

# Electronic Supplementary Information for

## Bimetallic Ni-Mo nitride@N-doped C as highly active and stable bifunctional electrocatalysts for full water splitting

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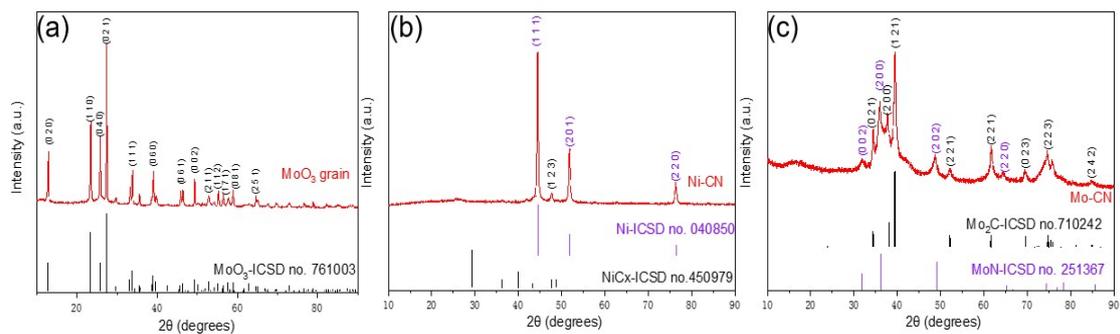


Figure S1 XRD pattern of (a) MoO<sub>3</sub> grain (b) Ni-CN (c) Mo-CN.

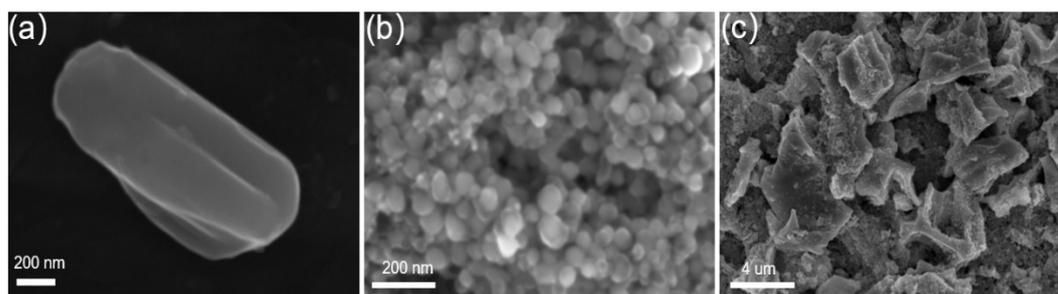


Figure S2 SEM images of (a) MoO<sub>3</sub> grain (b) Ni-CN (c) Mo-CN.

