

Supporting Information

Self-adaptive ternary NiCoMo-carbon composite as a bifunctional electrocatalyst for high-current-density water splitting

Yuchen Hao^{a, b}, Shujuan Wang^{b,*}, Xuewen Xia^a, Yang^b, YangHao Zhang^b, Yuanman Ni^b, Xiaolu Xiong^b, Chao Jing^b, Tongshuai Wang^b, Jianqiang Wang^b, Linjuan Zhang^b, Xingli Zou^a

^a State Key Laboratory of Advanced Refractories & School of Materials Science and Engineering, Shanghai University, Shanghai 200444, China.

^b Shanghai Institute of Applied Physics, Chinese Academy of Sciences, Shanghai 201800, China.

* Corresponding author. E-mail address: wangshujuan@sinap.ac.cn

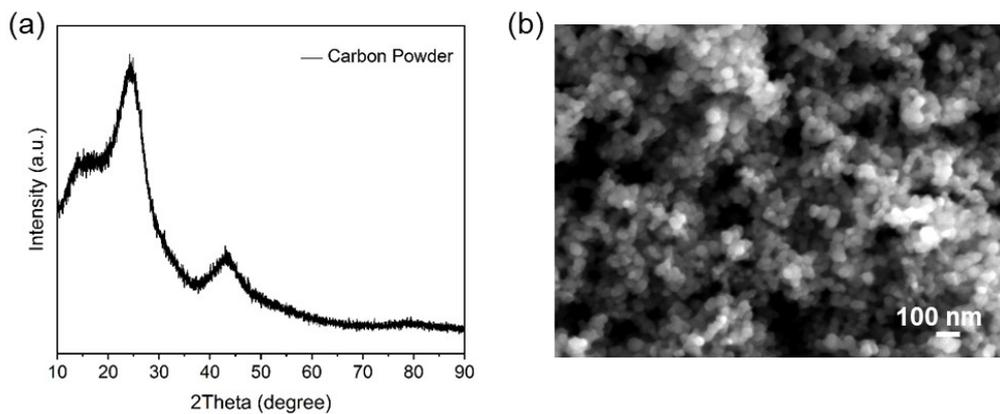


Fig. S1 (a) XRD pattern of carbon powders. (b) SEM image of carbon powders.

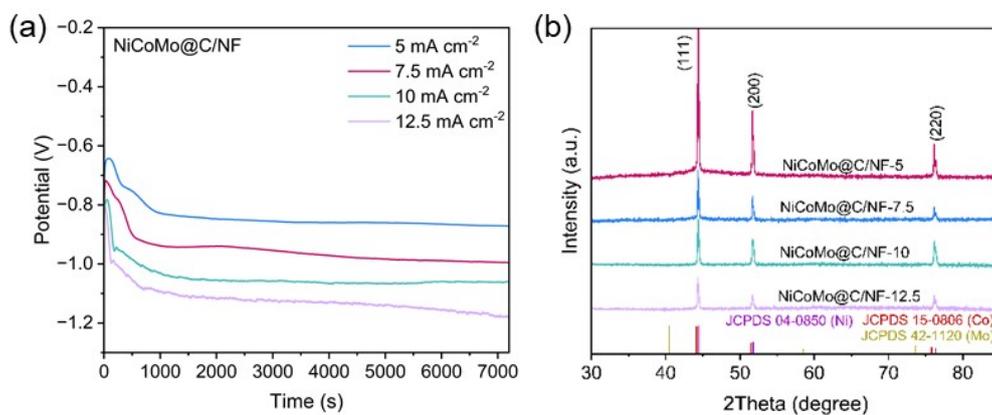


Fig. S2 (a) Voltage-time (V-t) curves of NiCoMo@C/NF at various current densities. (b) XRD patterns of NiCoMo@C/NF at various current densities.

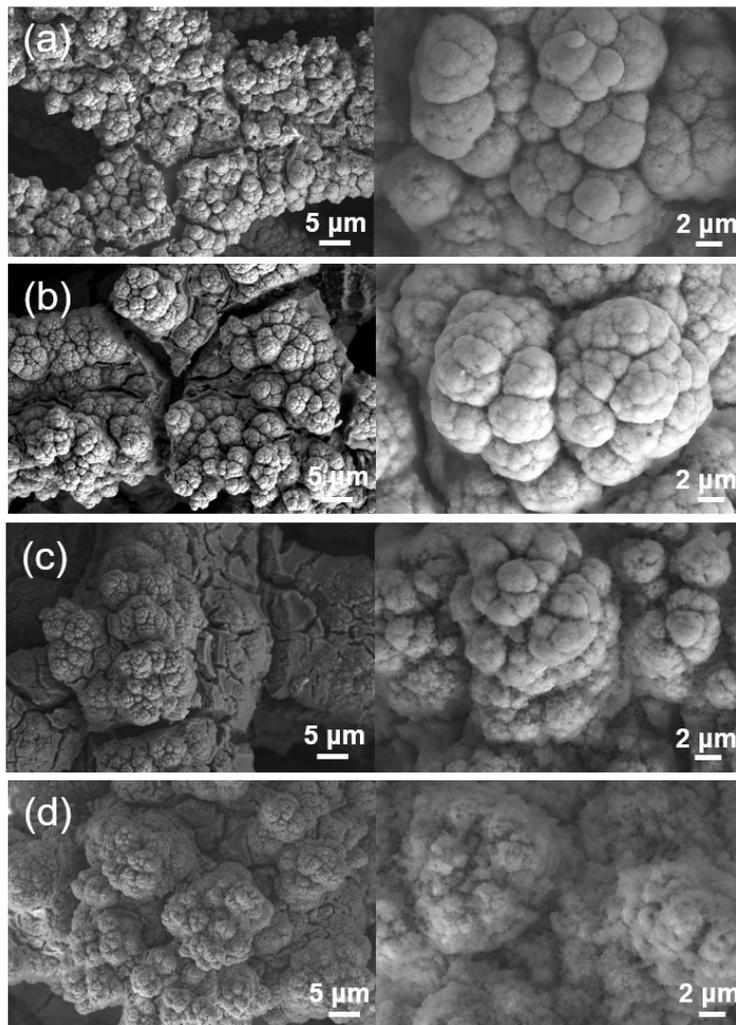


Fig. S3 SEM images of NiCoMo@C/NF at different densities: (a) -5 mA cm^{-2} ; (b) -7.5 mA cm^{-2} ; (c) -10 mA cm^{-2} ; (d) -12.5 mA cm^{-2} .

