Cobalt Incorporation and MoS_2-NiS_2 Heterostructure Synergistic Improving Full Water Electrolysis Efficiency

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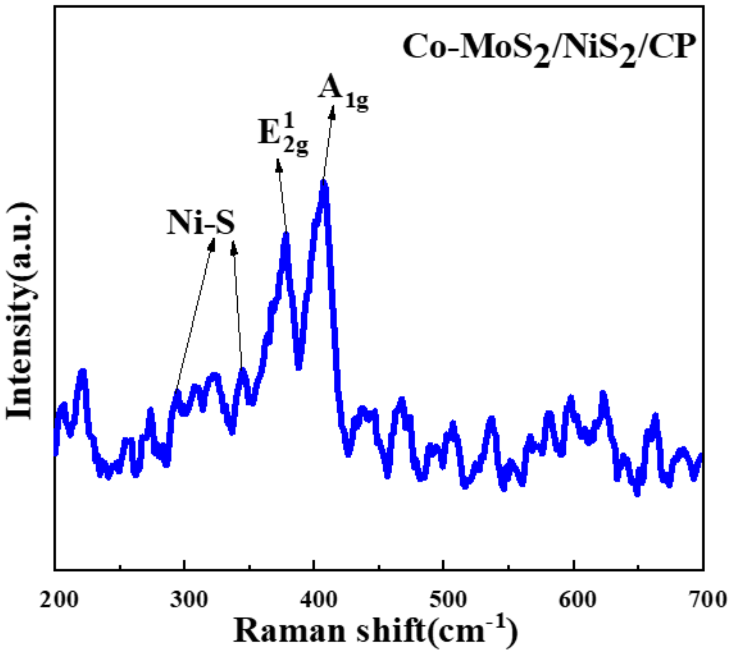

Fig. S1. Raman spectrum of Co-MoS_2/NiS_2/CP.

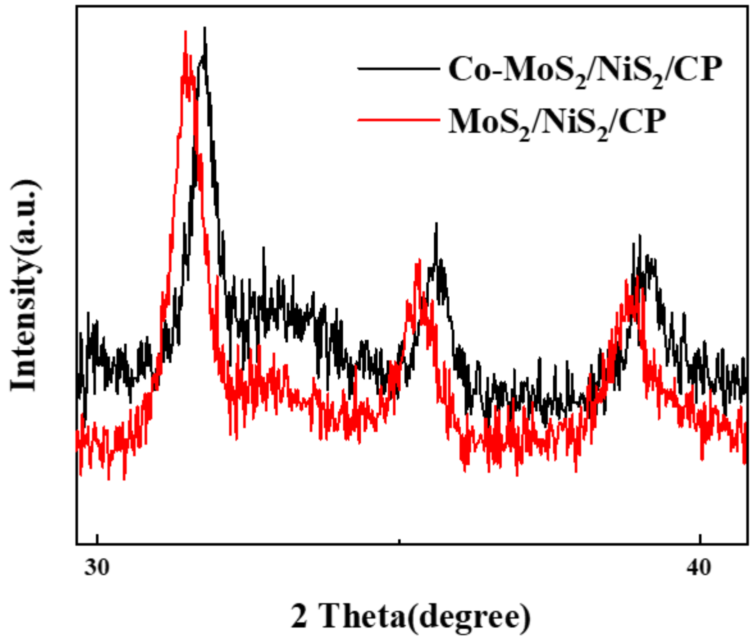

Fig. S2. XRD patterns of Co-MoS_2/NiS_2/CP and NiS_2/MoS_2/CP.

