Supplementary Information

Sulfur-doped $NiFe(CN)_5NO$ nanoparticles as efficient electrocatalysts for the oxygen evolution reaction

Yi Zhang,[a] Xiaoping Shen,*[b] Chunsen Song,[b] Zhenyuan Ji[b] and Fei-Hu Du*[a]

[a] School of Environmental and Chemical Engineering, Shanghai University, Shanghai 200444, PR China

[b] School of Chemistry and Chemical Engineering, Jiangsu University, Zhenjiang 212013, PR China

* Corresponding authors.

E-mail address: shenxp@ujs.edu.cn, xiaopingshen@163.com (X. Shen); fh_du@shu.edu.cn (F.-H. Du)

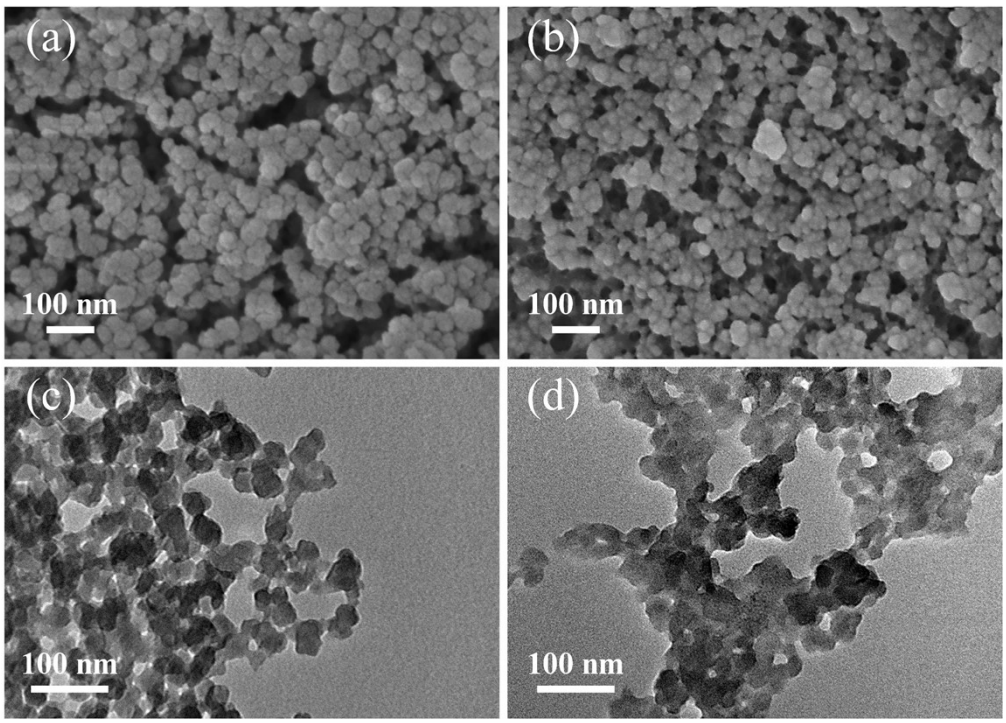

Fig. S1 SEM images of (a) S–NiFe(CN)$_5$NO-250 and (b) S–NiFe(CN)$_5$NO-750. TEM images of (c) S–NiFe(CN)$_5$NO-250 and (d) S–NiFe(CN)$_5$NO-750.

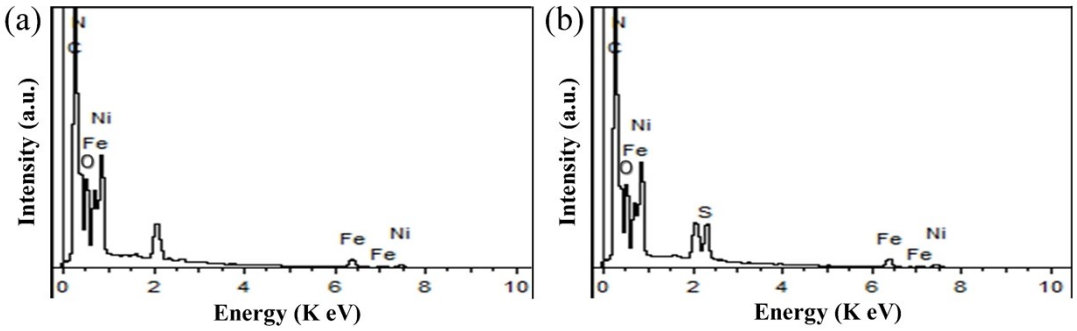

Fig. S2 EDS patterns of (a) $NiFe(CN)_5NO$ and (b) S–$NiFe(CN)_5NO$-500.