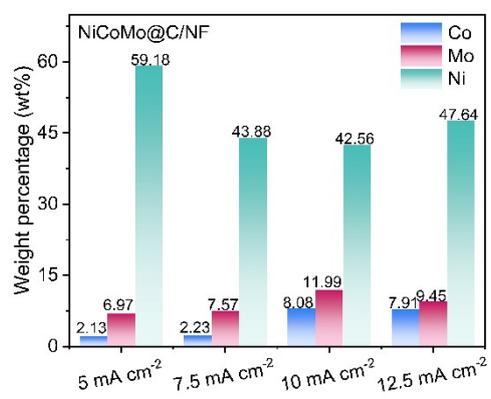


Fig. S4 Weight percentages of Ni, Co, and Mo in NiCoMo@C/NF under different current densities based on the EDX data.

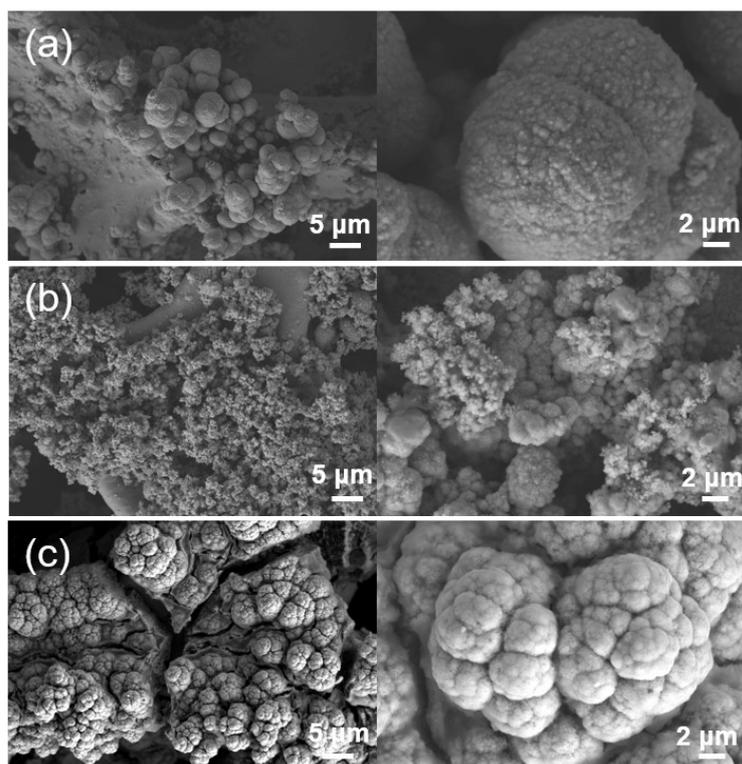


Fig. S5 SEM images of (a) Ni@C/NF, (b) NiCo@C/NF, and (c) NiCoMo@C/NF electrodeposited at a current density of -7.5 mA cm^{-2} .

