

Electronic Supplementary Material (ESI) for Journal of Materials Chemistry A.  
This journal is © The Royal Society of Chemistry 2023

## **One-step hydrothermal synthesis of Se-doped NiTe electrocatalysts for efficient hydrogen production from saline water assisted by the anodic iodide oxidation**

Hao Tan,<sup>a, b</sup> Zhipeng Yu,<sup>\*b</sup> Alec P. LaGrow,<sup>c</sup> Shiyu Ma,<sup>a</sup> Jingwei Wang,<sup>b</sup> Hong Li,<sup>a</sup> Dehua Xiong<sup>\*a</sup> and Lifeng Liu<sup>\*b, d</sup>

<sup>a</sup>State Key Laboratory of Silicate Materials for Architectures, Wuhan University of Technology, Wuhan 430070, P. R. China

<sup>b</sup>Songshan Lake Materials Laboratory, Dongguan 523808, P. R. China

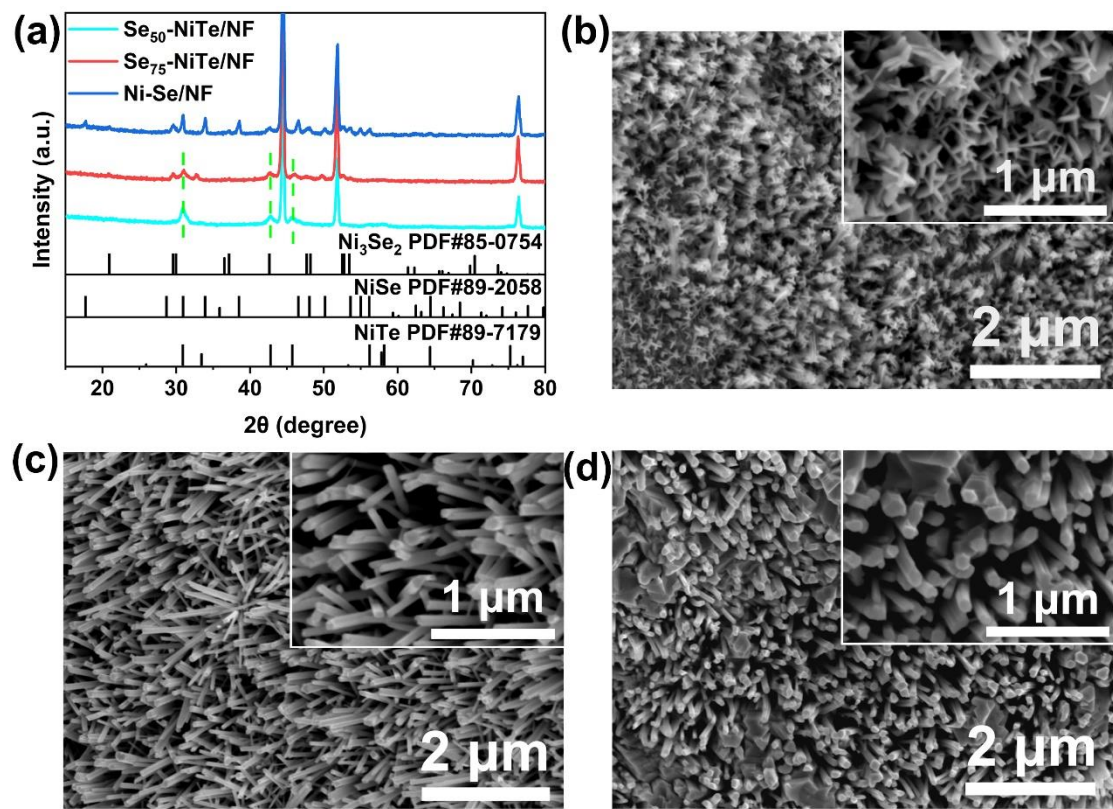
<sup>c</sup>Scientific Imaging Section, Okinawa Institute of Science and Technology Graduate University, Kunigami-gun, Okinawa 904-0412, Japan

<sup>d</sup>Clean Energy Cluster, International Iberian Nanotechnology Laboratory (INL), Braga 4715-330, Portugal

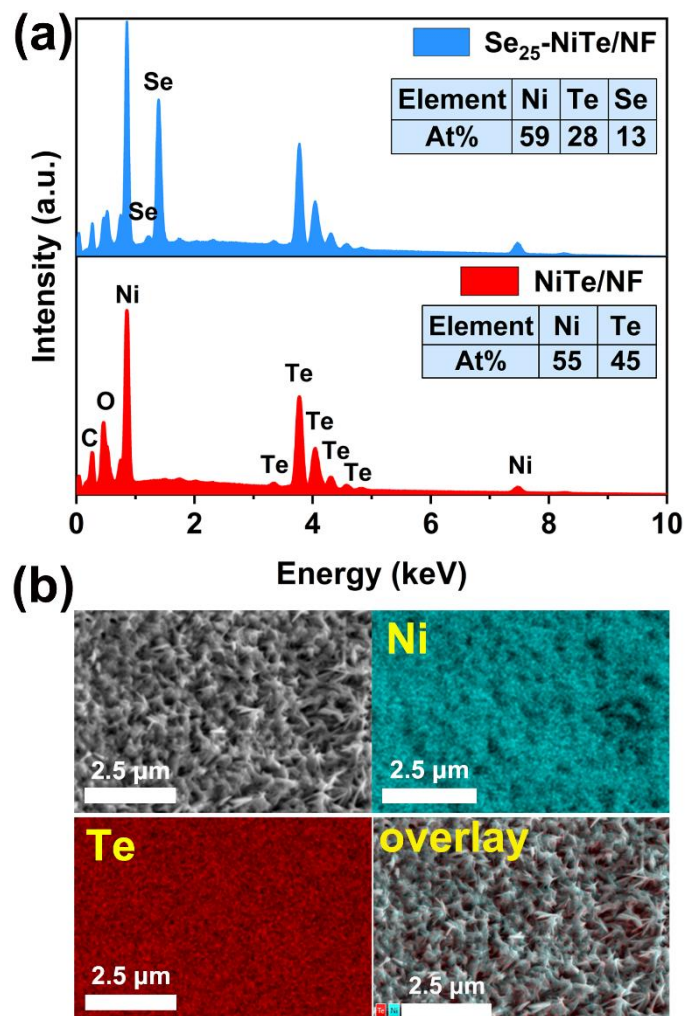
\*Corresponding authors:

E-mail address: [zhipeng-yu@outlook.com](mailto:zhipeng-yu@outlook.com) (Z. P. Yu); [xiongdehua@whut.edu.cn](mailto:xiongdehua@whut.edu.cn) (D. H. Xiong);

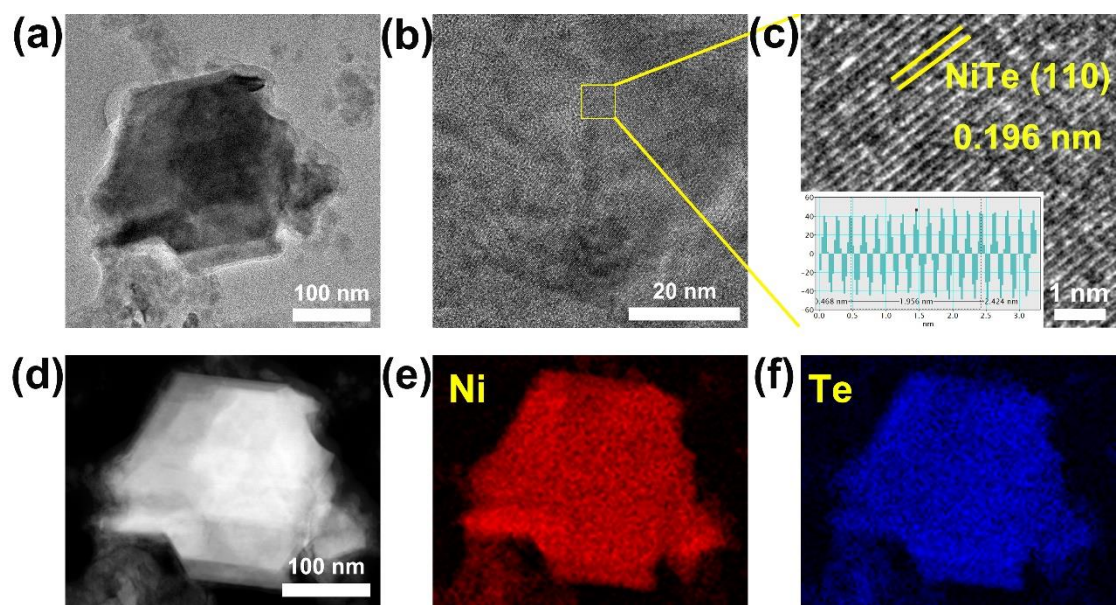
[liu.lifeng@sslslab.org.cn](mailto:liu.lifeng@sslslab.org.cn) (L. Liu)



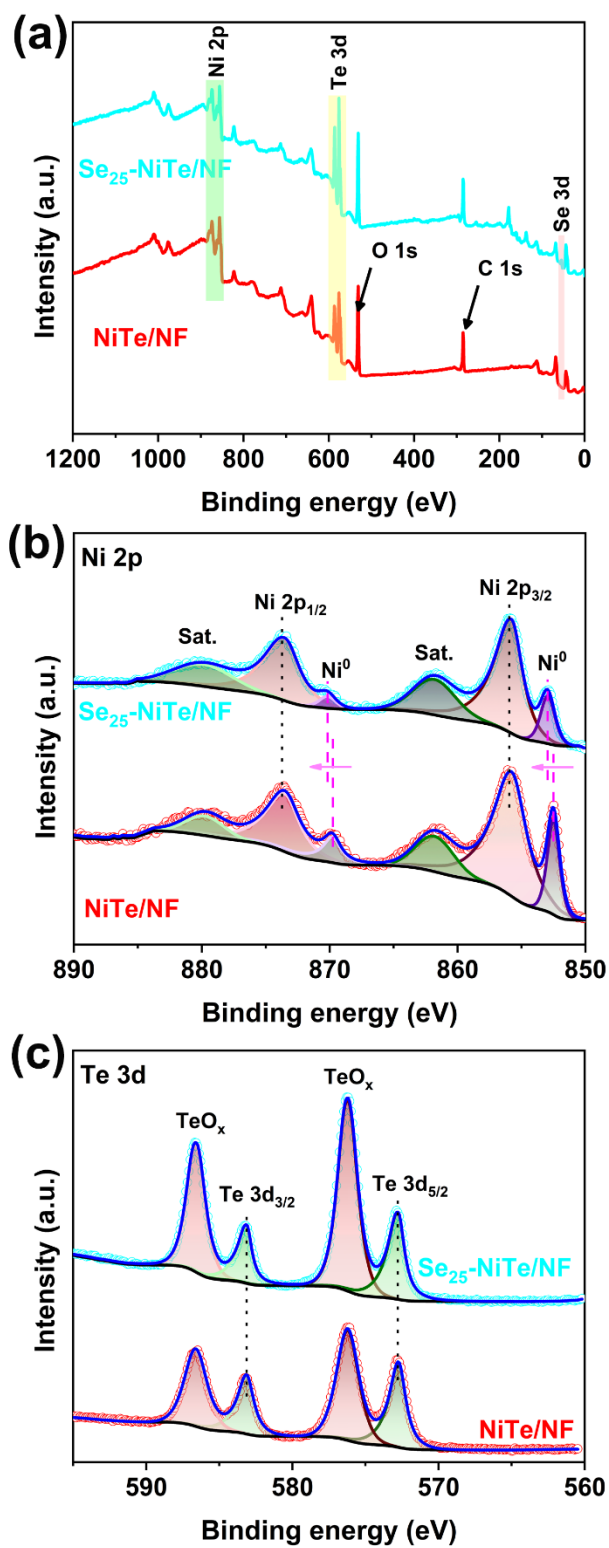
**Fig. S1** (a) XRD patterns and (b) SEM images of Se<sub>50</sub>-NiTe/NF, Se<sub>75</sub>-NiTe/NF and Ni-Se/NF electrodes.