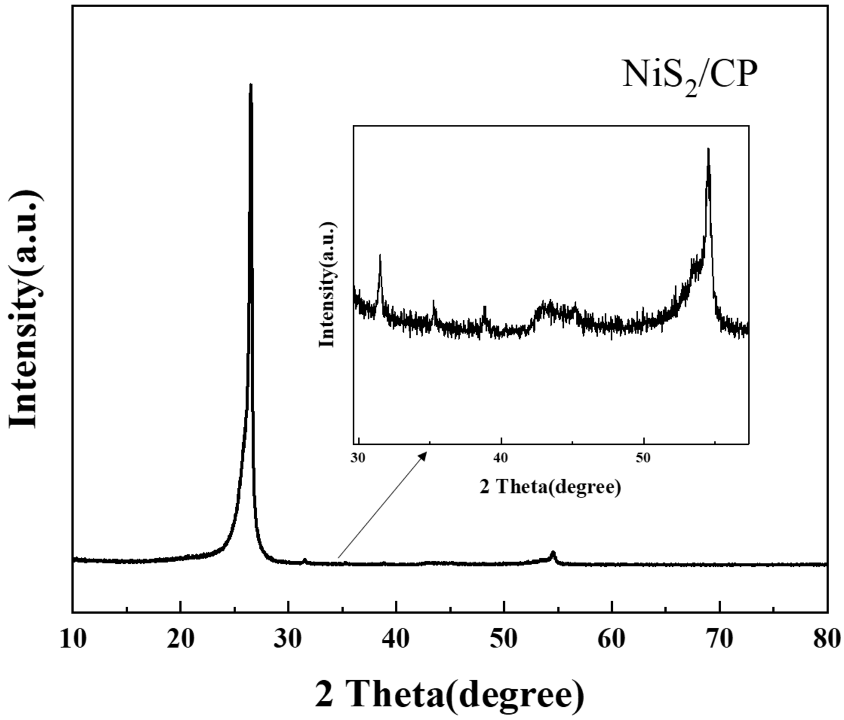

Fig. S3. XRD patterns of NiS_2/CP sample.

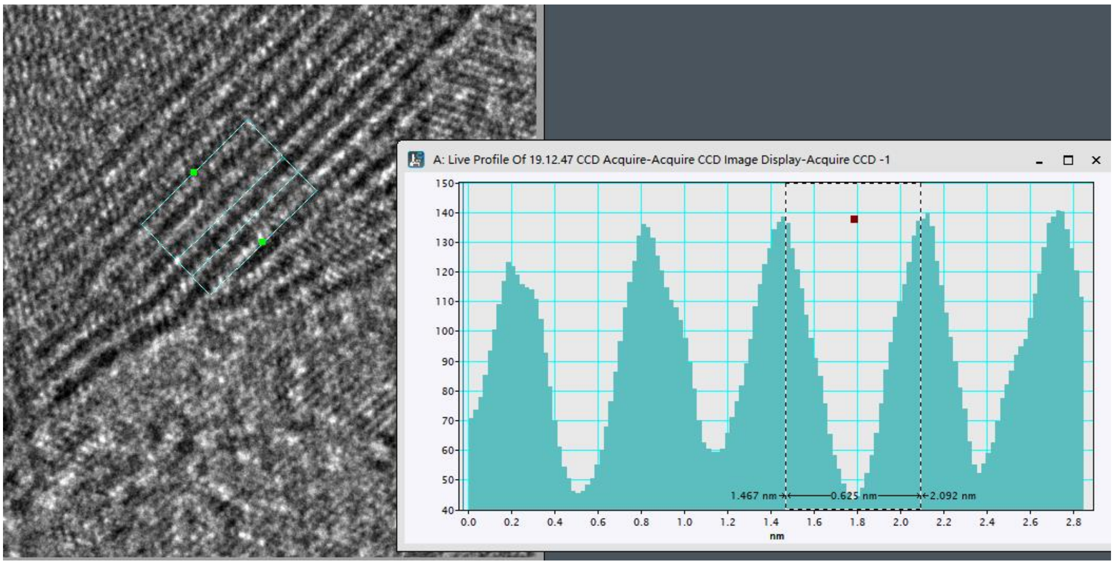

Fig. S4. The lattice distances of MoS_2 in HRTEM image, d=0.62nm.