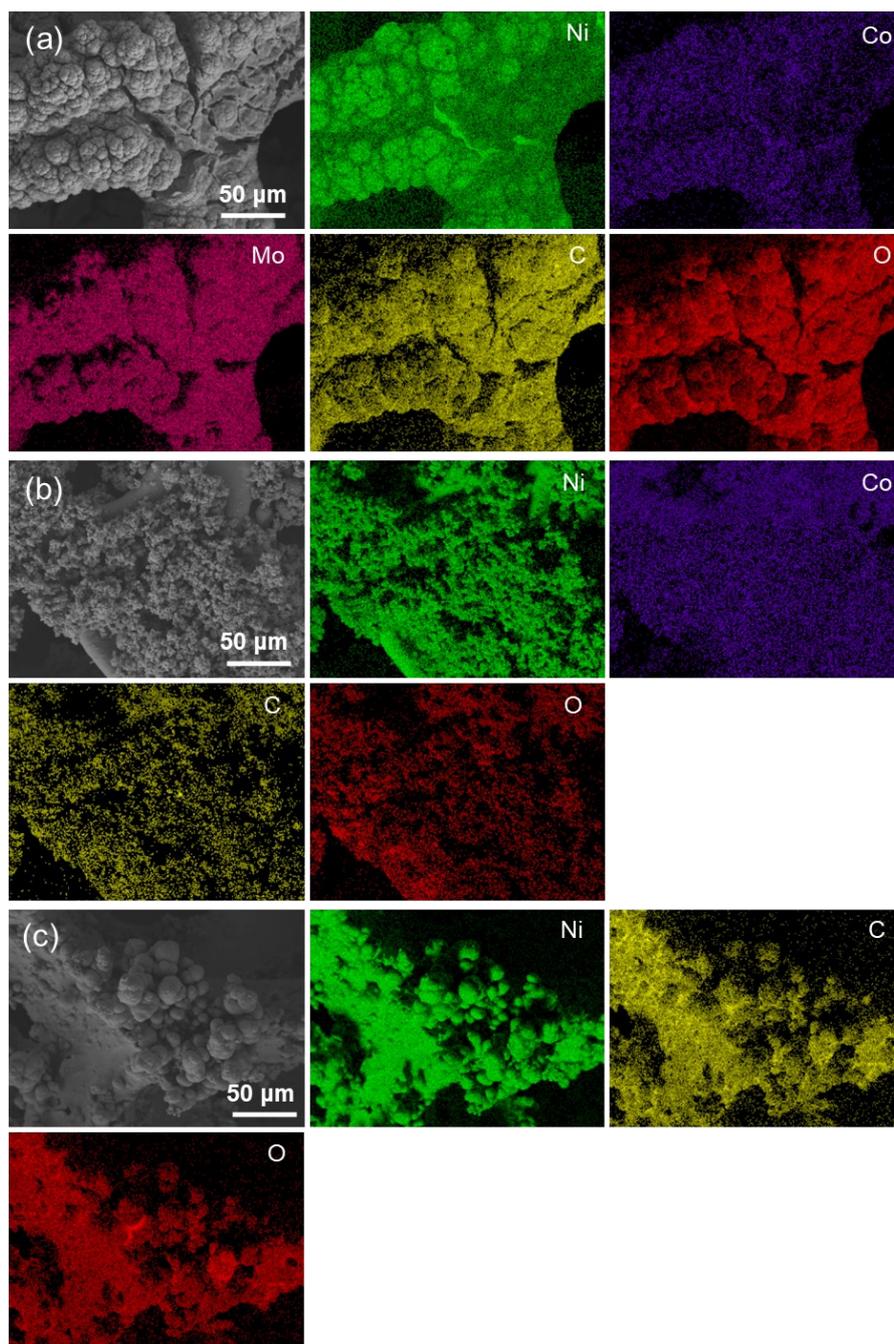


Fig. S6 (a) SEM and EDX elemental mapping images of NiCoMo@C/NF; (b) SEM and EDX elemental mapping images of NiCo@C/NF; (c) SEM and EDX elemental mapping images of Ni@C/NF.

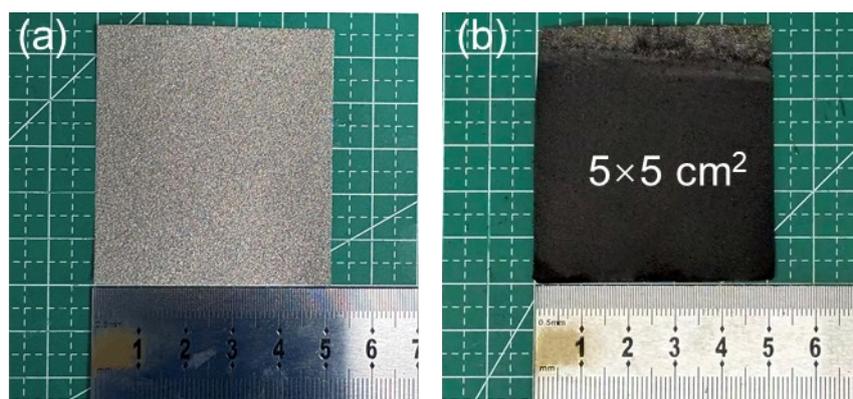


Fig. S7 Physical images of bare nickel foam and NiCoMo@C/NF with a size of 5 cm × 5 cm.

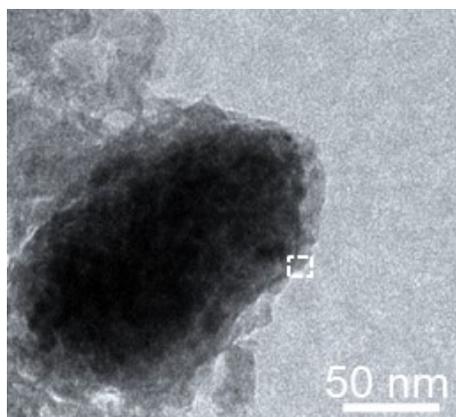


Fig. S8 TEM image of NiCoMo@C/NF.

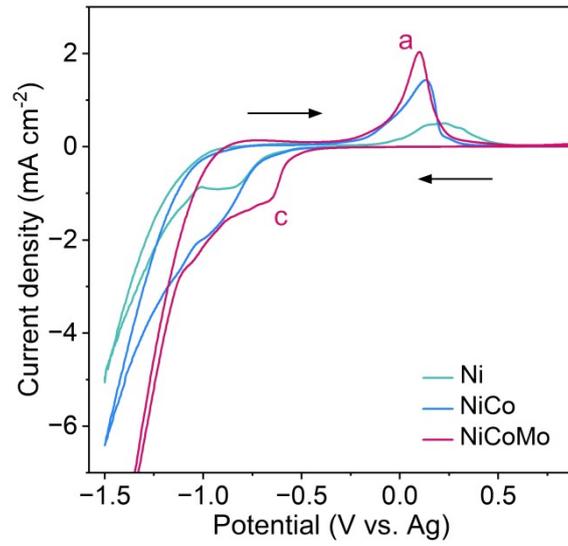


Fig. S9 CV curves in three ChCl-EG electrolytes containing NiCl_2 , $\text{NiCl}_2\text{-CoCl}_2$, and $\text{NiCl}_2\text{-CoCl}_2\text{-Na}_2\text{MoO}_4$ systems with C powders, respectively.

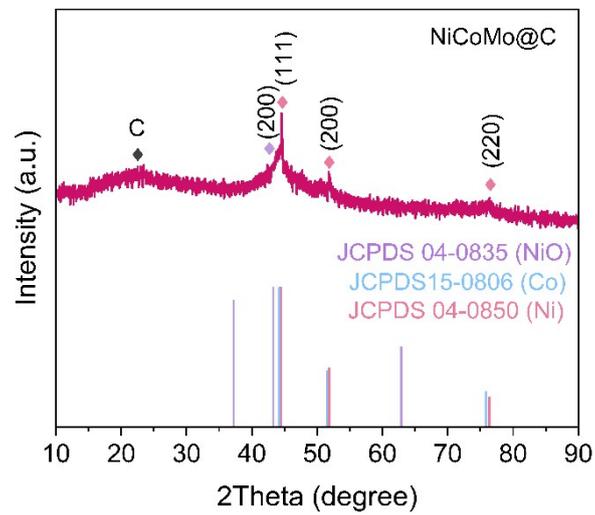


Fig. S10 XRD patterns of NiCoMo@C powders.