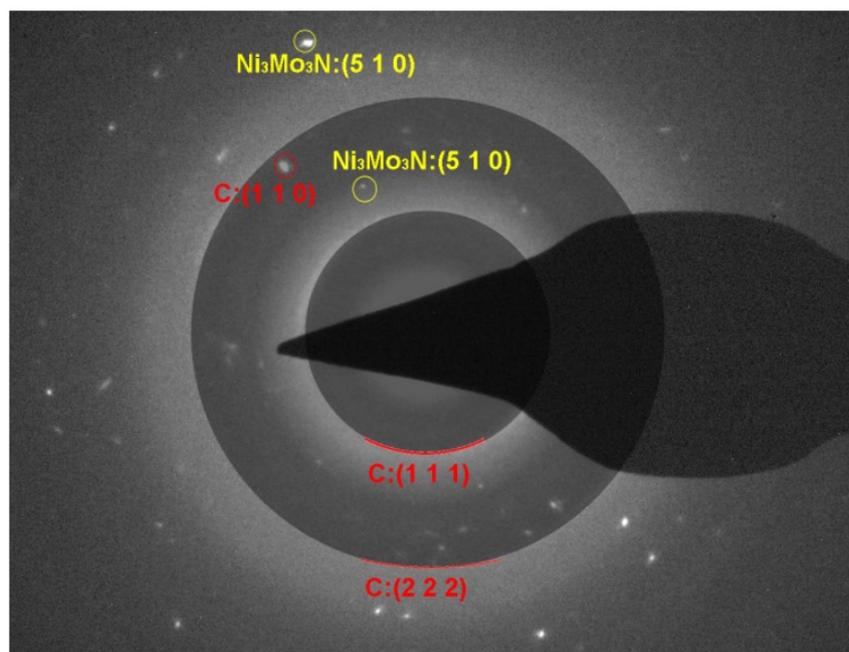
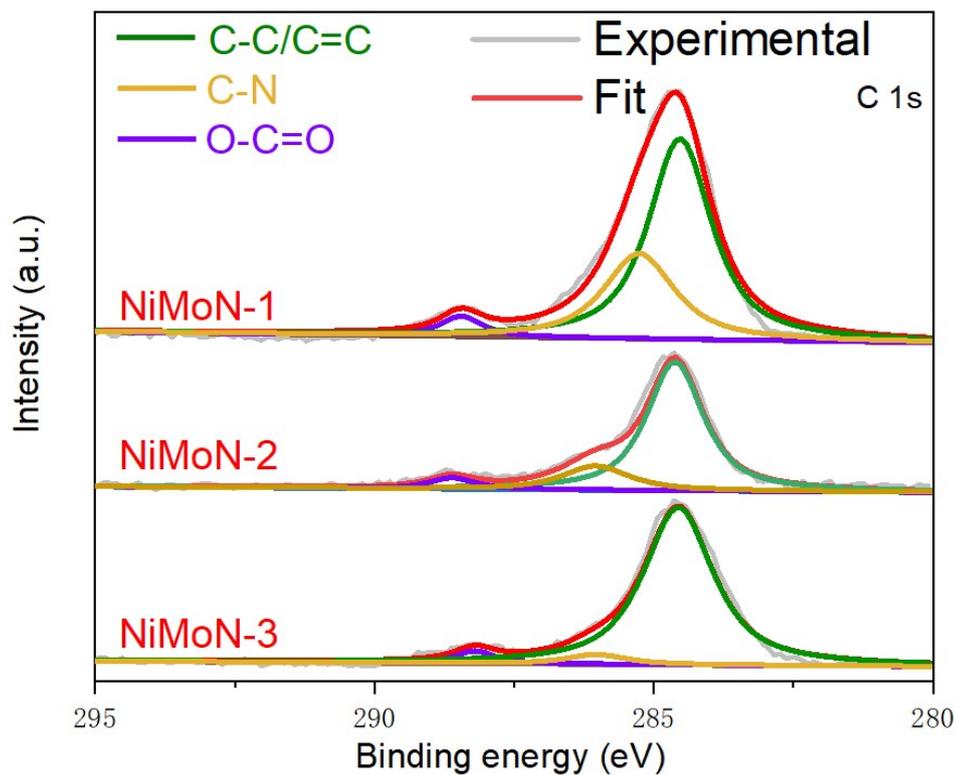
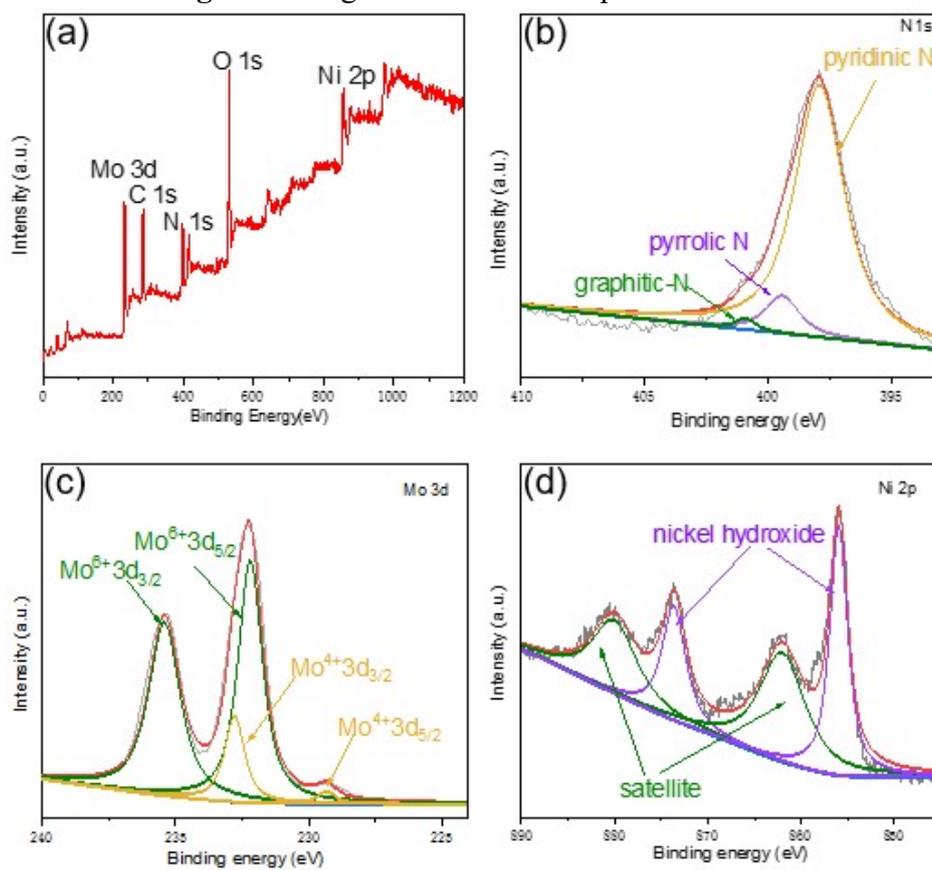


