

Supporting information

Preparation of Ni-Fe-based transition metal phosphide as efficient electrocatalyst for the oxygen evolution reaction

Huanhuan Tang,^{‡a} Yufan Qi,^{‡a} Danning Feng,^a Yangyang Chen,^a Liying Liu,^a Lei Hao,^a Kefen Yue,^{*a} Dongshen Li,^{*b} and Yaoyu Wang^a

^a College of Chemistry and Materials Science, Key Laboratory of Synthetic and Natural Functional Molecule of the Ministry of Education, National Demonstration Center for Experimental Chemistry Education, Shaanxi Key Laboratory of Physico-Inorganic Chemistry, Northwest University, Xi'an 710127, People's Republic of China.

Email: ykflyy@nwu.edu.cn

^b Dong-Sheng Li

College of Materials and Chemical Engineering, Hubei Provincial Collaborative Innovation Center for New Energy Microgrid, Key Laboratory of Inorganic Nonmetallic Crystalline and Energy Conversion Materials, China Three Gorges University, No. 8, Daxue Road, Yichang, 443002, China.

Email: lidongsheng1@126.com

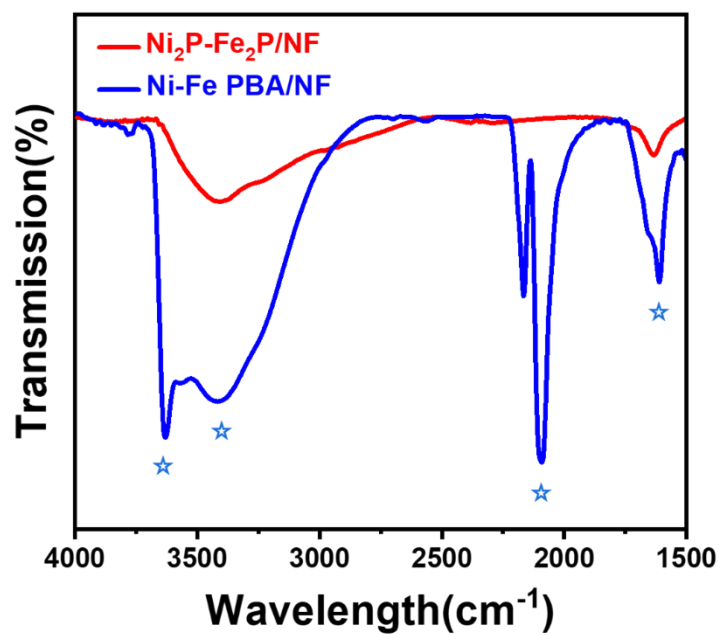


Fig. S1 FT-IR spectra of Ni₂P-Fe₂P/NF and Ni-Fe PBA/NF.

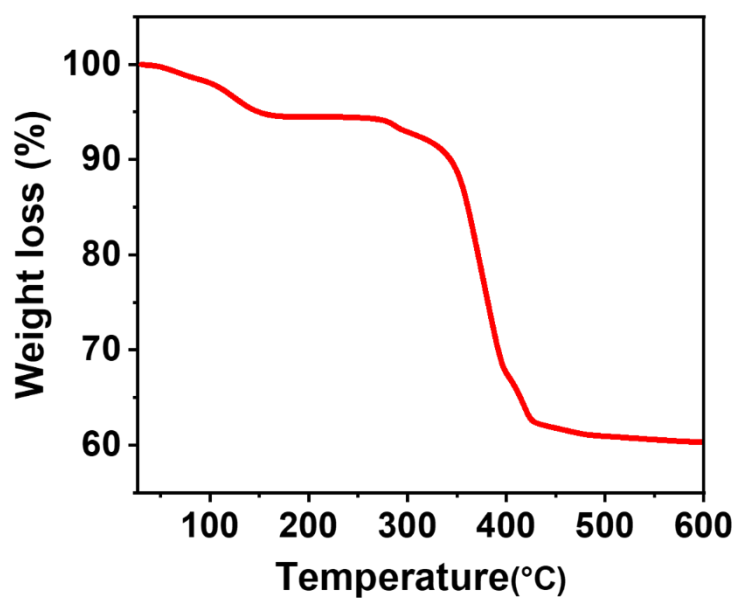


Fig. S2 TGA curve of Ni-Fe PBA precursor measured under a N₂ atmosphere.