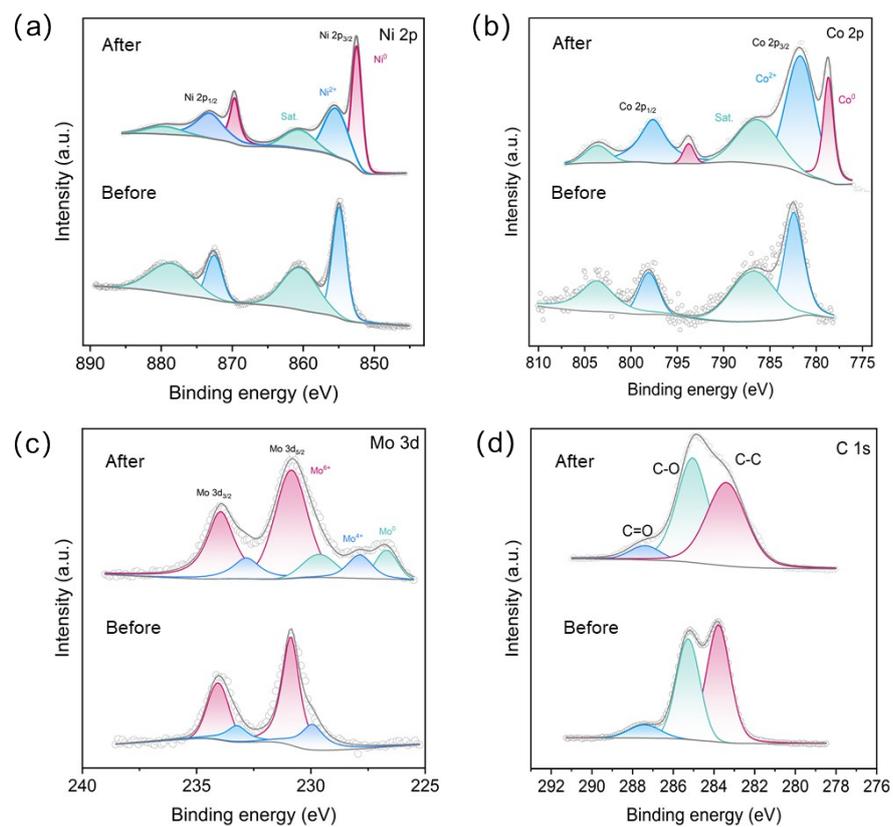


Fig. S11 XPS spectra of NiCoMo@C/NF before and after argon ion sputtering (with an etching depth of ~10 nm) : (a) Ni 2p; (b) Co 2p; (c) Mo 3d; (d) C 1s.

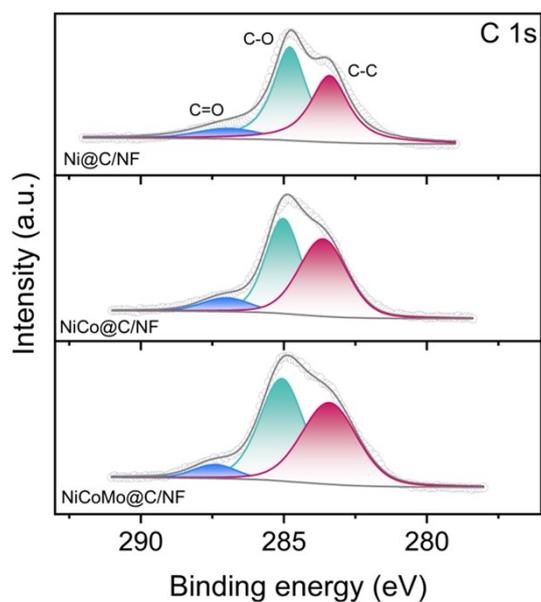


Fig. S12 XPS of C 1s region for Ni@C/NF, NiCo@C/NF, and NiCoMo@C/NF electrodeposited at a current density of -7.5 mA cm^{-2} .

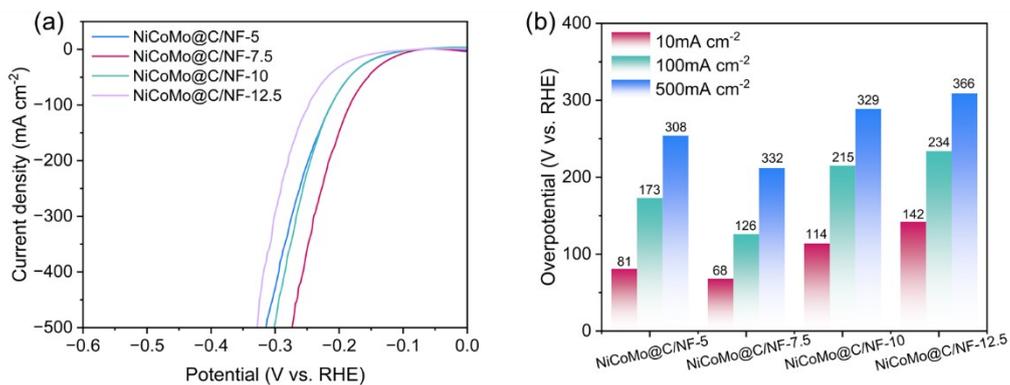


Fig. S13 (a) LSV curves for NiCoMo@C/NF electrodeposited at different current densities (-5 mA cm^{-2} , -7.5 mA cm^{-2} , -10 mA cm^{-2} , and -12.5 mA cm^{-2}); (b) Overpotentials of electrodes obtained at different current densities at 10 mA cm^{-2} , 100 mA cm^{-2} , and 1000 mA cm^{-2} for HER.

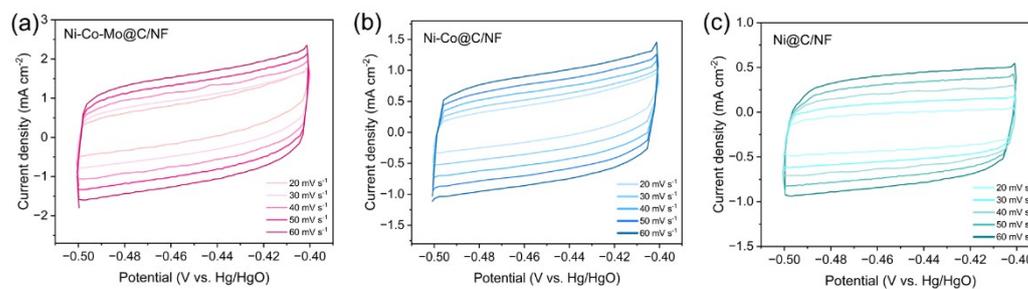


Fig. S14 Electrochemical active surface area analysis by the CV scans in a non-Faradaic potential range of as-prepared electrodes for HER: (a) NiCoMo@C/NF; (b) NiCo@C/NF; (c) Ni@C/NF in 1.0 M KOH at scan rate of 20 mV s^{-1} , 30 mV s^{-1} , 40 mV s^{-1} , 50 mV s^{-1} , and 60 mV s^{-1} .