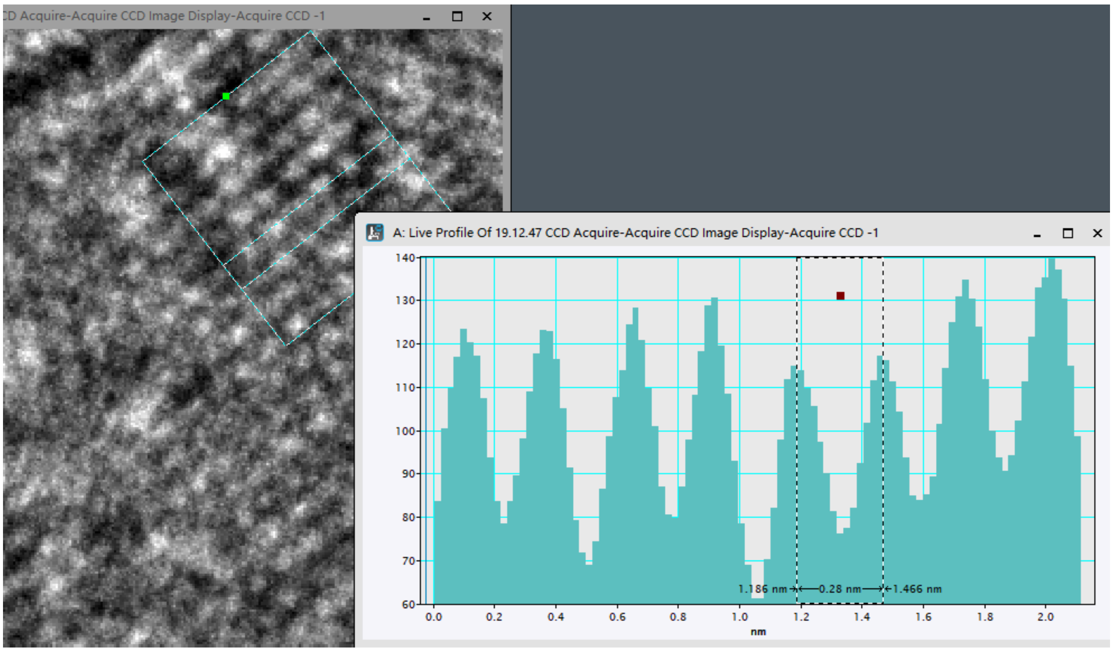

Fig. S5. The lattice distances of NiS_2 in HRTEM image, d=0.28nm.

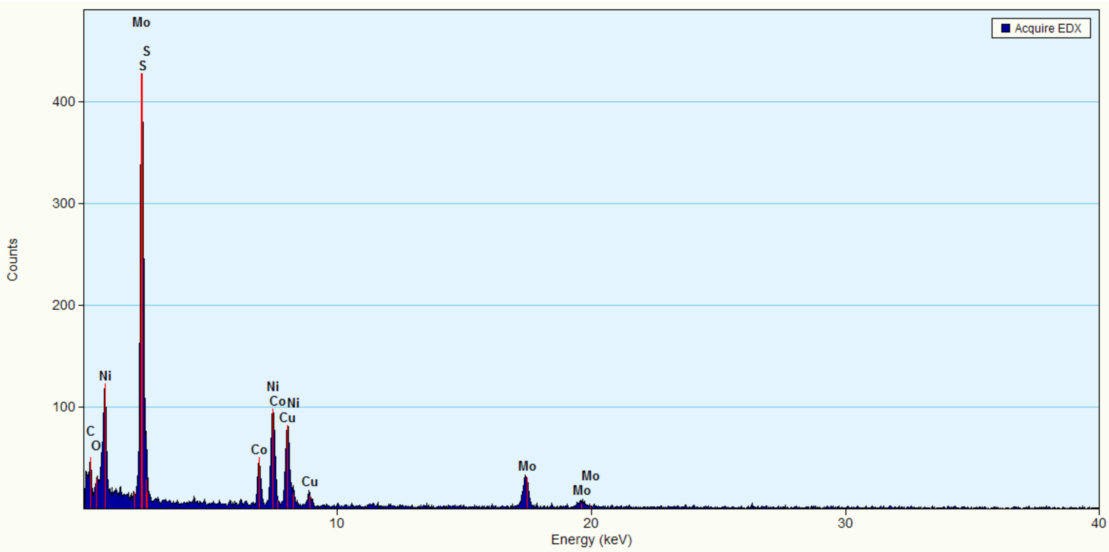

Fig. S6. EDS spectra of Co-MoS_2/NiS_2/CP sample.