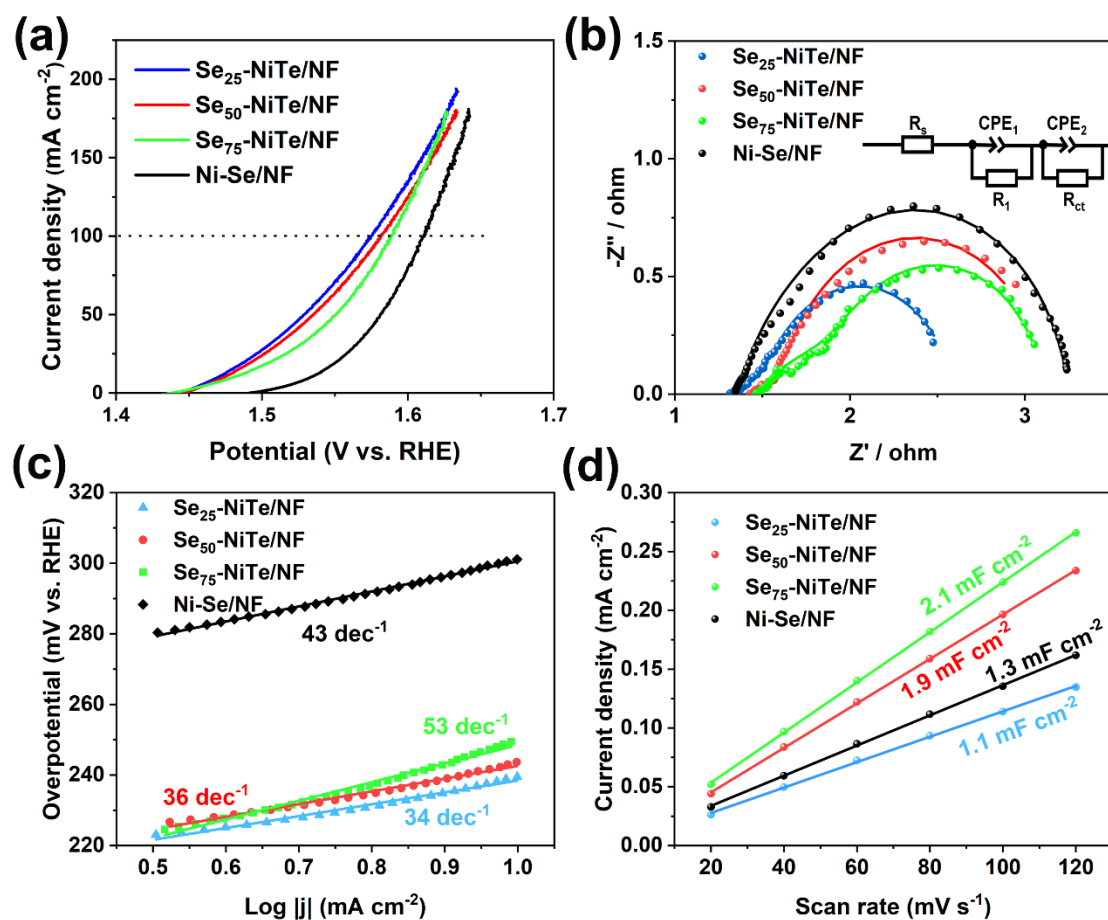
**Fig. S2** (a) EDS spectra of the NiTe/NF and Se<sub>25</sub>-NiTe/NF electrodes. (b) SEM image and the corresponding elemental maps of the NiTe/NF electrode.



**Fig. S3** (a) TEM image, (b-c) HRTEM images, (d) HAADF-STEM image and (e-f) the corresponding elemental maps of the NiTe/NF catalyst.