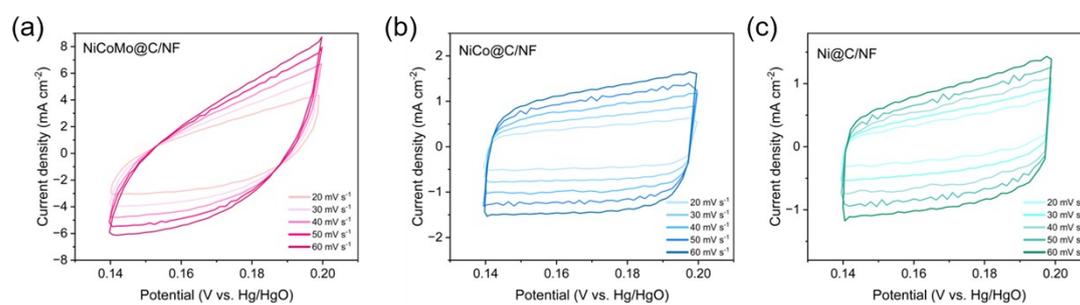


Fig. S15 Electrochemical active surface area analysis by the CV scans in a non-Faradaic potential range of as-prepared electrodes for OER: (a) NiCoMo@C/NF; (b) NiCo@C/NF; (c) Ni@C/NF in 1.0 M KOH at scan rate of 20 mV s^{-1} , 30 mV s^{-1} , 40 mV s^{-1} , 50 mV s^{-1} , and 60 mV s^{-1} .

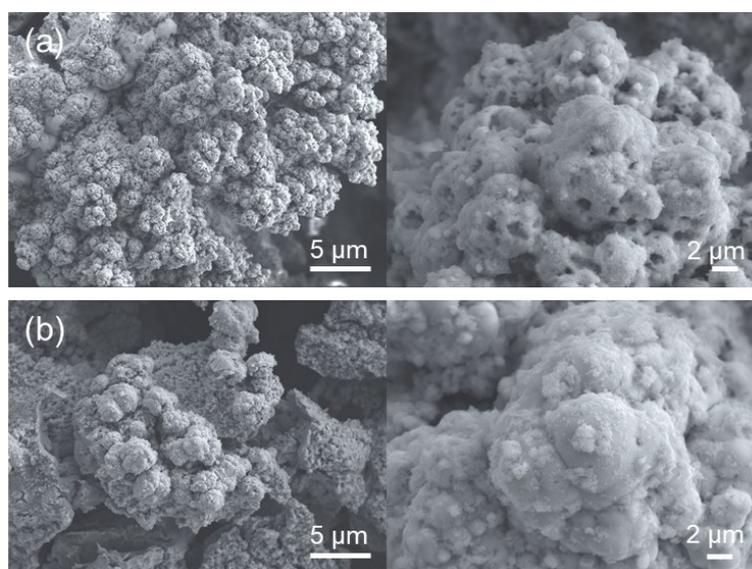


Fig. S16 SEM images of NiCoMo@C/NF after stability tests for (a) HER and (b) OER.

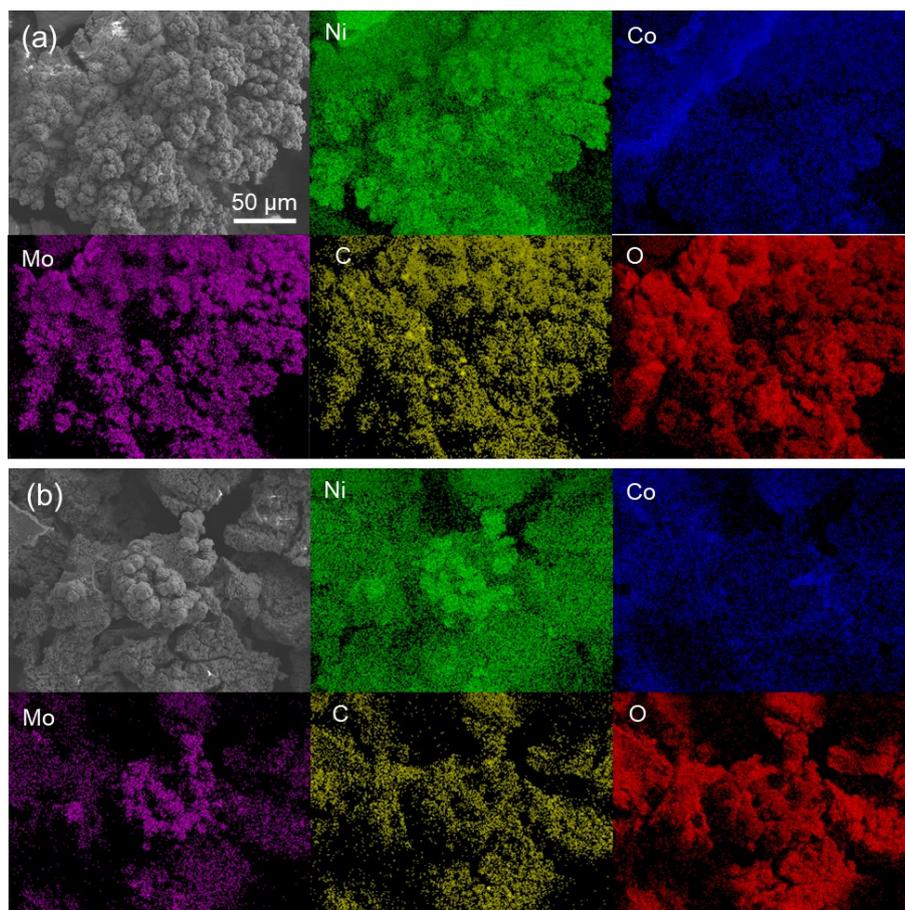


Fig. S17 SEM and EDX elemental mapping images of NiCoMo@C/NF after stability tests for (a) HER and (b) OER.