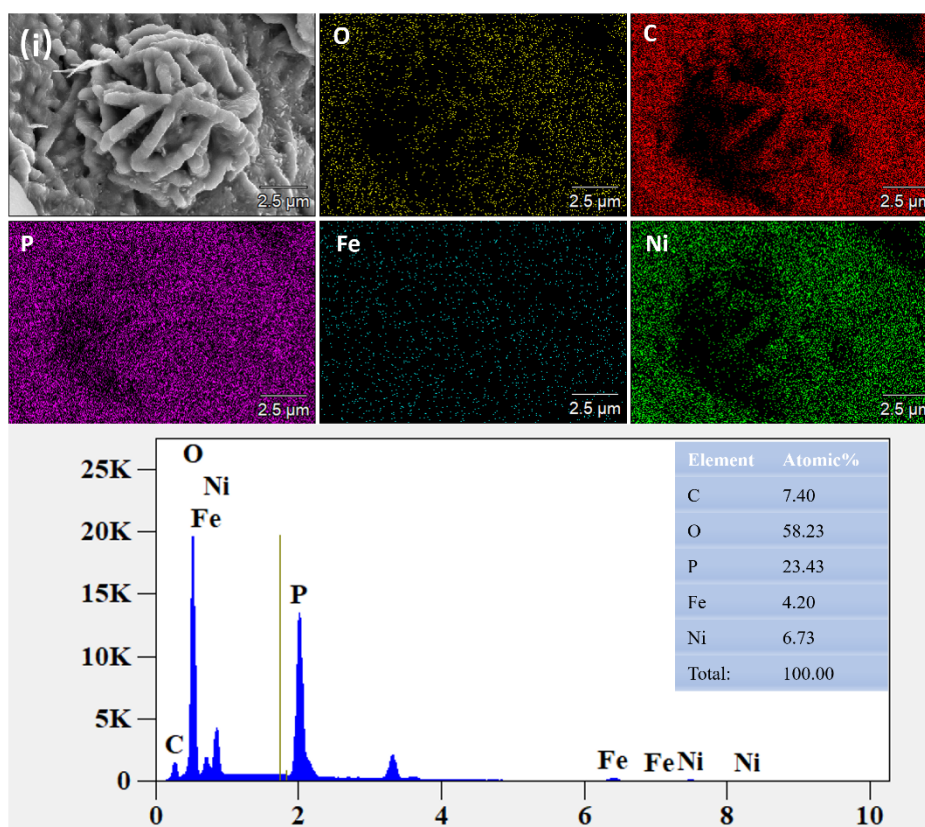


Fig. S3 EDX spectrum and corresponding elemental compositions of the $\text{Ni}_2\text{P-Fe}_2\text{P/NF}$.

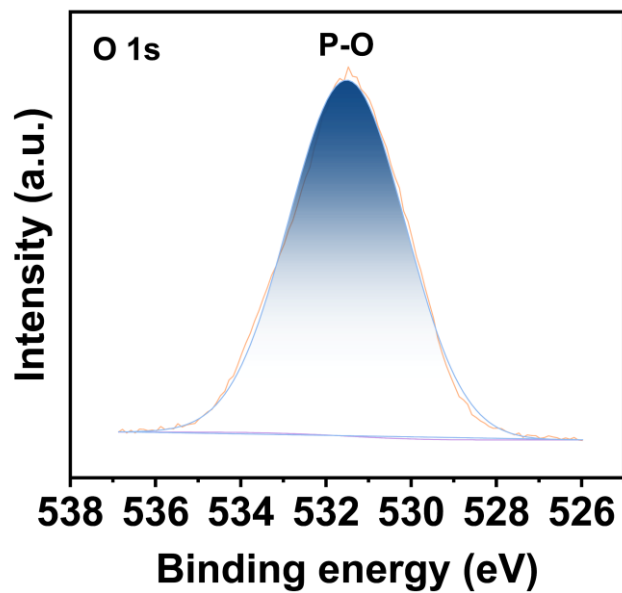


Fig. S4 High-resolution XPS spectrum of O 1s.