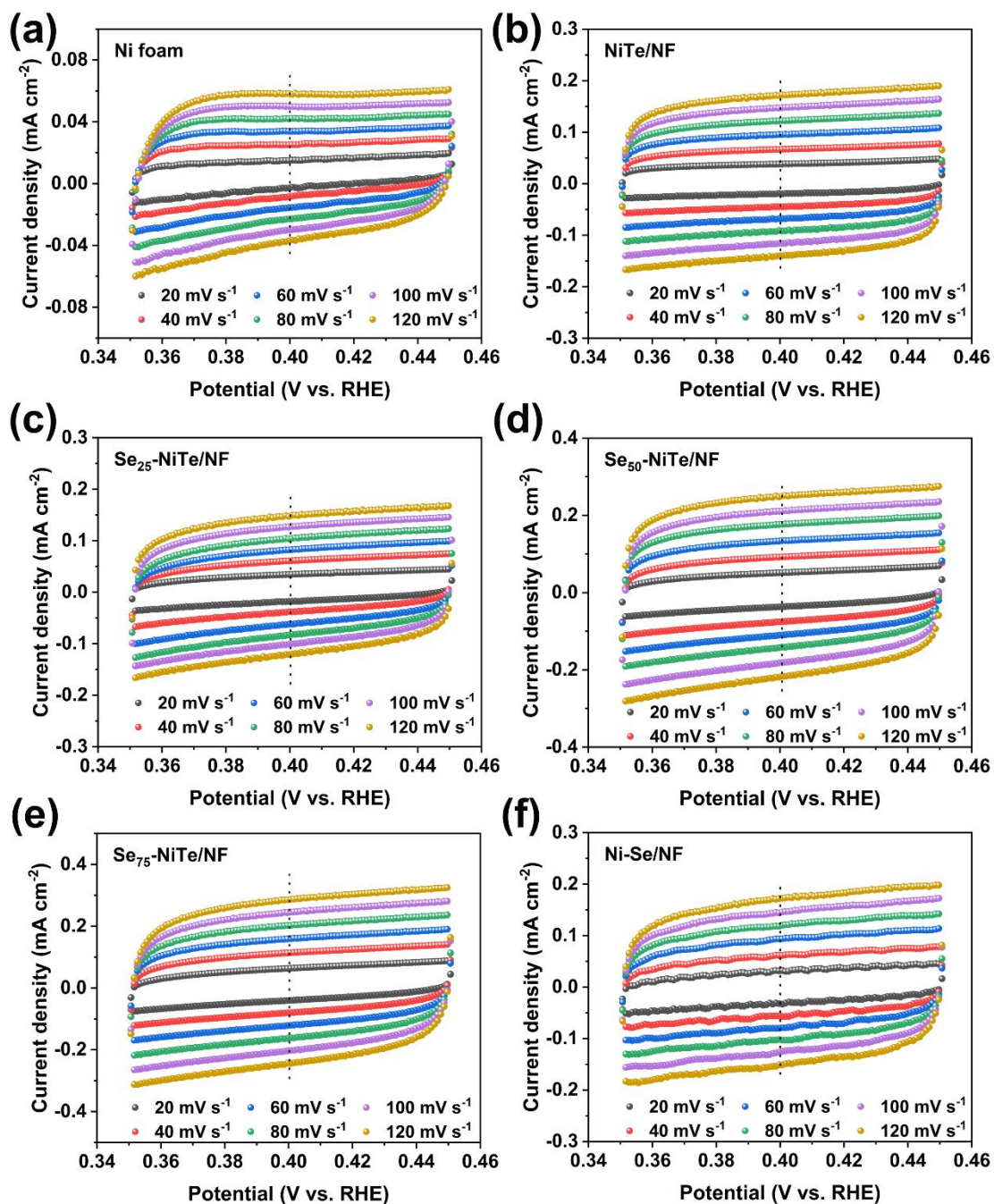


**Fig. S4** (a) XPS survey spectrum. High-resolution (b) Ni 2p and (c) Te 3d XPS spectra of the NiTe/NF and  $\text{Se}_{25}\text{-NiTe/NF}$  electrodes.

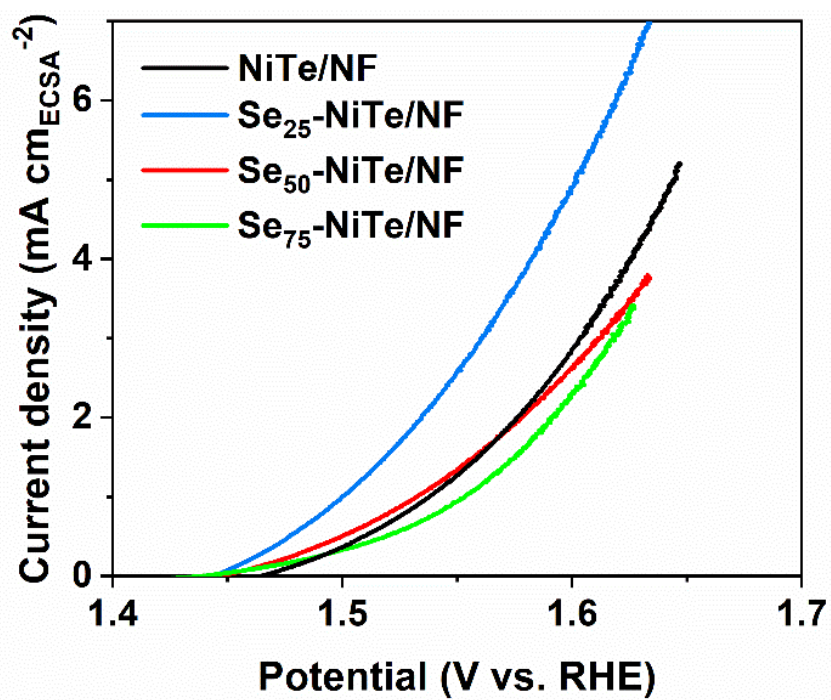


**Fig. S5** Electrocatalytic performance of the Se-NiTe/NF electrodes with different selenium doping amounts tested in 1.0 M KOH + 0.5 M NaCl electrolyte. (a) Polarization curves. (b) Nyquist plots. Inset: equivalent circuit model used for fitting. (c) Tafel plots, and (d)  $C_{dl}$  values.



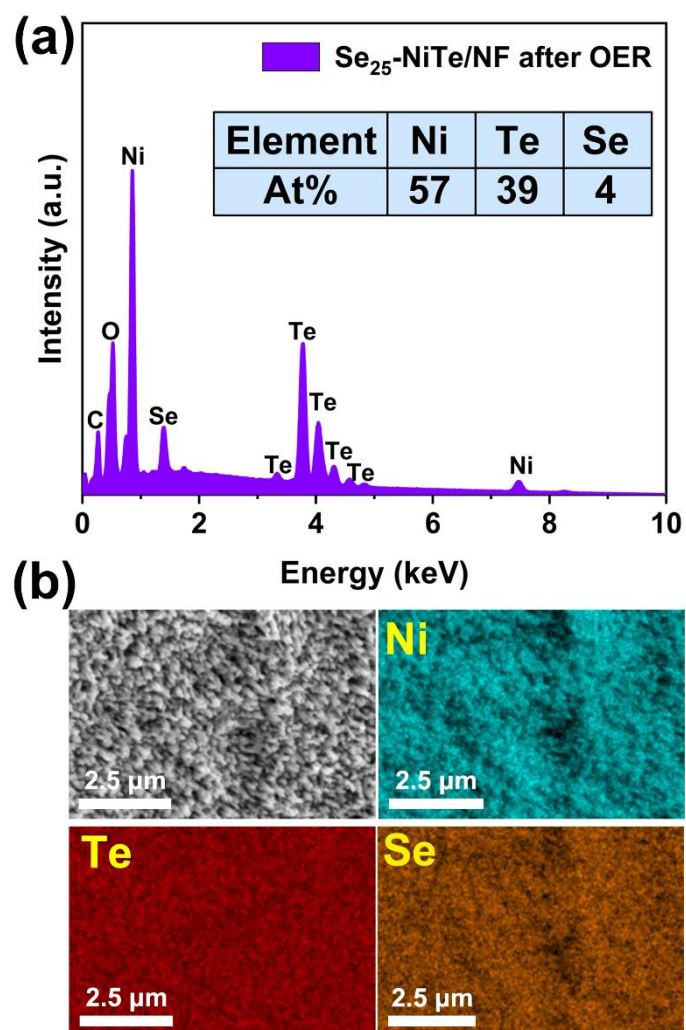


**Fig. S6** The CV curves (Potential ranging from 0.35 – 0.45 V vs. RHE) of different electrocatalysts recorded at various scan rates from 20 to 120 mV s<sup>-1</sup>. (a) Bare Ni foam, (b) NiTe/NF, (c) Se<sub>25</sub>-NiTe/NF, (d) Se<sub>50</sub>-NiTe/NF, (e) Se<sub>75</sub>-NiTe/NF, and (f) Ni-Se/NF.