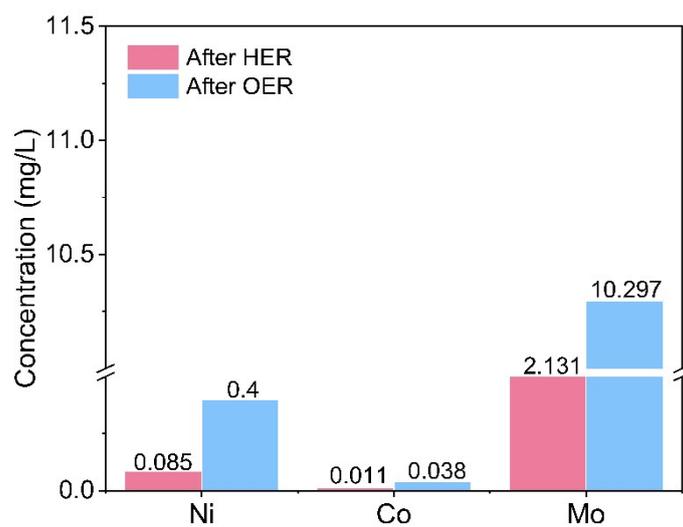


Fig. S18 Metal concentrations in the electrolyte after HER and OER stability testing.

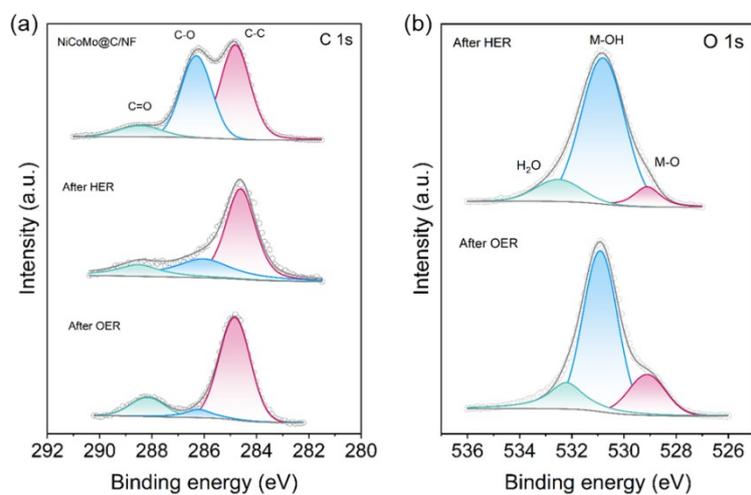


Fig. S19 XPS spectra of NiCoMo@C/NF before and after stability testing for HER and OER: (a) C 1s; (b) O 1s.

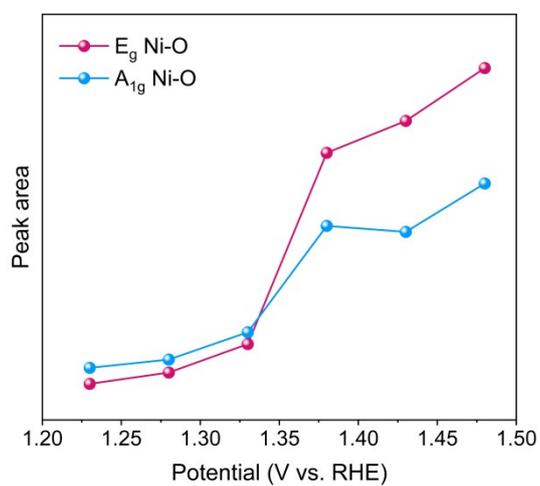


Fig. S20 Plot of the Ni-O characteristic peak area versus potential.

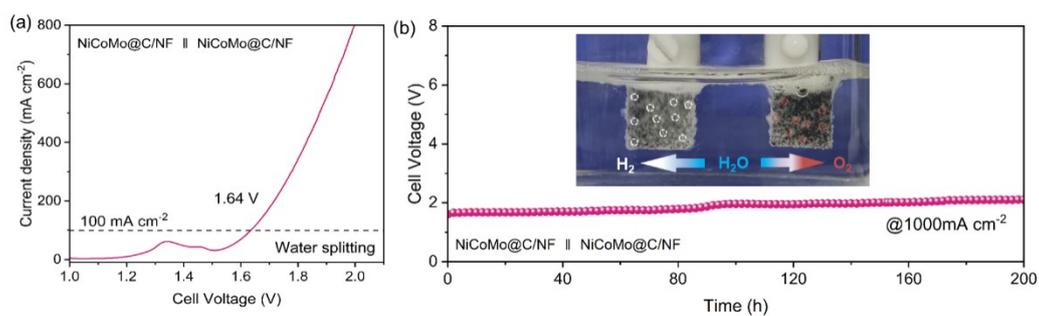


Fig. S21 (a) LSV curve of NiCoMo@C/NF || NiCoMo@C/NF for overall water splitting in 1.0 M KOH; (b) Long-term stability of NiCoMo@C/NF || NiCoMo@C/NF at 1000 mA cm⁻². The inset shows the process of overall water splitting on the NiCoMo@C/NF electrode.

Table S1. Comparisons of overpotentials and Tafel slopes for NiCoMo@C/NF at 10 mA cm⁻² with other reported electrocatalysts for HER in alkaline solutions.