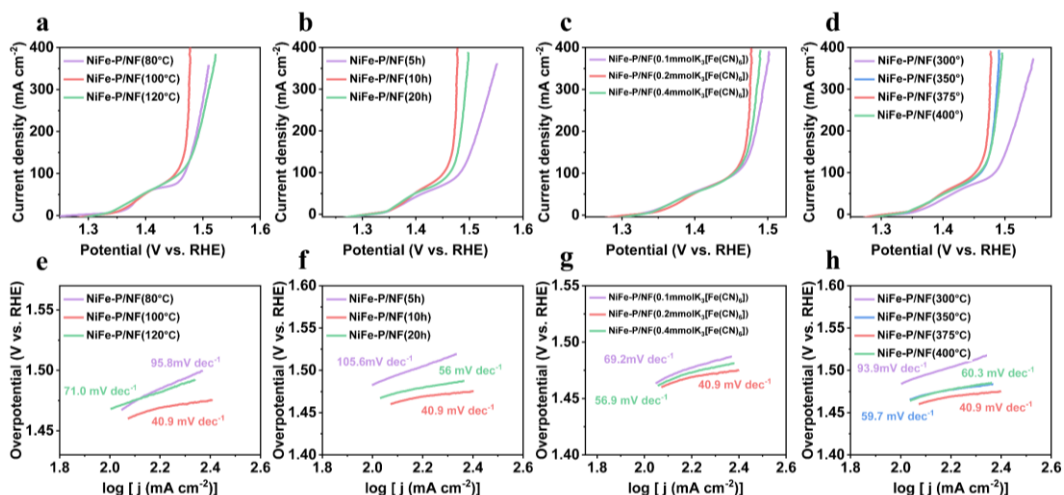


Fig. S5 Under different conditions, the LSV curves and Tafel slopes of mixed-metal phosphides.