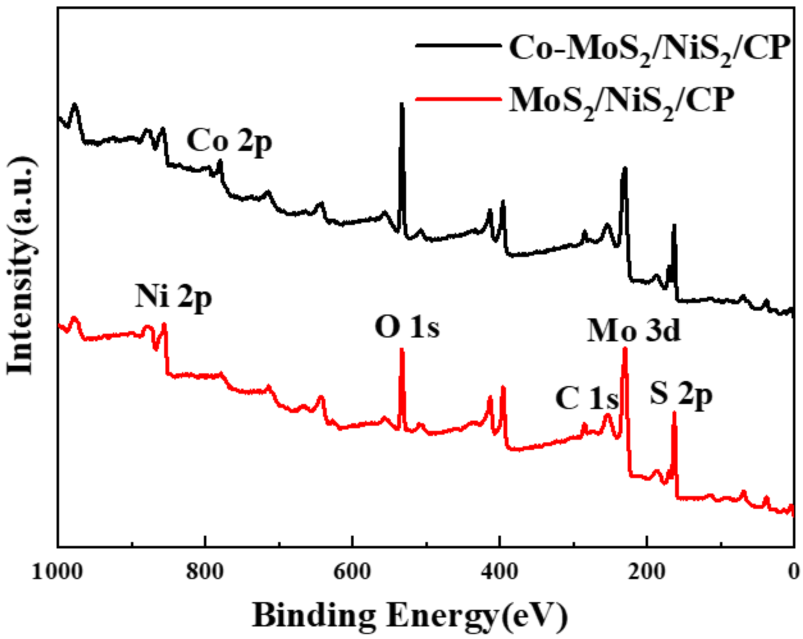

Fig. S7. XPS spectra of Co-MoS_2/NiS_2/CP and NiS_2/MoS_2/CP catalyst.

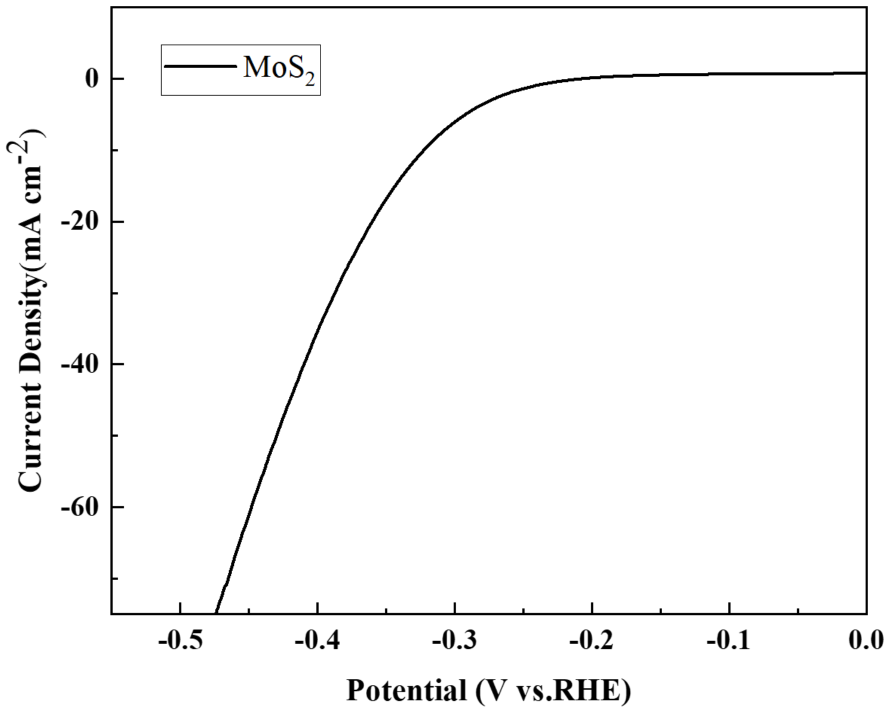

Fig. S8. LSV curve of pure MoS_2 in 1.0 M KOH for HER.

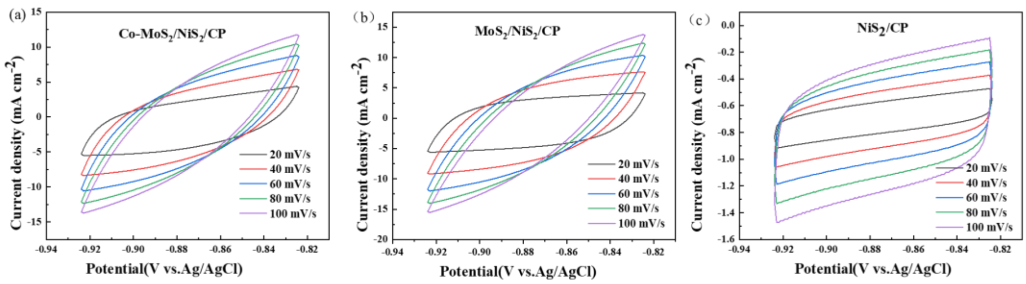

Fig. S9. The cyclic voltammetry (CV) curves of (a) Co-MoS_2/NiS_2/CP, (b) NiS_2/MoS_2/CP and (c) NiS_2/CP at various scan rates for the calculation of electrochemical double-layer capacitances.