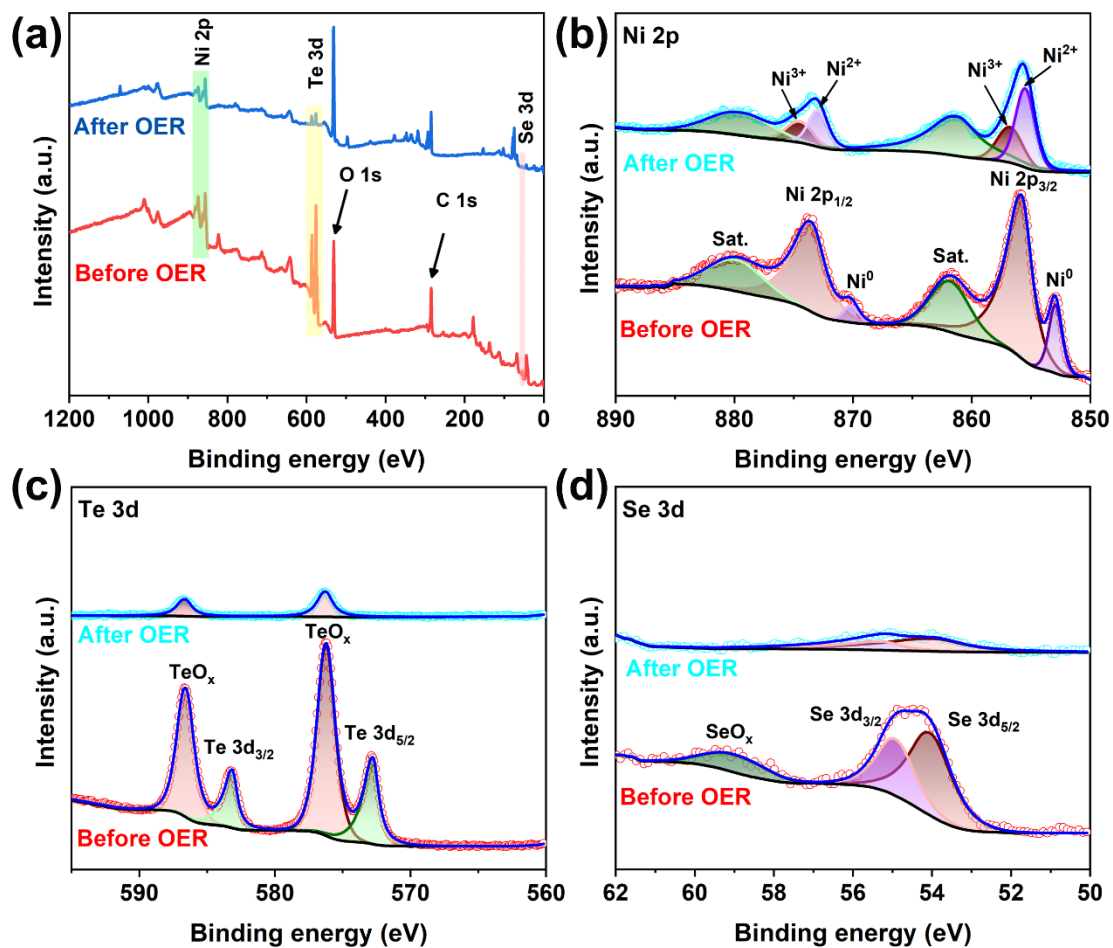


**Fig. S7** ECSA normalized specific activities of NiTe/NF, Se<sub>25</sub>-NiTe/NF, Se<sub>50</sub>-NiTe/NF, and Se<sub>75</sub>-NiTe/NF.