Electrocatalysts	Overpotential (mV)	Tafel slope (mV dec ⁻¹)	Test conditions	References
NiCoMo@C/NF	59	32.4	1.0 M KOH (with 95% IR compensation)	This work
Ni-Co-B-P	166	55.6	1.0 M KOH	1
Mn-Co-P@Ni-Co-NF	75	79	1.0 M KOH	2
Co-Ni-NF	68	131	0.1 M KOH (with 90% IR compensation)	3
NiCo-MOFs	125	78	N ₂ -saturated 1.0 M KOH	4
Ni ₁ Co ₂ -LDH/Ni/NiO-CNFs	152	50.5	1.0 M KOH	5
Ni-Co/CC	62	63.5	1.0 M KOH	6
Ni-Co/N@CW	143	105	1.0 M KOH (with 90% IR compensation)	7
NCMO@NC	92	115	1.0 M KOH + 1.0 M CH ₃ OH	8
Cu-Zn-Ni-Co	67	97.7	1.0 M KOH	9
NiCo(CrV)	87	96	1.0 M KOH	10
NiCo ₂ S ₄ /ReS ₂	85	78.3	1.0 M KOH	11
GO/Ni-Co/CW	70	70.8	1.0 M KOH	12
MOF/NiCo	98	48	1.0 M KOH (with 90% IR compensation)	13

NiCo-SAD-NC	61	31.5	1.0 M KOH	14
Mo-NiCo	235.8	161.1	1.0 M KOH	15
(with 90% IR compensation)				
Co ₁ Mo ₁ Ni _{0.5} Pi	96	145.3	1.0 M KOH	16

Table S2. Comparisons of overpotentials for NiCoMo@C/NF at at 1000 mA cm⁻² with other reported electrocatalysts for HER in 1.0 M KOH at room temperature.

Materials	Overpotential @1000 mA cm ⁻² (mV)	References
NiCoMo@C/NF	289	This work
Ni-WO ₃ /NF	~300	17
FeCoNiCrMn HEA/NM	425	18
Fe-rich MEA	343.6	19
Mn@Ni ₃ N-Co ₃ N	~350	20
NiCoMoO	566	21
ac-NiCo(OH) ₂ /NF	510	22
Fe-CoP@Fe-Ni ₂ P/NF	310	23
FeMoS@CoFe LDH	376	24
NiCo/V ₂ O ₃ /C	396	25
Cu-FeOOH/Fe ₃ O ₄	349	26

Table S3. Comparisons of overpotentials for NiCoMo@C/NF at 10 mA cm⁻² with other reported electrocatalysts for OER.

Electrocatalysts	Overpotential (mV)	Electrolyte	References
NiCoMo@C/NF	214	1.0 M KOH (with 95% IR compensation)	This work
NiCo	288	1.0 M KOH	27
EP-NiCo/EGR	300	1.0 M KOH	28
NiFeCr/NF	233	1.0 M KOH (with 90% IR compensation)	29
CoNi-Ti ₃ C ₂ T _x	241	N ₂ -saturated 1.0 M KOH	30
NiCo-CAT MOF	307	1.0 M KOH	31
NiCo(CrV)	320	1.0 M KOH	10
NiFeB	319	N ₂ -saturated 1.0 M KOH (with 85% IR compensation)	32
NiCo-NiCoO ₂ @NC	318	O ₂ -saturated 1.0 M KOH	33
Ni-60-V ₂ O ₅ @NC	300	1.0 M KOH	34
NF@NiMoCo	277	O ₂ -saturated 1.0 M KOH	35
(Ni, Cu)O@C	330	1.0 M KOH (with 90% IR compensation)	36

Table S4. Comparisons of overpotentials for NiCoMo@C/NF at 1000 mA cm⁻² with other reported electrocatalysts for OER in 1.0 M KOH at room temperature.

Materials	Overpotential @1000 mA cm ⁻² (mV)	References
NiCoMo@C/NF	354	This work
Ni-WO ₃ /NF	~550	17
FeCoNiCrMn HEA/NM	560	18
ac-NiCo(OH) ₂ /NF	364	22
NiCoMoO	631	21
Fe _{0.125} Ni _{0.375} Mo _{0.5} NFs	426	37
NiFe LDH-CeW@NFF	353.8	38
Fe _x Ni _{2-x} P ₄ O ₁₂ /RGO	380	39
CrO ²⁻ -NiFe LDH/Cr ₂ O ₃	355	40
Fe-NiCo-LDH	400	41

