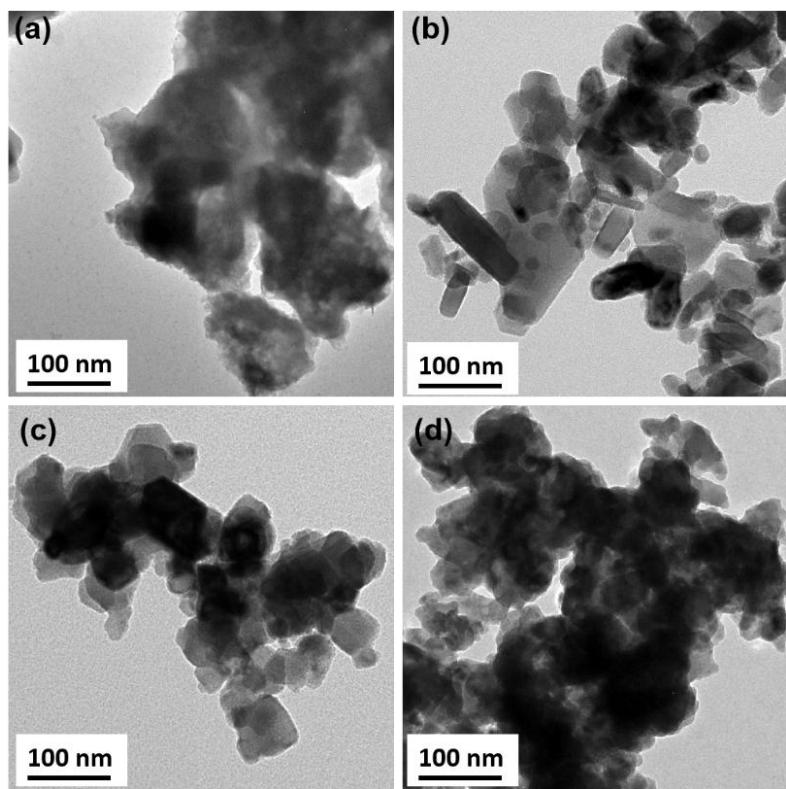
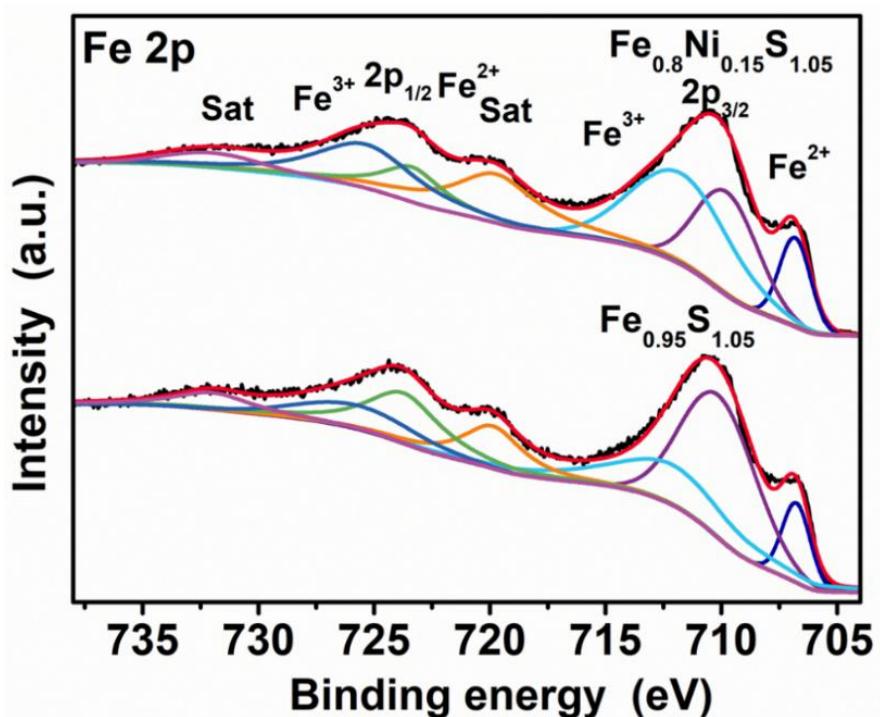