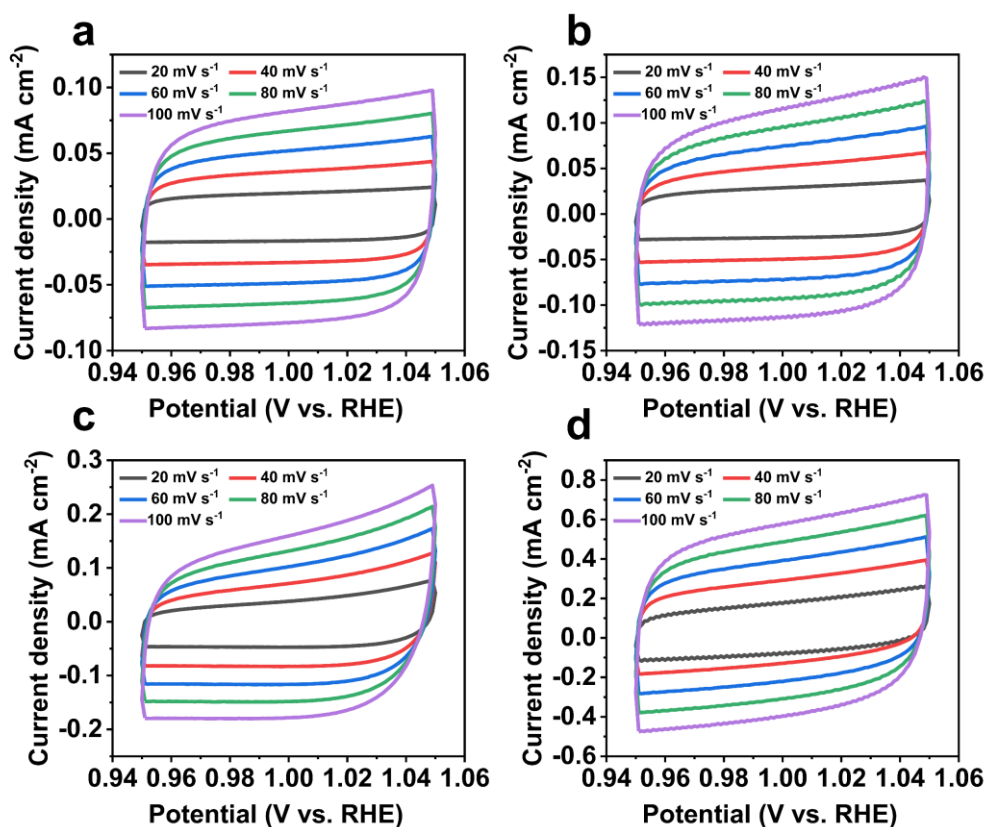


Fig. S6 The cyclic voltammograms (CVs) measurements with various scan rates for (a) NF, (b) Ni(OH)₂/NF, (c) Ni-Fe PBA/NF, (d) Ni₂P-Fe₂P/NF.

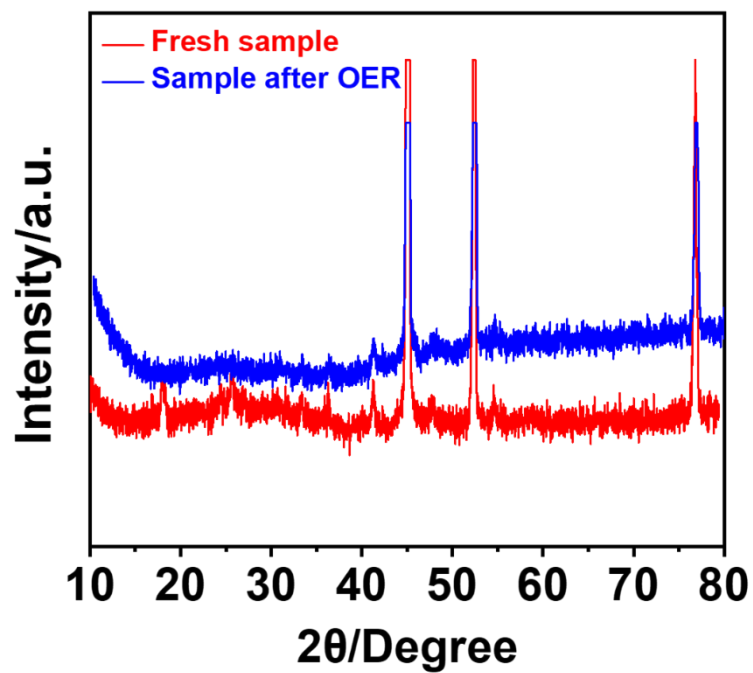


Fig. S7 The XRD patterns of fresh sample and sample after OER.