References

- 1 T. Liu, N. Li, B. Wu, X. Han, Q. Ding, Q. Zhao, Q. Cheng, R. Wang and D. Li, *Int. J. Hydrogen Energy*, 2025, **102**, 900-908.
- 2 R. Abedi and G. Barati Darband, *J. Power Sources*, 2025, **641**, 236840.
- 3 H. C. Novais, M. F. Montemor, A. J. S. Fernandes, C. Freire and D. M. Fernandes, *J. Power Sources*, 2025, **644**, 237141.
- 4 T. V. M. Sreekanth, G. K. Kiran, J. Kim and K. Yoo, *Inorg. Chem. Commun.*, 2024, **161**, 112128.
- 5 H. Cao, B. Liu, J. Bai, C. Li and G. Xu, *J. Alloys Compd.*, 2025, **1010**, 178041.
- 6 Y. Hu and C. Wang, *J. Mater. Chem. A*, 2024, **12**, 16769-16779.
- 7 C. Yang, R. Jin, Z. Liu, S. Li, D. Lv, J. Liu, J. Li, Z. Lin and L. Gao, *J. Mater. Chem. A*, 2024, **12**, 33222-33232.
- 8 S. E. Islam, D.-R. Hang, C.-T. Liang, K. H. Sharma, H.-C. Huang and M. M. C. Chou, *ACS Appl. Energy Mater.*, 2023, **6**, 9543-9555.
- 9 Y. Xie, A. Miche, V. Vivier and M. Turmine, *Int. J. Hydrogen Energy*, 2025, **127**, 95-106.
- 10 S. Ahmad, M. Egilmez, W. Abuzaid, F. Mustafa, A. M. Kannan and A. S. Alnaser, *Int. J. Hydrogen Energy*, 2024, **52**, 1428-1439.
- 11 C. Pei, M.-C. Kim, Y. Li, C. Xia, J. Kim, W. So, X. Yu, H. S. Park and J. K. Kim, *Adv. Funct. Mater.*, 2023, **33**, 2210072.
- 12 Y. Qian, M. Hu, L. Li, X. Liu, S. Cao and C. Guo, *Int. J. Hydrogen Energy*, 2023, **48**, 13543-13554.
- 13 L. Zhang, F. Ye, Z. Wu, L. Jiang, Q. Liu, R. Pang, Y. Liu and L. Hu, *Small Methods*, 2022, **6**, 2200515.
- 14 A. Kumar, V. Q. Bui, J. Lee, L. Wang, A. R. Jadhav, X. Liu, X. Shao, Y. Liu, J. Yu, Y. Hwang, H. T. D. Bui, S. Ajmal, M. G. Kim, S.-G. Kim, G.-S. Park, Y. Kawazoe and H. Lee, *Nat. Commun.*, 2021, **12**, 6766.
- 15 D. Gao, J. Guo, H. He, P. Xiao and Y. Zhang, *Chem. Eng. J.*, 2022, **430**, 133110.
- 16 P. Viswanathan and K. Kim, *ACS Appl. Mater. Interfaces*, 2023, **15**, 16571-16583.
- 17 W. Jiang, Z. Zhai, J. Wu and S. Yin, *J. Colloid Interface Sci.*, 2026, **702**, 138869.
- 18 Y. Zhang, Q. Wan, L. Huang, T. Jiang, S. Wu, D. Li, Y. Liu, H. Wu and F. Ren, *J. Mater. Chem. A*, 2025, **13**, 17384-17392.
- 19 Y. Shao, J. Ni, J. Yin, X. Liu, S. Guo, Y. Xu, B. Song, Y. Song, X. Li, L. Luo and C. Sun, *Small*, 2025, **21**, 2407061.
- 20 X. Wang, H. Hu, X. Yan, Z. Zhang and M. Yang, *Angew. Chem. Int. Ed.*, 2024, **63**, e202401364.
- 21 P. Wang, P. Wang, T. Wu, X. Sun and Y. Zhang, *Adv. Sci.*, 2024, **11**, 2407892.
- 22 S. Ju, Y. Liu, M. Pei, Y. Shuai, Z. Zhai, W. Yan, Y.-J. Wang and J. Zhang, *J. Colloid Interface Sci.*, 2024, **653**, 1704-1714.
- 23 Z. Li, C. Xu, Z. Zhang, S. Xia, D. Li, L. Liu, P. Chen and X. Dong, *Adv. Sci.*, 2024, **11**, 2308477.
- 24 C. Han, Y. Zhao, G. Chen, H. Song, X. Wu, Z. Guo and C. Chen, *J. Mater. Chem. A*, 2024, **12**, 26528-26535.
- 25 D. Li, J. Wang, S. Wang, B. Chu, R. Li, B. Li, L. Dong, M. Fan and Z. Chen, *J. Mater. Chem. A*, 2023, **11**, 23397-23404.
- 26 C. Yang, W. Zhong, K. Shen, Q. Zhang, R. Zhao, H. Xiang, J. Wu, X. Li and N. Yang, *Adv. Energy Mater.*, 2022, **12**, 2200077.
- 27 F. Zhu, X. Wen, X. Li, Y. Wang, K. Shao, S. Shen and X. Zhao, *ACS Appl. Energy Mater.*, 2025, **8**, 1210-1219.
- 28 A. A. Abdelraouf, A. M. Abdelrahim, M. G. Abd El-Moghny and M. S. El-Deab, *J. Environ. Chem. Eng.*, 2025, **13**, 117089.
- 29 Z. Zhang, Z. Yang, J. Gao, X. Wu, J. Yun and J. Zhang, *Mol. Catal.*, 2024, **557**, 113980.
- 30 X. Zhao, W.-P. Li, Y. Cao, A. Portniagin, B. Tang, S. Wang, Q. Liu, D. Y. W. Yu, X. Zhong, X. Zheng and A. L. Rogach, *ACS Nano*, 2024, **18**, 4256-4268.
- 31 W.-R. Yan, Y. Xue, M.-C. Liu, X. Qiao, C.-Y. Jing, Y. Yu, X.-C. Yan, J.-Z. Wei, H. Dong and F.-M. Zhang, *CrystEngComm*, 2024, **26**, 3185-3193.
- 32 H.-l. Li, Y.-y. Wang, C.-m. Liu, S.-m. Zhang, H.-f. Zhang and Z.-w. Zhu, *Int. J. Hydrogen Energy*, 2022, **47**, 20718-20728.

- 33 Y. Xiao, P. Zhang, X. Zhang, X. Dai, Y. Ma, Y. Wang, Y. Jiang, M. Liu and Y. Wang, *J. Mater. Chem. A*, 2017, **5**, 15901-15912.
- 34 W. Xue, H. Fu, G. Xue, J. Zhao, Y. Lian, Z. Wang, Y. Hu and H. Zhang, *J. Alloys Compd.*, 2025, **1027**, 180640.
- 35 K. Hu, M. Wu, S. Hinokuma, T. Ohto, M. Wakisaka, J.-i. Fujita and Y. Ito, *J. Mater. Chem. A*, 2019, **7**, 2156-2164.
- 36 A. Z. Alhakemy, M. H. Elsayed, F. K. Algethami and H. N. Abdelhamid, *Int. J. Hydrogen Energy*, 2025, **115**, 289-298.
- 37 M. Xu, W. Li, M. Zhong, J. Yang, M. Gao, N. Pinna and X. Lu, *ACS Mater. Lett.*, 2024, **6**, 3548-3556.
- 38 M. Li, H.-J. Niu, Y. Li, J. Liu, X. Yang, Y. Lv, K. Chen and W. Zhou, *Appl. Catal., B*, 2023, **330**, 122612.
- 39 L. Lin, Y. Wang, Q. Ye, Y. Zhao and Y. Cheng, *Appl. Catal., B*, 2023, **334**, 122834.
- 40 Z. Cai, J. Liang, Z. Li, T. Yan, C. Yang, S. Sun, M. Yue, X. Liu, T. Xie, Y. Wang, T. Li, Y. Luo, D. Zheng, Q. Liu, J. Zhao, X. Sun and B. Tang, *Nat. Commun.*, 2024, **15**, 6624.
- 41 H. Zhang, H. Guo, Y. Li, Q. Zhang, L. Zheng, L. Gu and R. Song, *Adv. Funct. Mater.*, 2023, **33**, 2304403.