Figure S5 TEM images of as-prepared products obtained via hydrothermal reaction after (a) 1 h, (b) 5 h, (c) 10 h and (d) 15 h



Figuer S6 Fe 2p and high-resolution XPS of $\text{Fe}_{0.8}\text{Ni}_{0.15}\text{S}_{1.05}$ catalyst and $\text{Fe}_{0.95}\text{S}_{1.05}$.

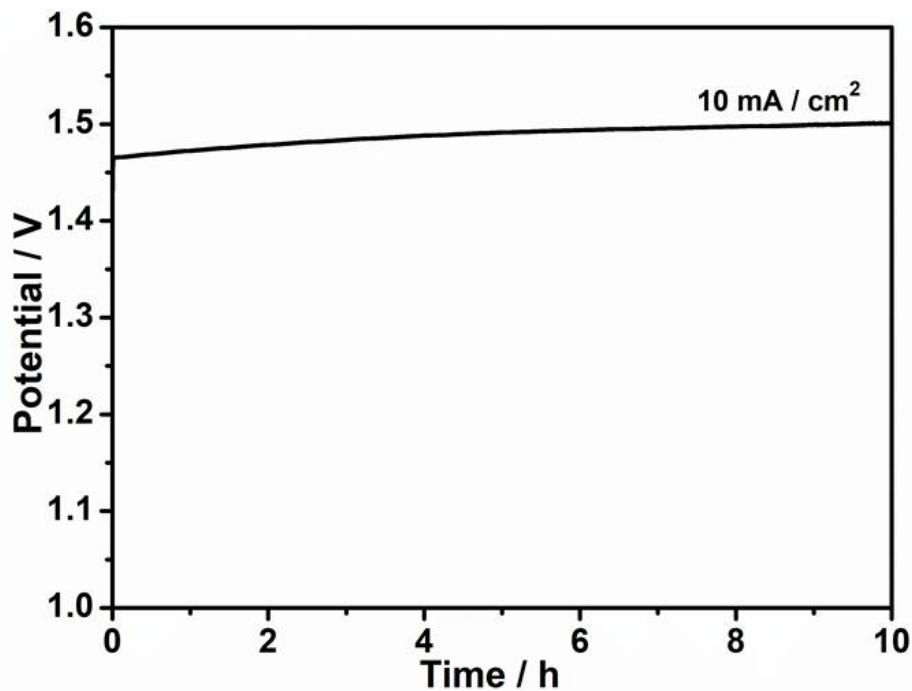


Figure S7 E - t curves of $\text{Fe}_{0.8}\text{Ni}_{0.15}\text{S}_{1.05}$ at a potential of 1.47 V for 10 h.