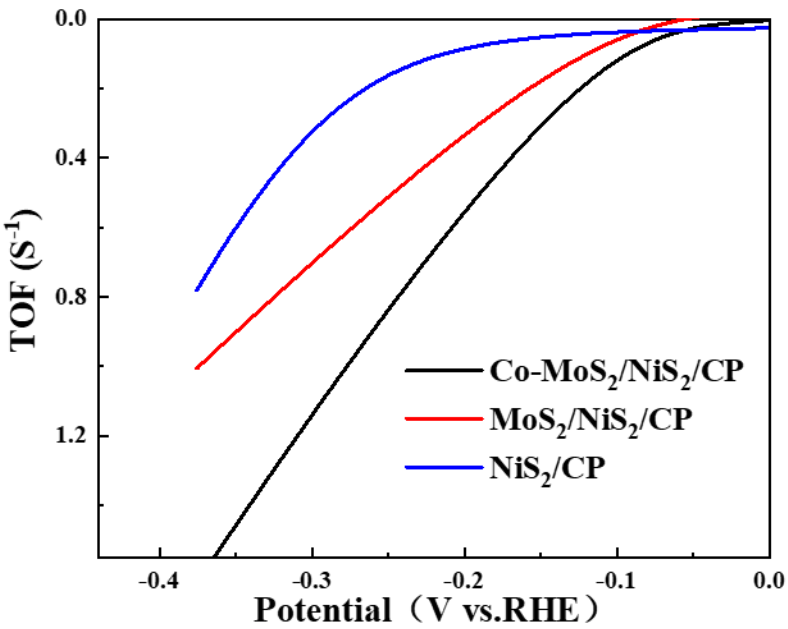

Fig. S10. TOF values of Co-MoS_2/NiS_2/CP, MoS_2/NiS_2/CP and NiS_2/CP for HER.

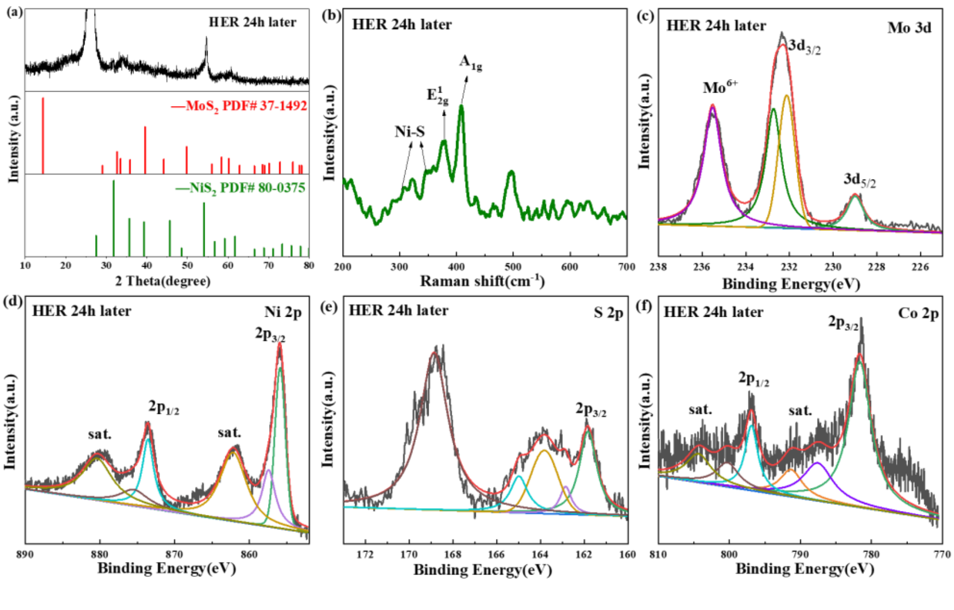

Fig. S11. (a) XRD, (b) Raman, and (c) Mo 3d, (d) Ni 2p, (e) S 2p, (f) Co 2p XPS spectra of Co-MoS_2/NiS_2/CP after 24h HER test.