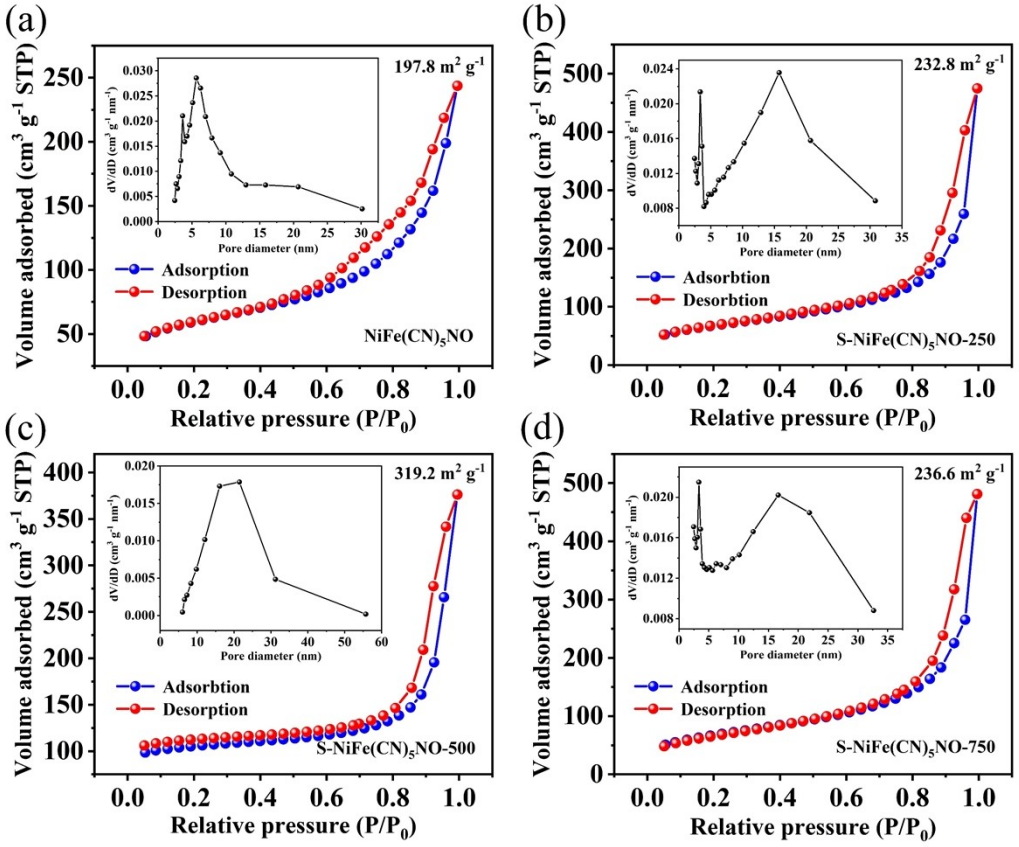

Fig. S3 N_2 adsorption-desorption isotherms for (a) $NiFe(CN)_5NO$, (b) S–$NiFe(CN)_5NO$-250, (c) S–$NiFe(CN)_5NO$-500 and (d) S–$NiFe(CN)_5NO$-750.

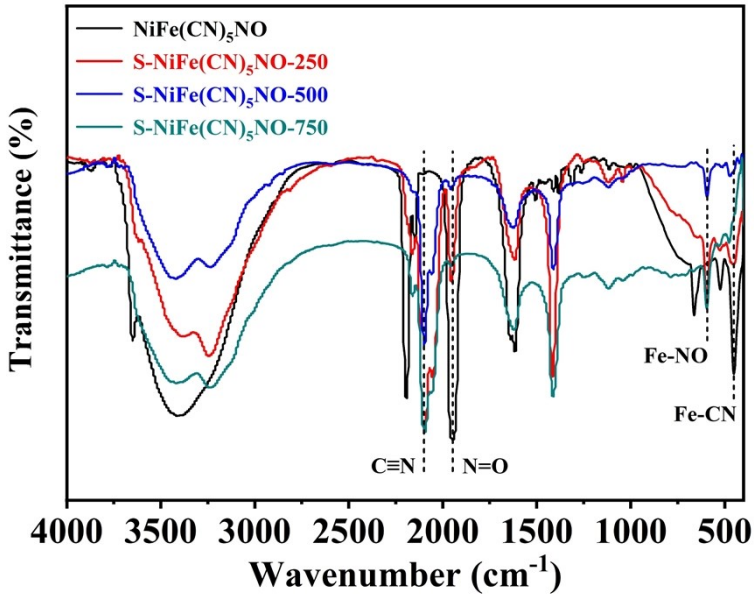

Fig. S4 FTIR spectra of $NiFe(CN)_5NO$, S–$NiFe(CN)_5NO$-250, S–$NiFe(CN)_5NO$-500 and S–$NiFe(CN)_5NO$-750.