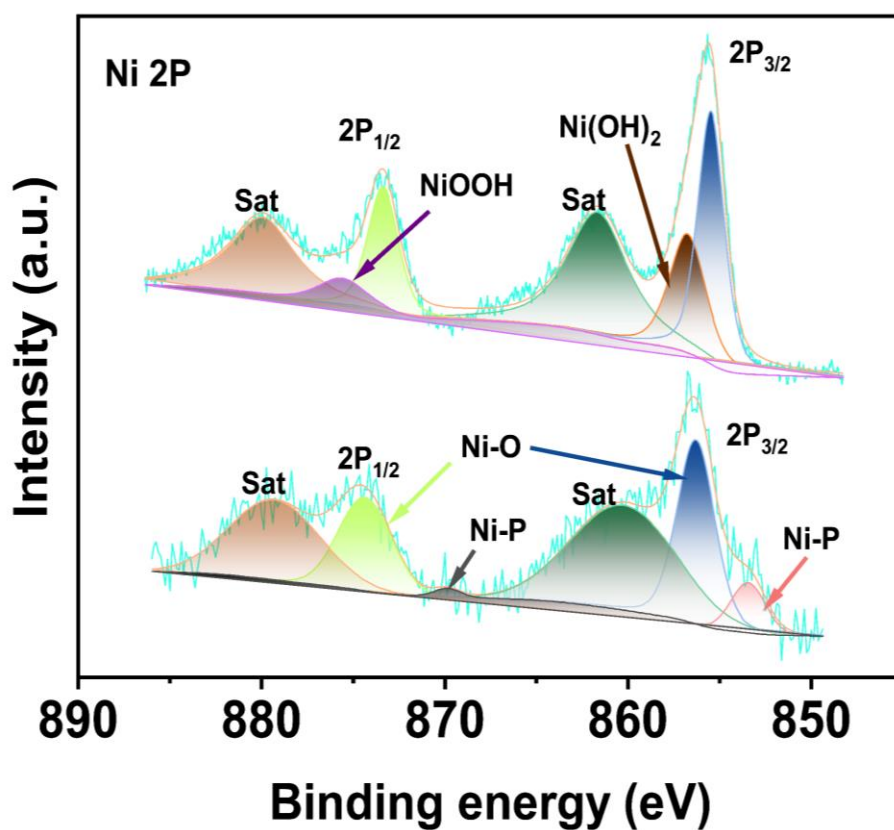


Fig. S8 The high resolution XPS of Ni 2p before (down) and after (up) OER test.

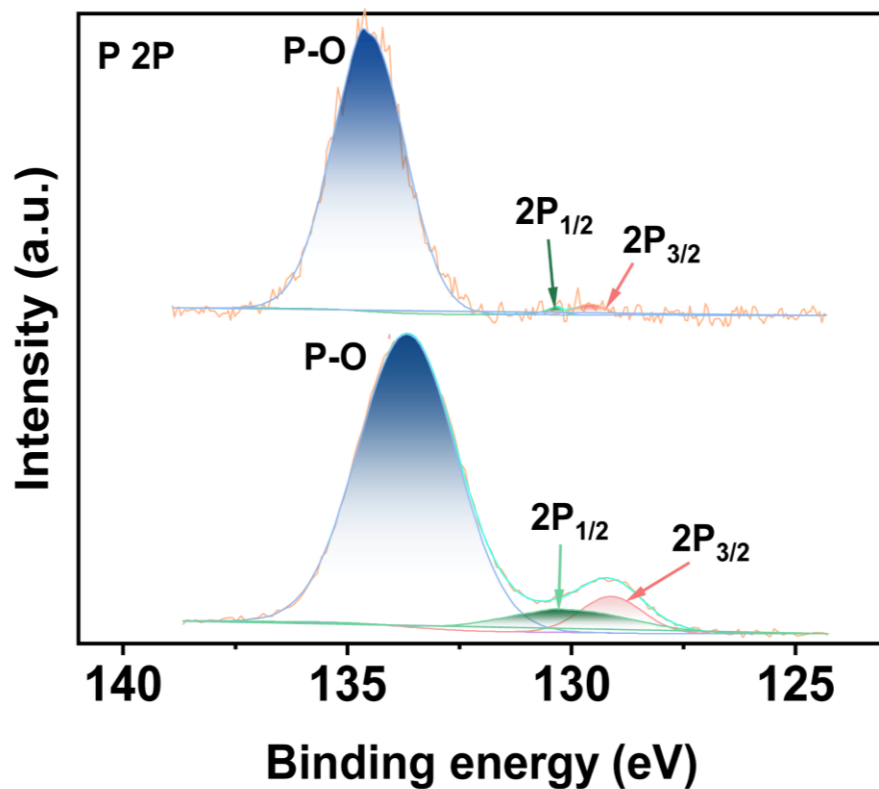


Fig. S9 The high resolution XPS of P 2p before (down) and after (up) OER test.