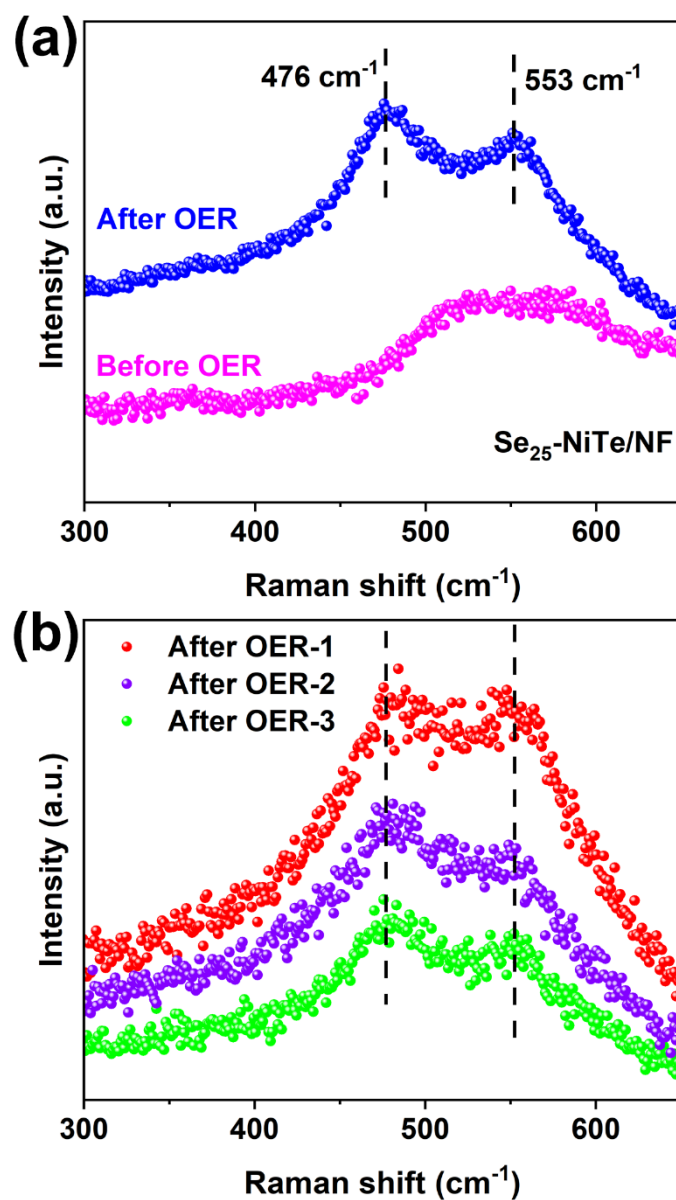




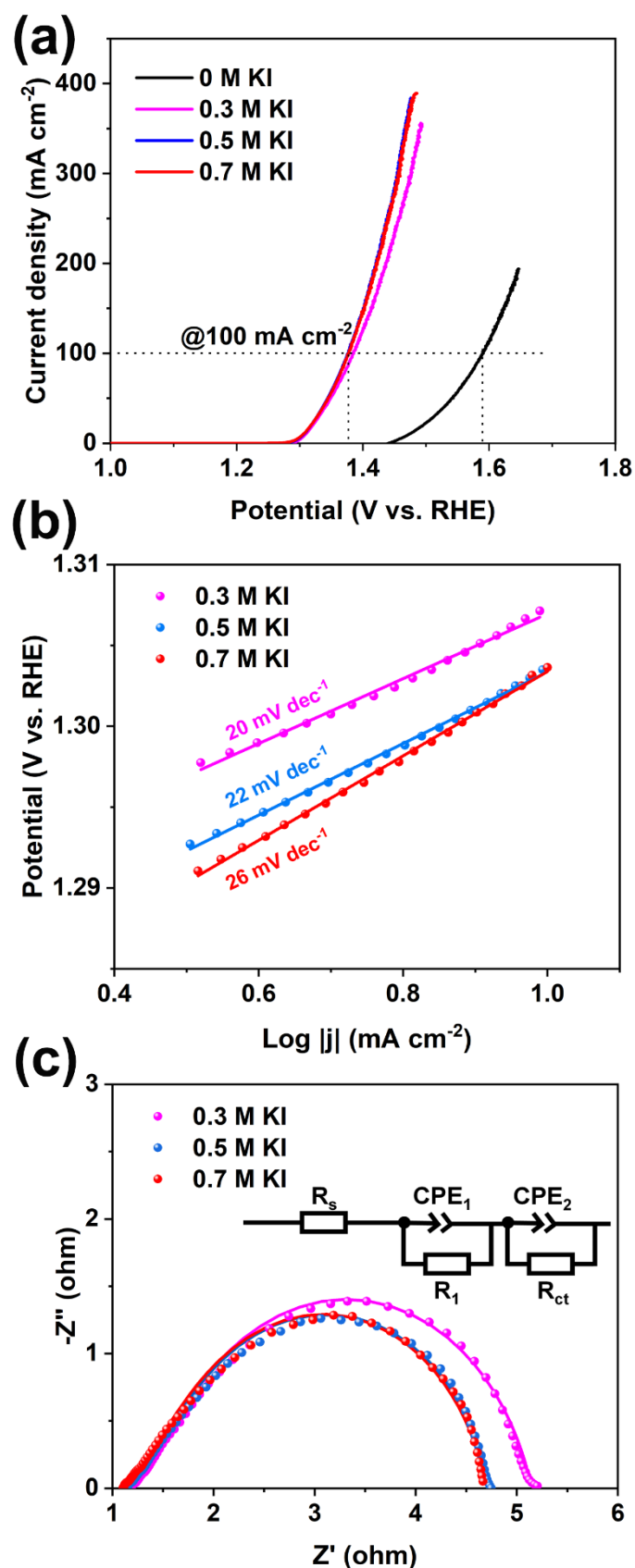
**Fig. S8** (a) EDS spectra and (b) SEM image and the corresponding elemental maps of the  $\text{Se}_{25}\text{-NiTe/NF}$  electrode after the OER stability test ( $100 \text{ mA cm}^{-2}$  for 200 hours in  $1.0 \text{ M KOH} + 0.5 \text{ M NaCl}$  electrolyte).



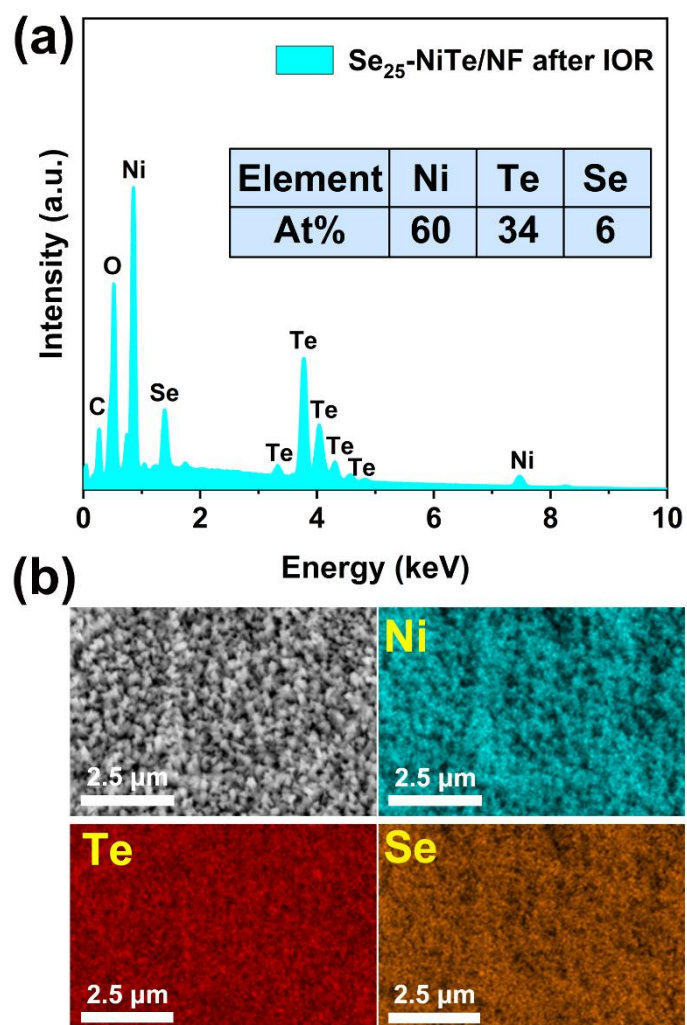
**Fig. S9** (a) XPS survey spectrum. High-resolution XPS spectra in the (b) Ni 2p, (c) Te 3d and (d) Se 3d regions acquired from the Se<sub>25</sub>-NiTe/NF electrode before and after the OER chronopotentiometry at a current density of 100 mA cm<sup>-2</sup> in 1.0 M KOH + 0.5 M NaCl electrolyte.