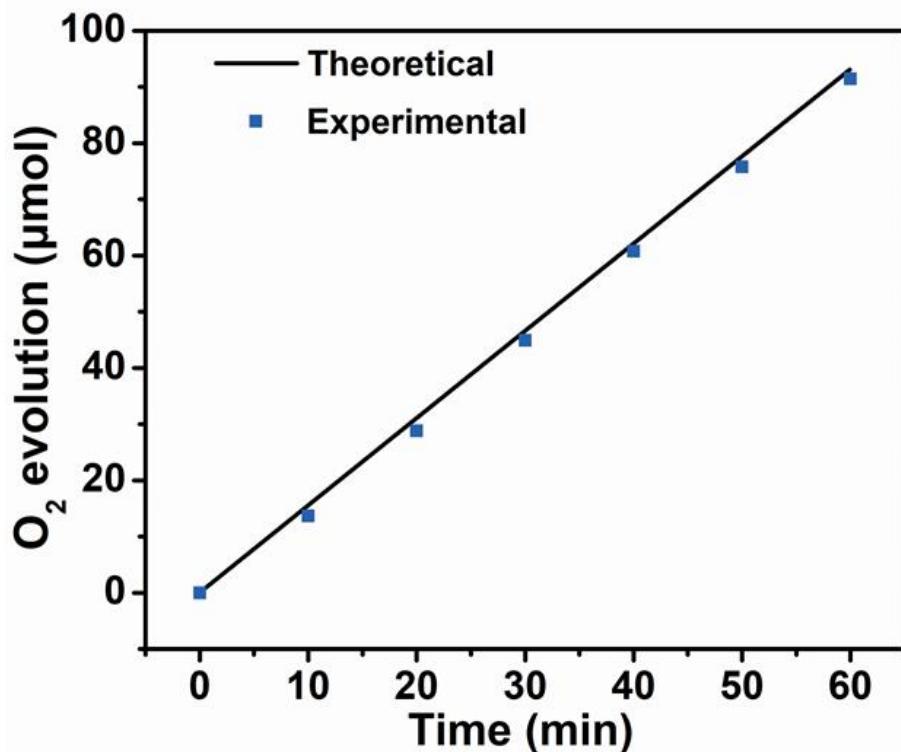


Figure S8 The Faradaic efficiency of $\text{Fe}_{0.8}\text{Ni}_{0.15}\text{S}_{1.05}$ for OER. Electrocatalytic Faradaic efficiencies of OER over $\text{Fe}_{0.8}\text{Ni}_{0.15}\text{S}_{1.05}$ at a current density of $10 \text{ mA} \cdot \text{cm}^{-2}$ measured for 60 min.