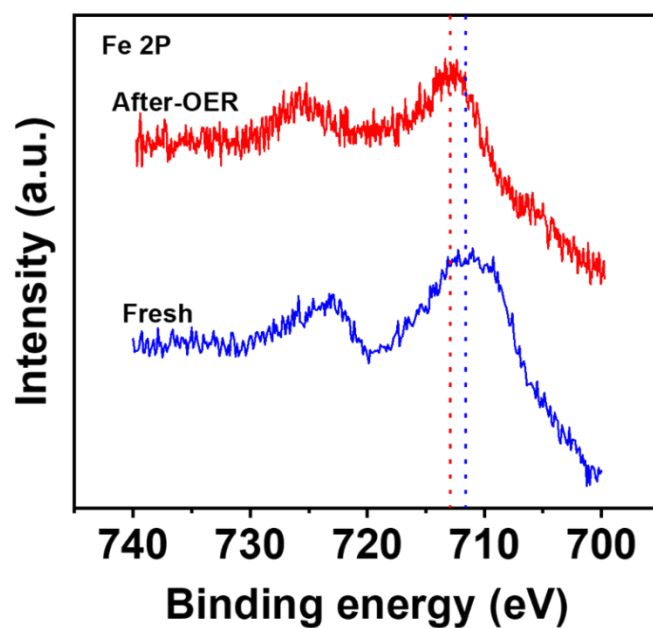


Fig. S10 The high resolution XPS of Fe 2p before (down) and after (up) OER test.

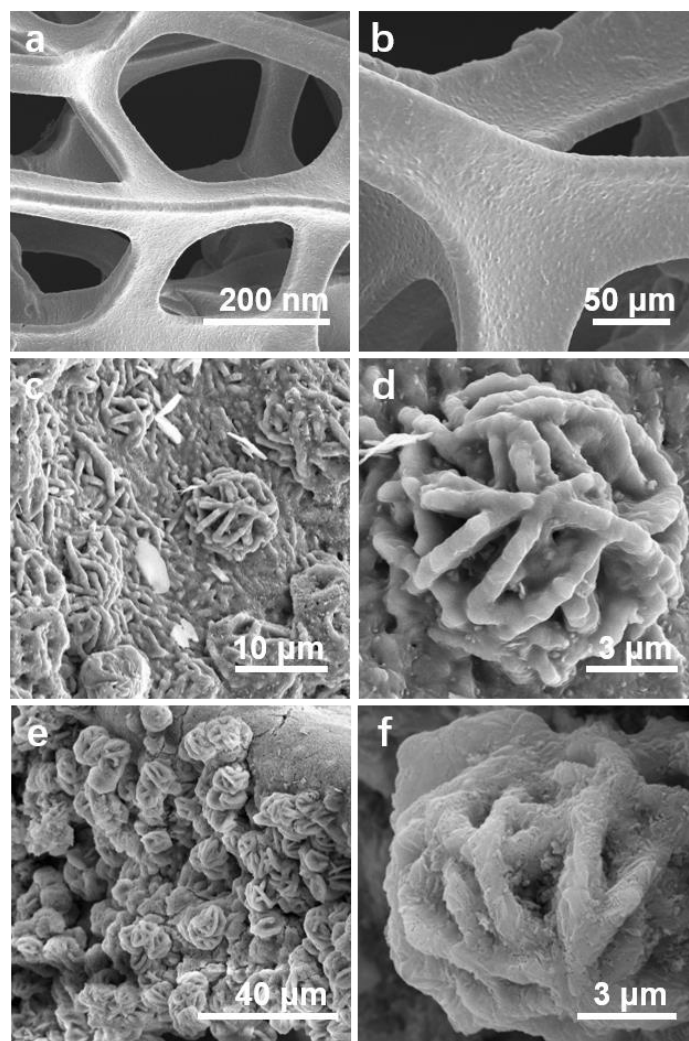


Fig. S11 The SEM images of (a,b)bare NF, (c,d) Ni₂P-Fe₂P/NF and (e,f) Ni₂P-Fe₂P/NF after OER test.