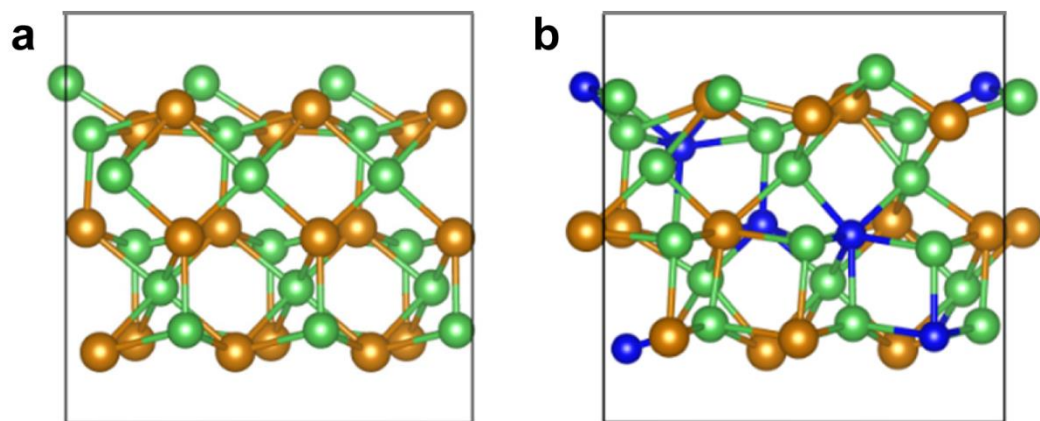
**Fig. S10** (a) Raman spectra of the Se<sub>25</sub>-NiTe/NF electrode before and after the OER stability test in alkaline-saline water solution (100 mA cm<sup>-2</sup> for 200 hours). (b) Raman spectra acquired at different positions over the same piece of electrode after the OER.



**Fig. S11** (a) IOR polarization curves, (b) Tafel plots, and (c) Nyquist plots of the  $\text{Se}_{25}\text{-NiTe/NF}$  electrode recorded in simulated seawater electrolyte (1.0 M KOH + 0.5 M NaCl) in the presence of different molar concentrations of KI.

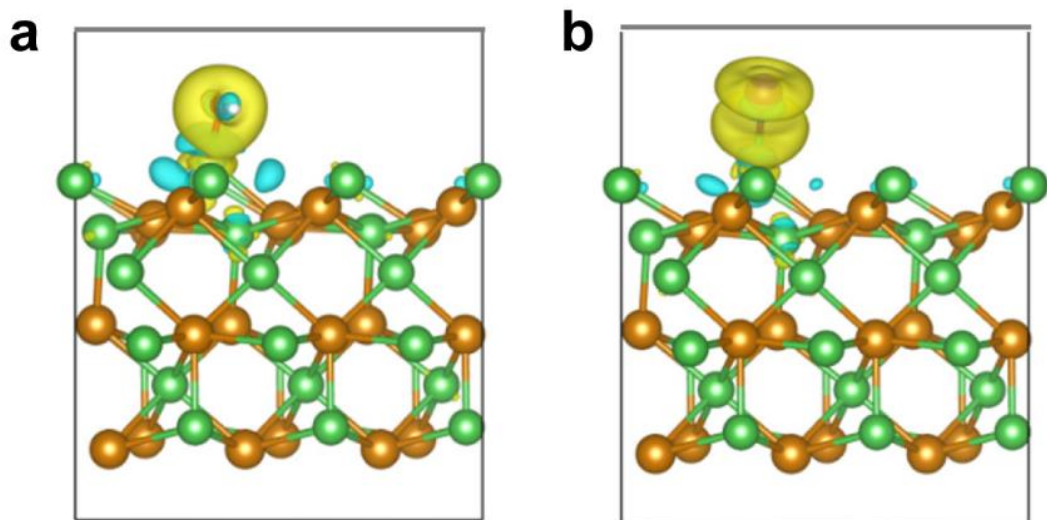


**Fig. S12** (a) EDS spectra and (b) SEM image and the corresponding elemental maps of the  $\text{Se}_{25}\text{-NiTe/NF}$  electrode after the IOR stability test ( $100 \text{ mA cm}^{-2}$  for 500 hours in  $1.0 \text{ M KOH} + 0.5 \text{ M NaCl} + 0.5 \text{ M KI}$  electrolyte).

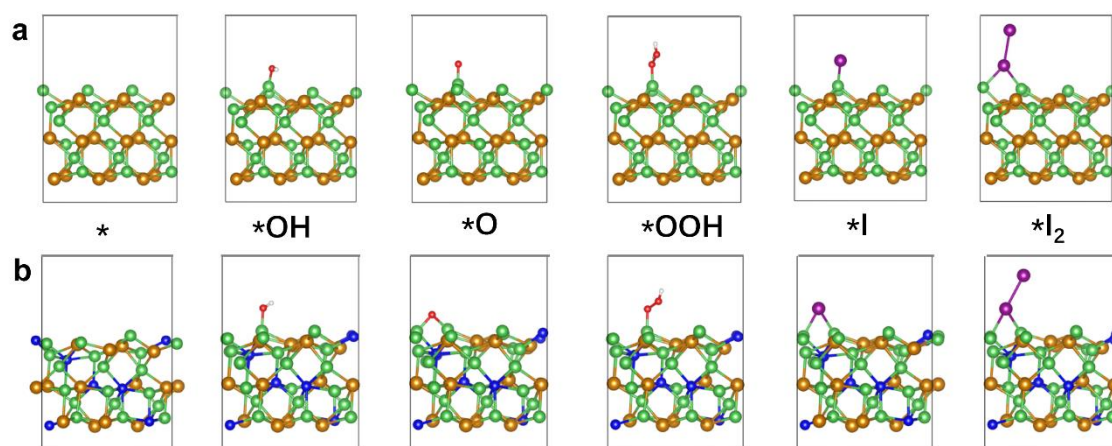


**Fig. S13** Optimized configurations for (a) the NiTe and (b) the Se-NiTe catalyst. The green, brown and blue spheres represent Ni, Te and Se, respectively.





**Fig. S14** The structural model and the corresponding charge density difference on pristine NiTe toward the (a)  $^*OH$  and (b)  $I^*$  adsorption. The green, brown, red, white and purple spheres represent Ni, Te, O, H and I, respectively. The yellow or cyan regions indicate the accumulation or depletion of the charges, respectively.