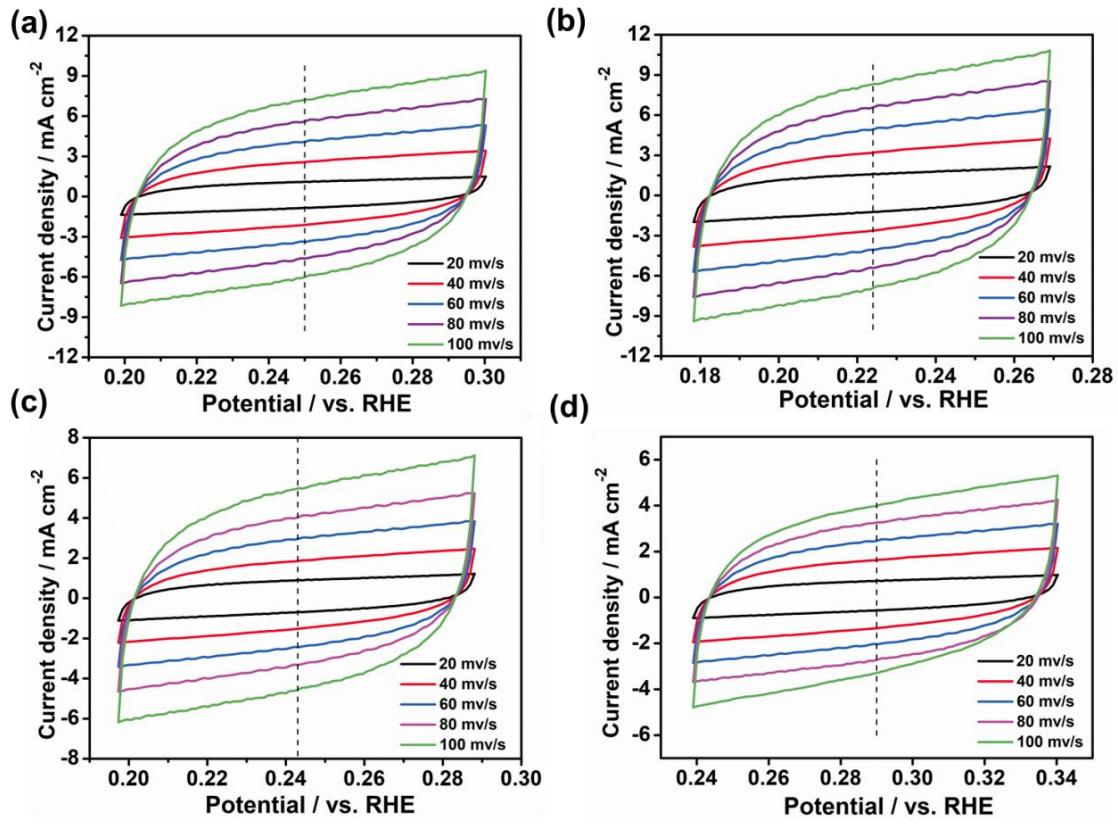


Figure S9 CV curves in a potential window of 200–300 mV of (a) $\text{Fe}_{0.75}\text{Ni}_{0.20}\text{S}_{1.05}$, (b) $\text{Fe}_{0.8}\text{Ni}_{0.15}\text{S}_{1.05}$, (c) $\text{Fe}_{0.85}\text{Ni}_{0.1}\text{S}_{1.05}$ and (d) $\text{Fe}_{0.9}\text{Ni}_{0.05}\text{S}_{1.05}$ electrode.

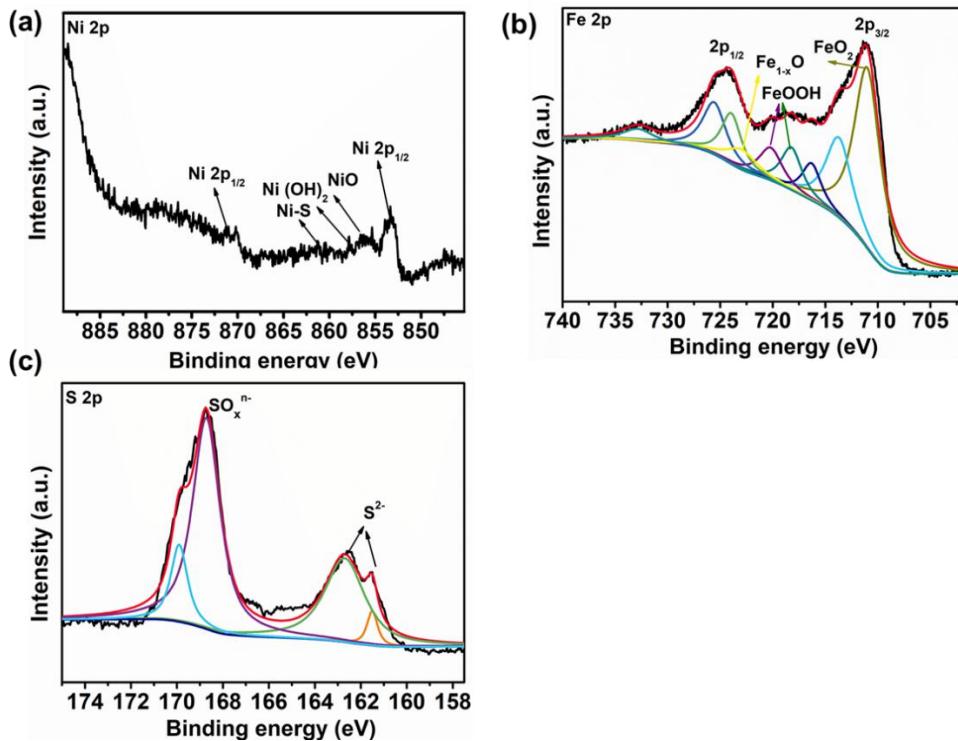


Figure S10 (a) Ni 2p, (b) Fe 2p and (c) S 2p high-resolution XPS of $\text{Fe}_{0.8}\text{Ni}_{0.15}\text{S}_{1.05}$ catalyst after OER test.