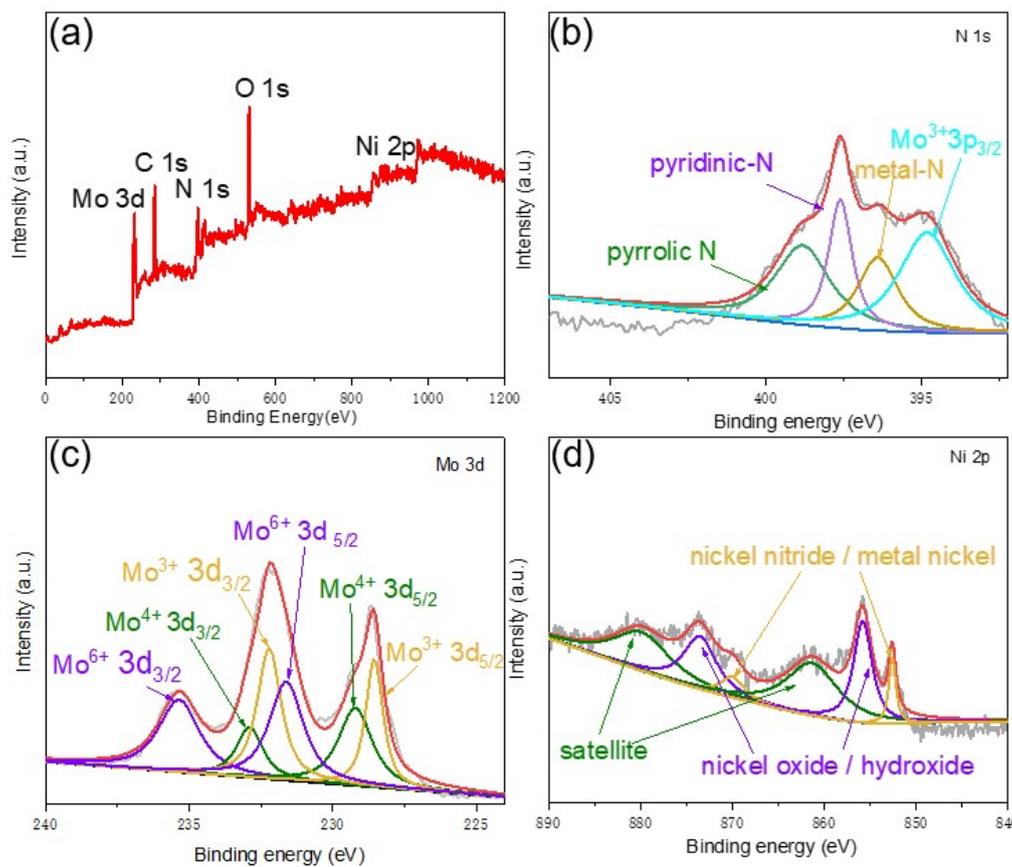
Figure S3 SAED pattern of NiMoN -2.