Table S1 Average mass loading of catalysts on NF substrates.

Samples	Mass loading (mg cm ⁻²)
Ni(OH) ₂ /NF	3.19
Ni-Fe PBA/NF	2.02
Ni ₂ P-Fe ₂ P/NF	2.63

Table S2 The simulated series resistance (R_s) and charge transfer resistance (R_{ct}) values based on the fitting models.

Samples	R_s (Ω)	R_{ct} (Ω)
NF	1.258	5.68
Ni(OH) ₂ /NF	1.276	5.50
Ni-Fe PBA/NF	1.497	1.18
Ni ₂ P-Fe ₂ P/NF	1.288	0.23

Table S3 The activity comparison of PBA precursors on the surface of NF for OER in 1.0 M KOH solution.

Catalysis	Electrolyte	Overpotential	Tafel slope	Ref
Ni₂P-Fe₂P/NF	1 M KOH	222 mV 100 mA cm ⁻²	40.9 mV dec ⁻¹	This work
NiFeP@NiP@NF	1 M KOH	252 mV 100 mA cm ⁻²	56 mV dec ⁻¹	1
NiFe₂O₄@NPNiFePB A/NF	1 M KOH	304 mV 100 mA cm ⁻²	80 mV dec ⁻¹	2
Ni(OH)₂@Ni₃S₂/NF	1 M KOH	210 mV 100 mA cm ⁻²	62.0 mV dec ⁻¹	3
NiSe₂/CoSe/NF	1 M KOH	270 mV 100 mA cm ⁻²	69.77 mV dec ⁻¹	4
Ni-Fe-P@NC/NF	1 M KOH	245 mV 100 mA cm ⁻²	81.0 mV dec ⁻¹	5
(Mo, Fe)P₂O₇@NF	1 M KOH	250 mV 100 mA cm ⁻²	40.0 mV dec ⁻¹	6
NiFeP_x/NF	1 M KOH	258 mV 100 mA cm ⁻²	29 mV dec ⁻¹	7
FeCoNi-LDH/NF	1.0 M KOH	230 mV	45.76 mV dec ⁻¹	8

	+ 0.5 M urea	100 mA cm ⁻²		
FeCoNiN/NF	1 M KOH	267 mV 50 mA cm ⁻²	60mV dec ⁻¹	9
Ni₃S₂@MIL-53(NiFeCo)/NF	1 M KOH	236 mV 50 mA cm ⁻²	14.8 mV dec ⁻¹	10
MOF CoFeP	1 M KOH	140 mV 50 mA cm ⁻²	40 mV dec ⁻¹	11
NiFeP@NC/NF	1 M KOH	286 mV 20 mA cm ⁻²	69 mV dec ⁻¹	12
Ru–MnFeP/NF	1 M KOH	191 mV 20 mA cm ⁻²	69 mV dec ⁻¹	13
PBA-SMo /NF-10 h	1 M KOH	252 mV 20 mA cm ⁻²	64 mV dec ⁻¹	14
CuFe-P/NF	1 M KOH	231 mV 10 mA cm ⁻²	63.0 mV dec ⁻¹	15
Fe-CoP/NF	1 M KOH	190 mV 10 mA cm ⁻²	92 mV dec ⁻¹	16
Ni_xCo_{3-x}O₄/NF	1 M KOH	287 mV 10 mA cm ⁻²	88 mV dec ⁻¹	17
CoFePBA@NiCoFe-LTH/NF	1 M KOH	228 mV 10 mA cm ⁻²	36 mV dec ⁻¹	18
(NiCo)₂P/NF	1 M KOH	162 mV 10 mA cm ⁻²	135 mV dec ⁻¹	19

References

- 1 F. Diao, W. Huang, G. Ctistis, H. Wackerbarth, Y. Yang, P. Si, J. Zhang, X. Xiao and C. Engelbrekt, *ACS Appl Mater Interfaces*, 2021, **13**, 23702-23713.
- 2 X. Zhang, I. U. Khan, S. Huo, Y. Zhao, B. Liang, K. Li and H. Wang, *Electrochimica Acta*, 2020, **363**, 137221.