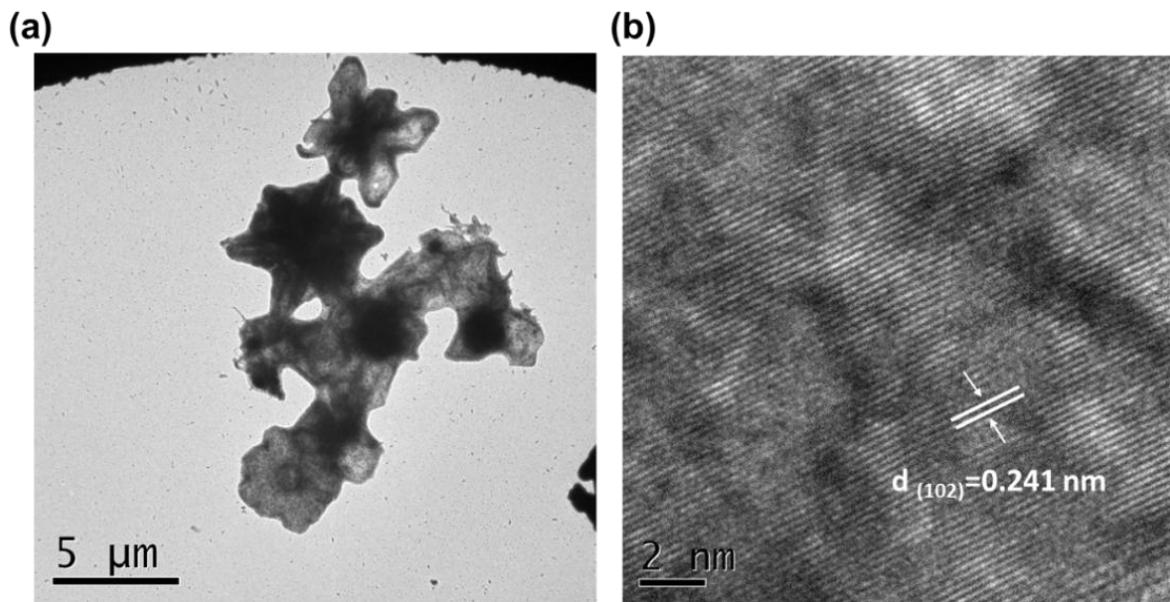


Figure S11 TEM images of $\text{Fe}_{0.8}\text{Ni}_{0.15}\text{S}_{1.05}$ catalyst after OER test.

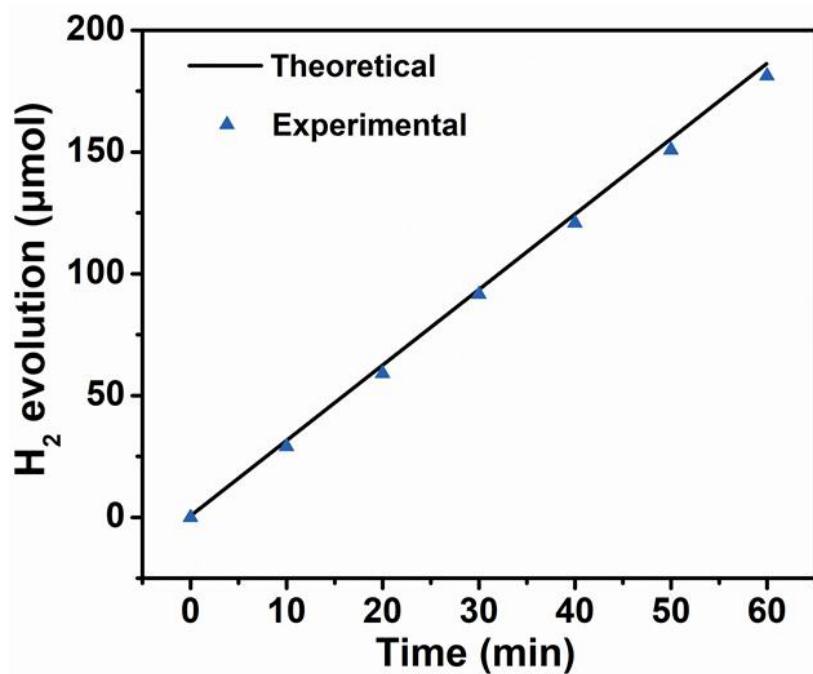
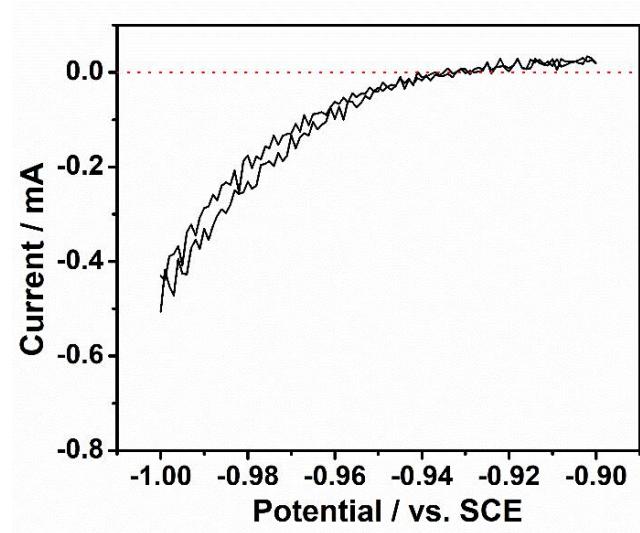