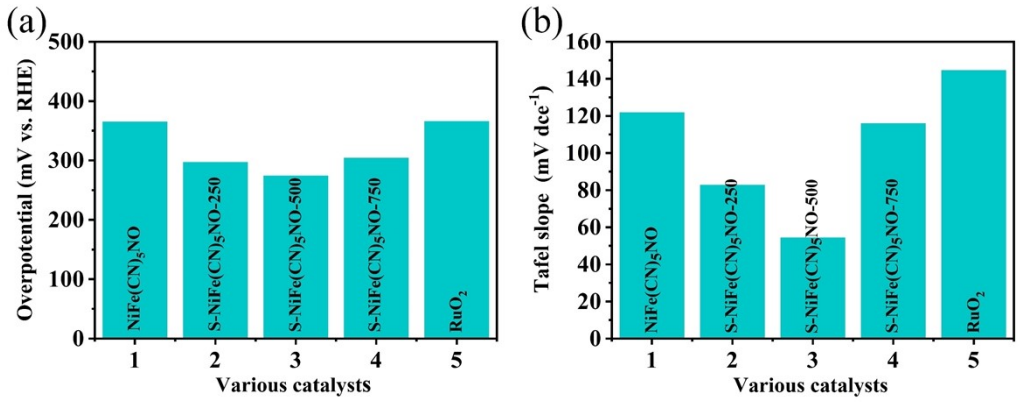

Fig. S5 (a) Overpotential values at 10 mA cm^{-2} and (b) Tafel slopes of $NiFe(CN)_5NO$, S–$NiFe(CN)_5NO$-250, S–$NiFe(CN)_5NO$-500, S–$NiFe(CN)_5NO$-750 and RuO_2.

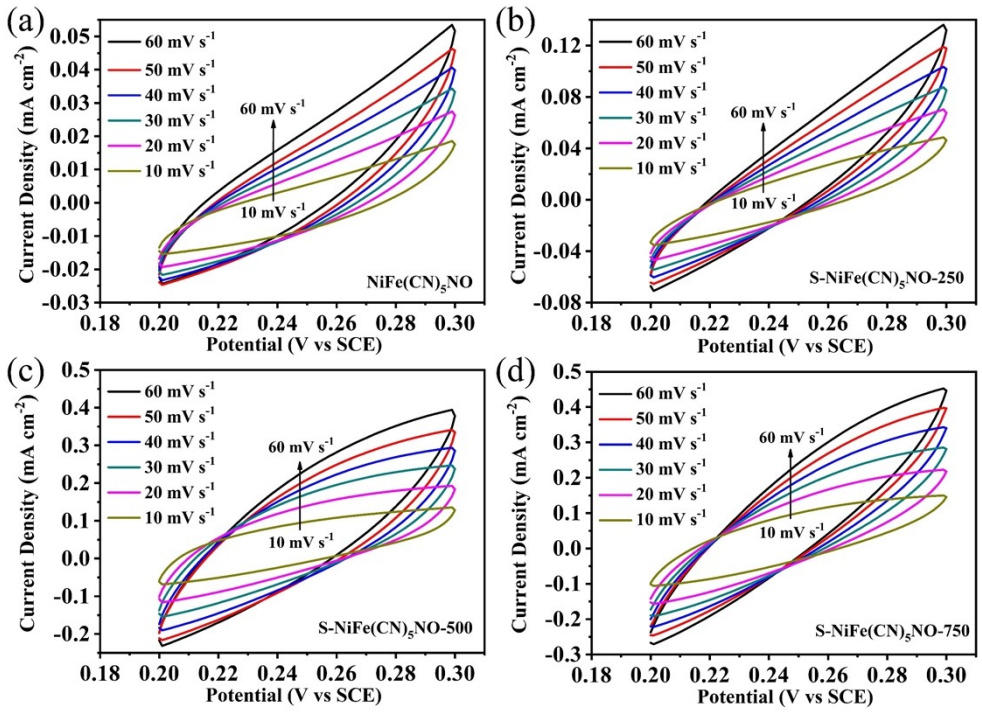

Fig. S6 CV curves of the catalysts with different scanning rates. (a) $NiFe(CN)_5NO$, (b) S–$NiFe(CN)_5NO$-250, (c) S–$NiFe(CN)_5NO$-500 and (d) S–$NiFe(CN)_5NO$-750.