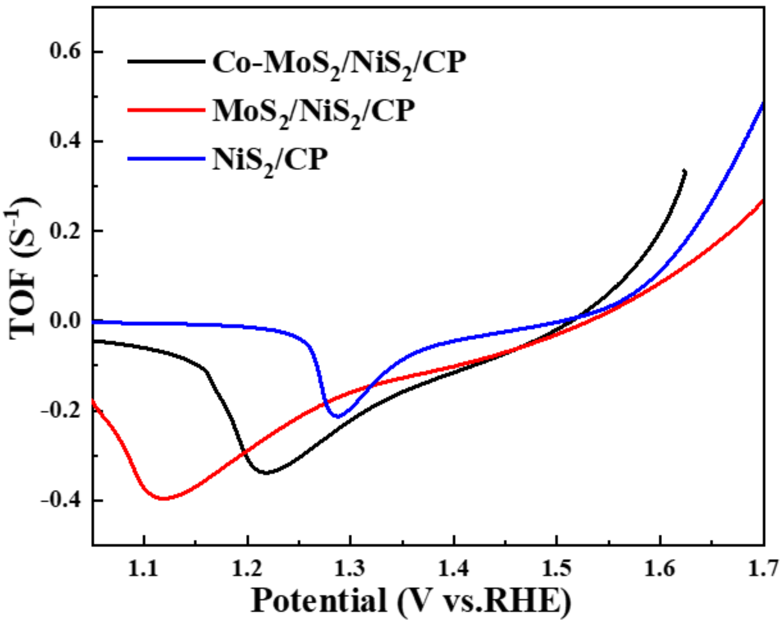

Fig. S12. TOF values of Co-MoS_2/NiS_2/CP, MoS_2/NiS_2/CP and NiS_2/CP for OER.

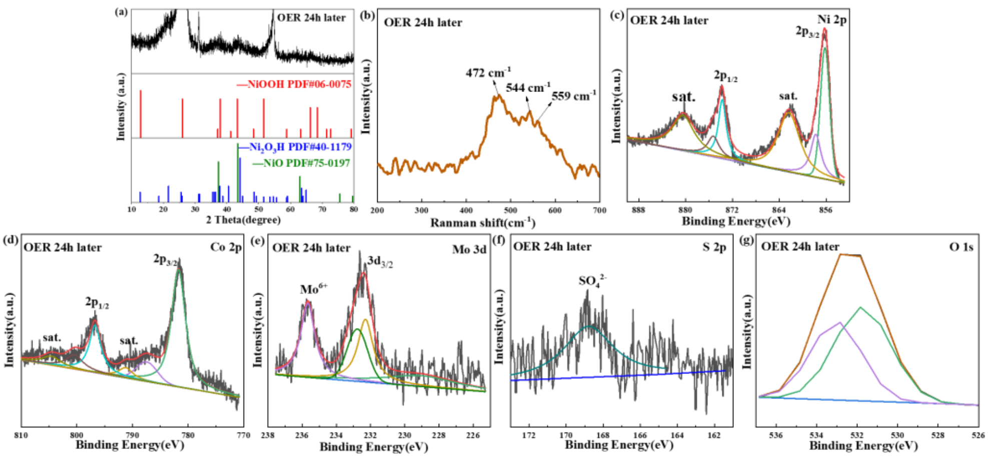

Fig. S13. (a) XRD, (b) Raman, and (c) Ni 2p, (d) Co 2p, (e) Mo 3d, (f) S 2p, (g) O 1s XPS spectra of Co-MoS_2/NiS_2/CP after 24h OER test.