Figure S12 The Faradaic efficiency of $\text{Fe}_{0.8}\text{Ni}_{0.15}\text{S}_{1.05}$ for HER. Electrocatalytic Faradaic efficiencies of HER over $\text{Fe}_{0.8}\text{Ni}_{0.15}\text{S}_{1.05}$ at a current density of $10 \text{ mA}\cdot\text{cm}^{-2}$ measured for 60 min.



RHE calibration

In all electrochemical tests, we use Hg/HgO electrode as the reference electrode. The calibration was performed using a Platinum wire as the working electrode in 1 M KOH solutions under H₂-saturated condition. The CV curves were test in 1.0 mol/L (M) KOH at a scan rate of 1 mV/s. The average value of the two potentials when the current crosses zero is used as the thermodynamic potential of the hydrogen electrode reaction.

$$E_{RHE} = E_{Hg/HgO} + 0.928$$

Table S1ICP results for $\text{Fe}_{0.95-x}\text{Ni}_x\text{S}_{1.05}$ catalysts.

	Fe	Ni	S
lin bk	< 0.00011	< -0.00059	< -0.00639
$\text{Fe}_{0.95}\text{S}_{1.05}$	1.2666	< -0.00077	1.4132
$\text{Fe}_{0.9}\text{Ni}_{0.05}\text{S}_{1.05}$	1.2131	0.0711	1.4666
$\text{Fe}_{0.85}\text{Ni}_{0.1}\text{S}_{1.05}$	1.1343	0.1346	1.4936
$\text{Fe}_{0.8}\text{Ni}_{0.15}\text{S}_{1.05}$	1.0785	0.2113	1.4864
$\text{Fe}_{0.75}\text{Ni}_{0.2}\text{S}_{1.05}$	1.0132	0.2438	1.4568

Table S2The R_{ct} value of $\text{Fe}_{0.95-x}\text{Ni}_x\text{S}_{1.05}$ catalysts.

Catalysts	$R_{ct} (\Omega)$
$\text{Fe}_{0.95}\text{S}_{1.05}$	22.5
$\text{Fe}_{0.9}\text{Ni}_{0.05}\text{S}_{1.05}$	4.593
$\text{Fe}_{0.85}\text{Ni}_{0.1}\text{S}_{1.05}$	5.293
$\text{Fe}_{0.8}\text{Ni}_{0.15}\text{S}_{1.05}$	1.553
$\text{Fe}_{0.75}\text{Ni}_{0.2}\text{S}_{1.05}$	3.909

References

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