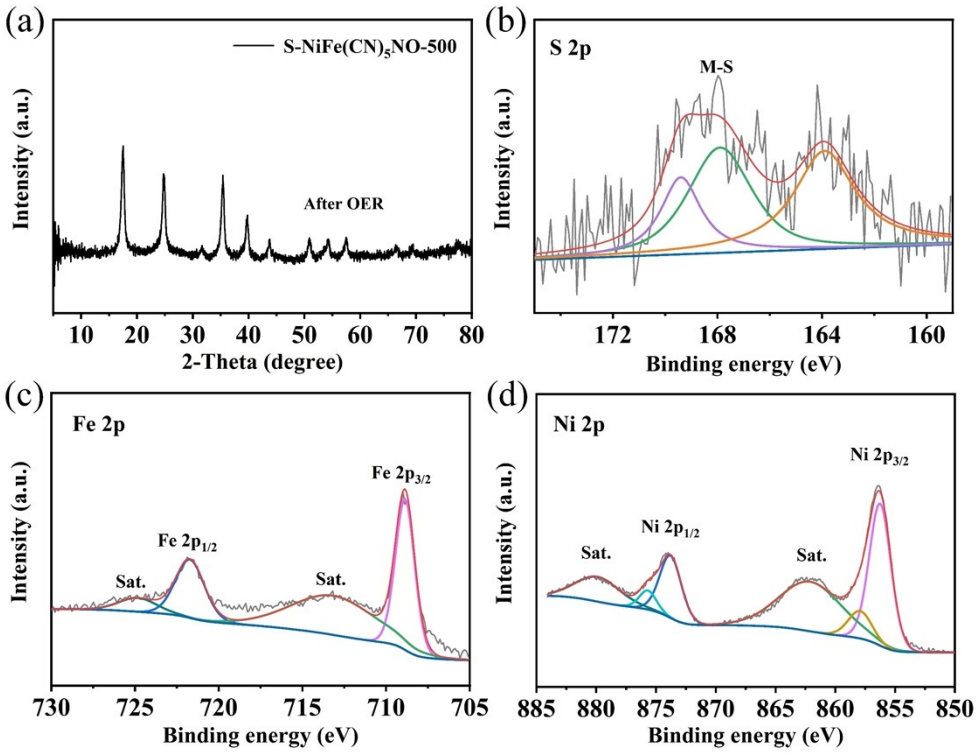

Fig. S7 (a) XRD pattern and XPS spectra of (b) S 2p, (c) Ni 2p, (d) Fe 2p for S–$NiFe(CN)_5NO$-500 after stability test.

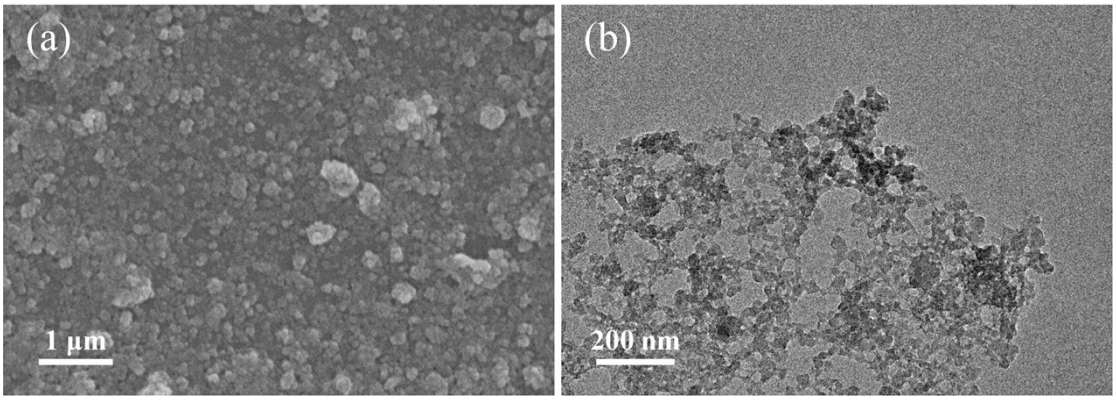

Fig. S8 (a) SEM and (b) TEM images of S–$NiFe(CN)_5NO$-500 after stability test.