Table S1. *The HER performance of Co-MoS_2/NiS_2/CP compared with other catalysts*

Catalysts	Electrolyte	$\eta_{j=10\ mA\ cm^{-2}}$ (mV)	TOF (H_2 S^{-1})	Ref
Co-MoS_2/NiS_2/CP	1.0M KOH	109	1.47 H_2 s^{-1} at 350 mV	This work
MoS_2/NiS_2/CP	1.0M KOH	129	0.91 H_2 s^{-1} at 350 mV	This work
NiS_2/CP	1.0M KOH	311	0.62 H_2 s^{-1} at 350 mV 0.146	This work
Co-Ni_3N	1.0 M KOH	194	H_2 s^{-1} at 290 mV 0.093 H_2	1
NiCoN/C	1.0 M KOH	103	s^{-1} at 200 mV 0.55 H_2 s^{-1} at	2
Co-NiS_2 NSs	1.0 M KOH	80	100 mV 5.89 H_2 s^{-1} at	3
Co_1/PCN	0.5 M H_2SO_4	151	100 mV 6.5 H_2 s^{-1} at	4
CoN_x/C	0.5 M H_2SO_4	133	200 mV	5

Calculated on the basis of the assumption of 100% participation of all Ni active site in the HER.

Table S2. *The OER performance of Co-MoS_2/NiS_2/CP compared with other catalysts*

Catalysts	Electrolyte	$\eta_{j=10\ mA\ cm^{-2}}$ (mV)	TOF (O_2 S^{-1})	Ref
Co-MoS_2/NiS_2/CP	1.0M KOH	323	0.159 O_2 s^{-1} at 350 mV^a 0.092	This work
MoS_2/NiS_2/CP	1.0M KOH	351	O_2 s^{-1} at 350 mV^a 0.071 O_2 s^{-1}	This work
NiS_2/CP	1.0M KOH	397	at 350 mV^a 0.036 O_2 s^{-1} at	This work
α-$Ni(OH)_2$ hollow spheres	1.0 M KOH	331	350 mV^a 0.003 O_2 s^{-1} at 350	6
β-$Ni(OH)_2$ hexagonal NPs	1.0 M KOH	444	mV^a 0.14 O_2 s^{-1} at 300 mV^b	6
Fe,Ni-CoS2	1.0 M KOH	242	4.71 O_2 s^{-1} at 1.45 V^b	7
β-$Ni(OH)_2$ nanoburls	1.0 M KOH	300		8

NiFe-LDH-V	1.0 M KOH	-	0.165 O_2 s^{-1} at 1.50 V^b	9

[a]Calculated on the basis of the assumption of 100% participation of all Ni active site in the OER. [b] Calculated using the ORR current from the RRDE experiment.

References

1 X. Q. Zheng, L. S. Peng, L. Li, N. Yang, Y. J. Yang, J. Li, J. C. Wang and Z. D. Wei, *Chem. Sci.*, 2018, **9**, 1822-1830.

2 J. X. Feng, J. Q. Wu, Y. X. Tong and G.-R. Li, *J. Am. Chem. Soc.*, 2018, **140**, 610-617.

3 J. Yin, J. Jin, H. Zhang, M. Lu, Y. Peng, B. Huang, P. Xi and C. H. Yan, *Angew. Chem. Int. Ed.*, 2019, **58**, 18676-18682.

4 L. Zeng, K. Sun, Z. Yang, S. Xie, Y. Chen, Z. Liu, Y. Liu, J. Zhao, Y. Liu and C. Liu, *J. Mater. Chem. A*, 2018, **6**, 4485-4493.

5 J. Dong, F. Q. Zhang, Y. Yang, Y. B. Zhang, H. He, X. Huang, X. Fan and X. M. Zhang, *Appl. Catal. B*, 2019, **243**, 693-702.

6 M. Gao, W. Sheng, Z. Zhuang, Q. Fang, S. Gu, J. Jiang and Y. Yan, *J. Am. Chem. Soc.*, 2014, **136**, 7077-7084.

7 W. Peng, A. Deshmukh, N. Chen, Z. Lv, S. Zhao, J. Li, B. Yan, X. Gao, L. Shang, Y. Gong, L. Wu, M. Chen, T. Zhang and H. Gou, *Acs Catal.*, 2022, **12**, 3743-3751.

8 S. Anantharaj, P. E. Karthik and S. Kundu, *Catal. Sci. Technol.*, 2017, **7**, 882-893.

9 D. Chen, J. Qiu, X. Chen, S. Chen, J. Zhang and Z. Peng, *J. Phys. Chem. Lett.*, 2023, **14,** 2148−2154.