**Fig. S15** The 3D configurations of (a) the NiTe and (b) the Se-NiTe catalyst during the OER and IOR. The green, brown, blue, red, white and purple spheres represent Ni, Te, Se, O, H and I, respectively.

**Table S1.** The fitting parameters of the EIS spectra of all samples under investigation.

Electrodes	$R_s(\Omega)$	$CPE_1$	$R_1(\Omega)$	$CPE_2$	$R_{ct}(\Omega)$	Electrolyte
Ni foam	1.43	0.00042	0.019	0.01	2.74	
NiTe/NF	1.42	1.52	0.50	3.34	1.27	
Se <sub>25</sub> -NiTe/NF	1.33	1.70	0.38	3.81	0.91	1.0 M KOH + 0.5 M NaCl
Se <sub>50</sub> -NiTe/NF	1.44	1.92	0.32	3.75	1.39	
Se <sub>75</sub> -NiTe/NF	1.48	0.56	0.60	2.56	1.06	
Ni-Se/NF	1.34	0.96	0.44	0.53	1.48	
Ni foam	1.15	0.015	0.75	0.0037	4.21	
NiTe/NF	1.15	0.021	2.56	0.036	1.87	1.0 M KOH + 0.5 M NaCl + 0.5 M KI
Se <sub>25</sub> -NiTe/NF	1.15	0.16	0.65	0.078	2.94	
Se <sub>25</sub> -NiTe/NF	1.18	0.19	0.51	0.088	3.45	1.0 M KOH + 0.5 M NaCl + 0.3 M KI
Se <sub>25</sub> -NiTe/NF	1.10	0.14	0.71	0.070	2.89	1.0 M KOH + 0.7 M NaCl + 0.7 M KI

**Table S2.** Comparison of the OER or SMOR performance of the Se<sub>25</sub>-NiTe/NF electrode with that of other catalysts reported recently in the literature.

Catalysts/catalytic electrodes	Electrolyte	Potential @ 10 or 100 mA cm <sup>-2</sup> (V vs. RHE)	Stability	References
Se <sub>25</sub> -NiTe/NF	1.0 M KOH + 0.5 M NaCl	1.47 @10 mA cm <sup>-2</sup>	100 mA cm <sup>-2</sup> for 200 hours	This work
	1.0 M KOH + 0.5 M NaCl +0.5 M KI	1.38 @100 cm <sup>-2</sup>	100 mA cm <sup>-2</sup> for 500 hours	
NiMn-LDH	1.0 M KOH + 3 M CH <sub>3</sub> OH	1.41 @100 cm <sup>-2</sup>	\	S1
N-Co <sub>9</sub> S <sub>8</sub> /Ni <sub>3</sub> S <sub>2</sub> /NF	1.0 M KOH + 0.5 M CO(NH <sub>2</sub> ) <sub>2</sub>	1.37 @100 cm <sup>-2</sup>	20 mA cm <sup>-2</sup> for 20 hours	S2
Ni <sub>3</sub> N/Mo <sub>2</sub> N	1.0 M KOH+ 0.33 M CO(NH <sub>2</sub> ) <sub>2</sub>	1.36 @100 cm <sup>-2</sup>	1.38 V for 40 hours	S3
Ni(OH) <sub>2</sub> /NF	1.0 M KOH + 0.5 M CH <sub>3</sub> OH	1.36 @100 cm <sup>-2</sup>	\	S4
V <sub>8</sub> C <sub>7</sub> /CoP-0.18	1.0 M KOH+ 0.33 M CO(NH <sub>2</sub> ) <sub>2</sub>	1.67 @100 cm <sup>-2</sup>	10 mA cm <sup>-2</sup> for 20 hours	S5
Ni-Mo-N/CFC	1.0 M KOH + 0.1 M C <sub>3</sub> H <sub>5</sub> (OH) <sub>3</sub>	1.51 @100 cm <sup>-2</sup>	\	S6
Fe-NiO/NiS <sub>2</sub>	1.0 M KOH	1.50 @10 mA cm <sup>-2</sup>	10 mA cm <sup>-2</sup> for 100 hours	S7
CoO@S-CoTe	1.0 M KOH	1.476 @10 mA cm <sup>-2</sup>	50 mA cm <sup>-2</sup> for 36 hours	S8
Ni <sub>2</sub> P-CoCH/CFP	1.0 M KOH	1.50 @10 mA cm <sup>-2</sup>	20 mA cm <sup>-2</sup> for 50 hours	S9

## References

- S1. B. Zhu, B. Dong, F. Wang, Q. Yang, Y. He, C. Zhang, P. Jin and L. Feng, *Nat Commun*, 2023, **14**, 1686.
- S2. H. Xie, Y. Feng, X. He, Y. Zhu, Z. Li, H. Liu, S. Zeng, Q. Qian and G. Zhang, *Small*, 2023, **19**, e2207425.
- S3. T. Wang, L. Miao, S. Zheng, H. Qin, X. Cao, L. Yang and L. Jiao, *Acs Catal*, 2023, **13**, 4091-4100.
- S4. J. Hao, J. W. Liu, D. Wu, M. X. Chen, Y. Liang, Q. Wang, L. Wang, X. Z. Fu and J. L. Luo, *Appl Catal B-Environ*, 2021, **281**, 119510.
- S5. L. S. Wu, M. T. Zhang, Z. H. Wen and S. Q. Ci, *Chemical Engineering Journal*, 2020, **399**, 125728.
- S6. Y. Li, X. Wei, L. Chen, J. Shi and M. He, *Nat Commun*, 2019, **10**, 5335.
- S7. N. Zhang, Y. Hu, L. An, Q. Li, J. Yin, J. Li, R. Yang, M. Lu, S. Zhang, P. Xi and C. H. Yan, *Angew Chem Int Ed Engl*, 2022, **61**, e202207217.
- S8. X. Wang, Z. Mao, X. Mao, X. Hu, F. Gao, M. Gao, Q. L. Wu, X. Lyu, A. Du, X. Xu, Y. Jia and L. Wang, *Adv Sci (Weinh)*, 2023, **10**, e2206204.
- S9. S. Zhang, C. Tan, R. Yan, X. Zou, F. L. Hu, Y. Mi, C. Yan and S. Zhao, *Angew Chem Int Ed Engl*, 2023, **62**, e202302795.