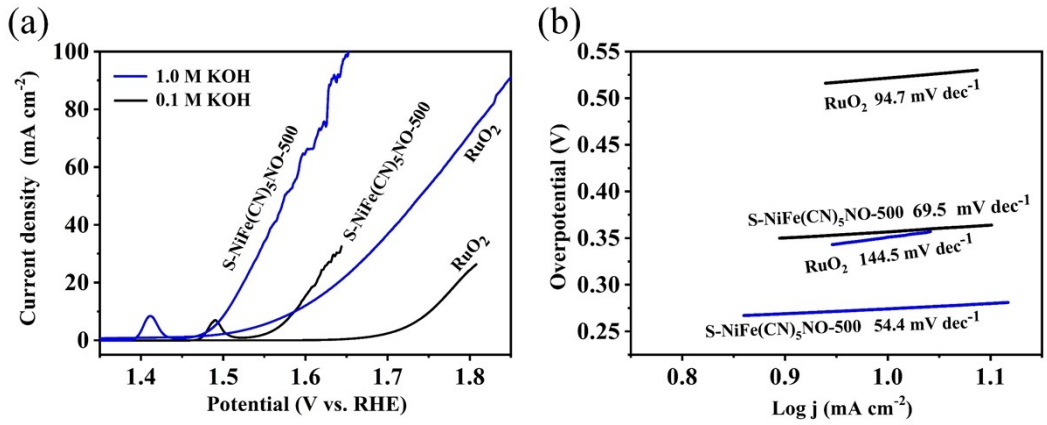

Fig. S9 (a) LSV curves and (b) corresponding Tafel slopes of S–$NiFe(CN)_5NO$-500 and RuO_2 for 1.0 and 0.1 M KOH solutions.

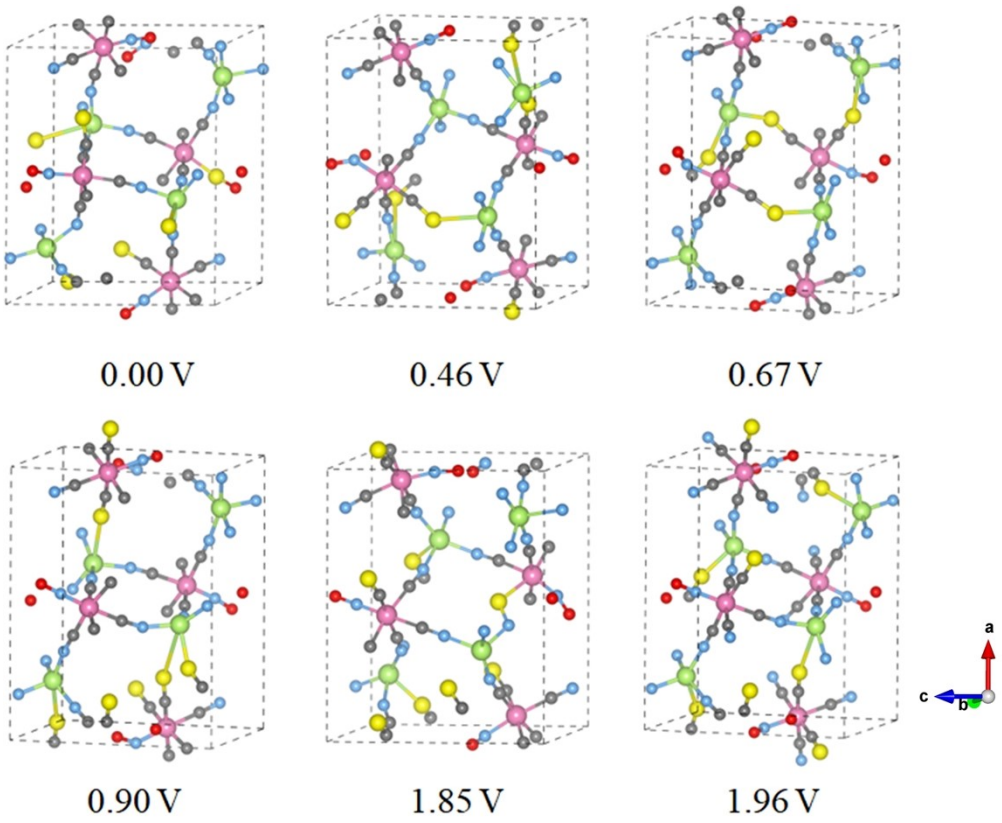

Fig. S10 Structures and energetics of S–$NiFe(CN)_5NO$. Energies are relative to the most stable isomer.