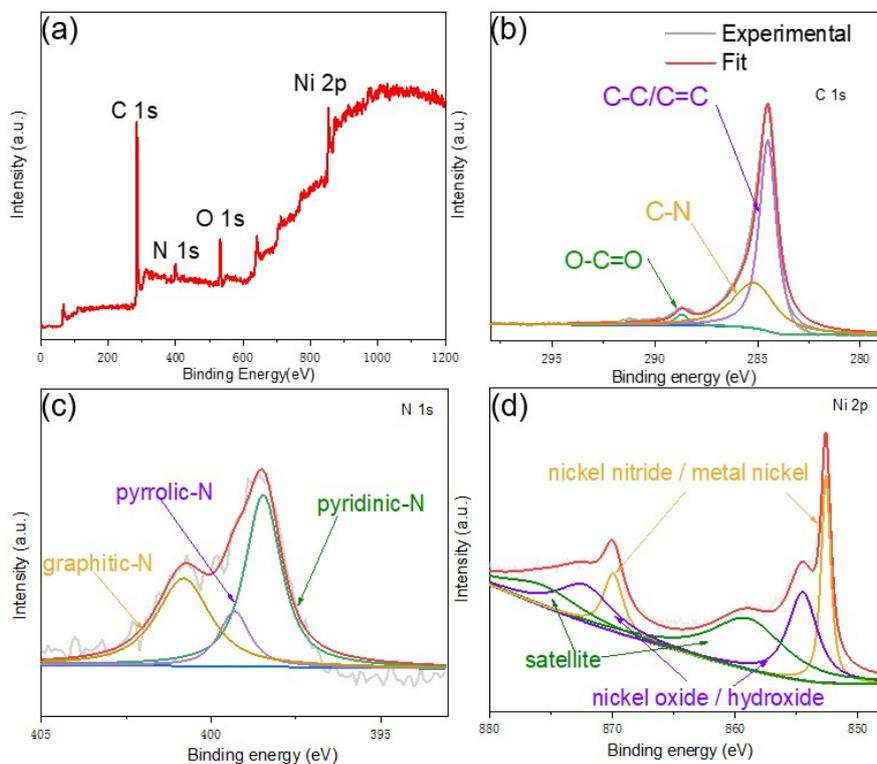
**Figure S4** High-resolution XPS spectra of C 1s.