- 3 X. Chen, L. Yang, Y. Huang, S. Ge, H. Zhang, Y. Cui, A. Huang and Z. Xiao, *Chem. Eur. J*, 2020, **26**, 1111-1116.
- 4 J. Zhang, L. Jin, P. Gu, L. Hu, D. Chen, J. He, Q. Xu and J. Lu, *ACS Appl. Nano Mater*, 2021, **4**, 12407-12414.
- 5 Y. Wang, S. Zhao, Y. Zhu, R. Qiu, T. Gengenbach, Y. Liu, L. Zu, H. Mao, H. Wang, J. Tang, D. Zhao and C. Selomulya, *iScience*, 2020, **23**, 100761.
- 6 J. Wang, J. Huang, S. Zhao, I. P. Parkin, Z. Tian, F. Lai, T. Liu and G. He, *Green Energy Environ*, 2022, **02**, 014.
- 7 X. Y. Zhang, B. Y. Guo, X. Y. Chen, L. Zhao, B. Dong, M. Yang, J. F. Yu, L. Wang, C. G. Liu and Y. M. Chai, *Mater. Today Energy*, 2020, **17**, 100468.
- 8 B. Yuan, F. Sun, C. Li, W. Huang and Y. Lin, *Electrochim. Acta*, 2019, **313**, 91-98.
- 9 Z. Wang, S. Jiao, B. Wang, Y. Kang, W. Yin, X. Lv, Q. Zhang, Z. Zhang, Y. Chen and G. Pang, *Int. J. Hydrog. Energy*, 2021, **46**, 8345-8355.
- 10 B. Yuan, C. Li, L. Guan, K. Li and Y. Lin, *J. Power Sources*, 2020, **451**, 227295.
- 11 A. Muthurasu, G. P. Ojha, M. Lee and H. Y. Kim, *J. Phys. Chem. C*, 2020, **124**, 14465-14476.
- 12 R. Yue, Z. Mo, C. Shuai, S. He, W. Liu, G. Liu, Y. Du, Q. Dong, J. Ding, X. Zhu, N. Liu and R. Guo, *J. Electroanal. Chem*, 2022, **918**, 116427.
- 13 D. Chen, Z. Pu, R. Lu, P. Ji, P. Wang, J. Zhu, C. Lin, H. W. Li, X. Zhou, Z. Hu, F. Xia, J. Wu and S. Mu, *Adv. Energy Mater*, 2020, **10**, 2000814.
- 14 C. Zhang, J. Chen, J. Zhang, Y. Luo, Y. Chen, Y. Xue, Y. Yan, Y. Jiao, G. Wang and R. Wang, *J Colloid Interface Sci*, 2022, **607**, 967-977.
- 15 X. Xing, Y. Song, W. Jiang and X. Zhang, *Sustain. Energy Fuels*, 2020, **4**, 3985-3991.
- 16 L. M. Cao, Y. W. Hu, S. F. Tang, A. Iljin, J. W. Wang, Z. M. Zhang and T. B. Lu, *Adv Sci*, 2018, **5**, 1800949.
- 17 Y. Shen, S. G. Guo, F. Du, X. B. Yuan, Y. Zhang, J. Hu, Q. Shen, W. Luo, A. Alsaedi, T. Hayat, G. Wen, G. L. Li, Y. Zhou and Z. Zou, *Nanoscale*, 2019, **11**, 11765-11773.
- 18 T. Wang, Q. Pang, B. Li, Y. Chen and J. Z. Zhang, *Appl. Phys. Lett*, 2021, **118**, 233903.
- 19 G. Yan, X. Zhang and L. Xiao, *J Mater Sci*, 2019, **54**, 7087-7095.