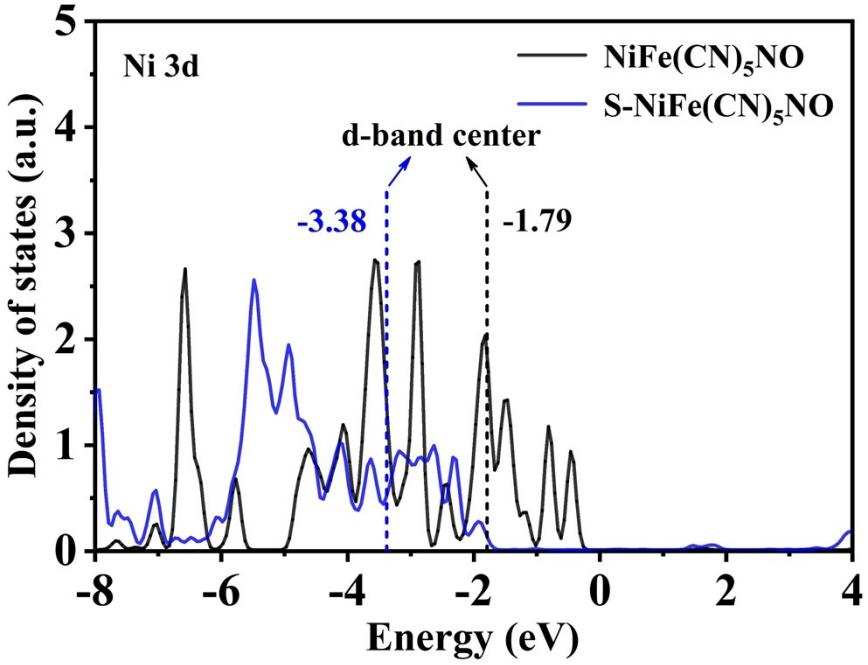

Fig. S11 Calculated PDOS of Ni 3d for $NiFe(CN)_5NO$ and S–$NiFe(CN)_5NO$.

Table S1. Contents of Ni, Fe and S in $NiFe(CN)_5NO$, S–$NiFe(CN)_5NO$-250, S–$NiFe(CN)_5NO$-500 and S–$NiFe(CN)_5NO$-750.

Weight%	Ni	Fe	S
$NiFe(CN)_5NO$	21.57%	18.30%	0
S–$NiFe(CN)_5NO$-250	23.71%	17.69%	1.82%
S–$NiFe(CN)_5NO$-500	22.54%	18.87%	2.34%
S–$NiFe(CN)_5NO$-750	25.83%	20.25%	2.49%

Table S2. The electrocatalytic parameters of $NiFe(CN)_5NO$, S–$NiFe(CN)_5NO$-250, S–$NiFe(CN)_5NO$-500, S–$NiFe(CN)_5NO$-750 and RuO_2 catalysts for the OER in 1.0 M KOH.

Catalyst	η_{10} (mV)	Tafel slope (mV dec^{-1})	C_{dl} (mF cm^{-2})
$NiFe(CN)_5NO$	365	121.8	0.28
S–$NiFe(CN)_5NO$-250	297	82.8	0.30
S–$NiFe(CN)_5NO$-500	274	54.4	1.67
S–$NiFe(CN)_5NO$-750	304	115.9	1.24
RuO_2	366	144.5	—

Table S3. Electrocatalytic OER activities of some materials similar to S–$NiFe(CN)_5NO$-500 in 1.0 M KOH. GC: glassy carbon, NF: Ni foam, CC: carbon cloth.

Catalyst	Substrate	Overpotential (mV)	Tafel slope (mV dec^{-1})	Ref.
S–$NiFe(CN)_5NO$-500	GC	η_{10}=274	54.4	—
Fe–MOF/NF	NF	η_{50}=240	72	38
Ni–MOF/NF	NF	η_{20}=350	98	39
Ni–MOF@CNT	NF	η_{10}=370	138.2	40
NiFeSe@NiSe|O	CC	η_{10}=270	63.2	41
Ni_3S_4	GC	η_{10}=307	67	42
$NiCo_2S_4$	CC	η_{100}=370	95.76	43
S–FeNi LDH@PBA/NF	NF	η_{50}=243	83.1	34