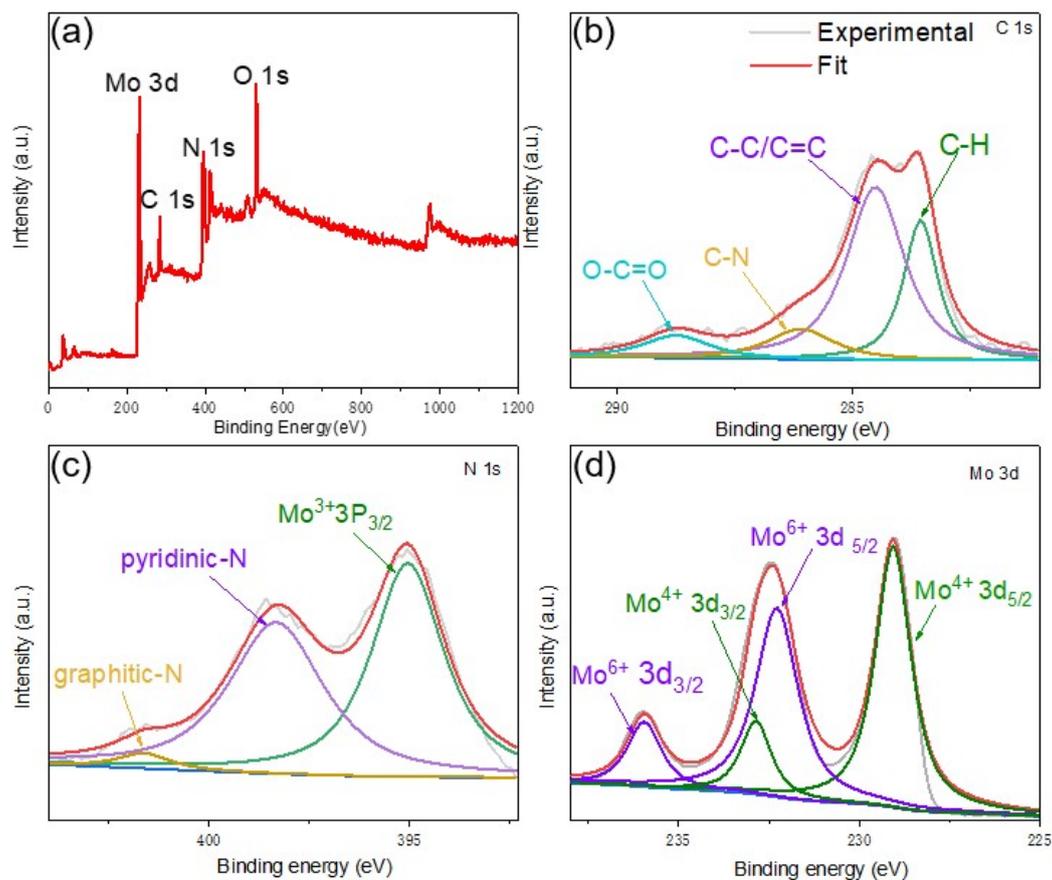
**Figure S5** XPS spectra of the bimetallic NiMoN-1 catalysts :  
 (a) survey spectrum, (b) N 1s (c) Mo 3d, and (d) Ni 2p .



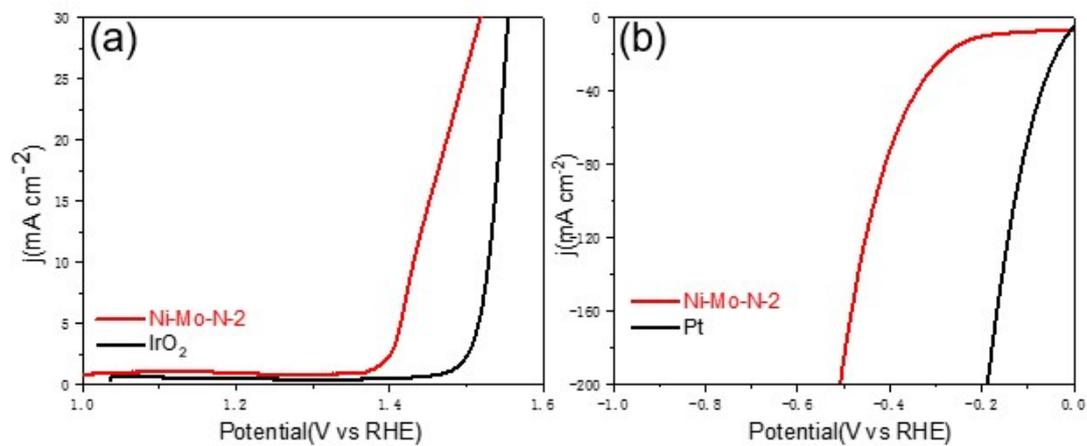
**Figure S6** XPS spectra of the bimetallic NiMoN-3 catalysts :  
 (a) survey spectrum, (b) N 1s (c) Mo 3d, and (d) Ni 2p .



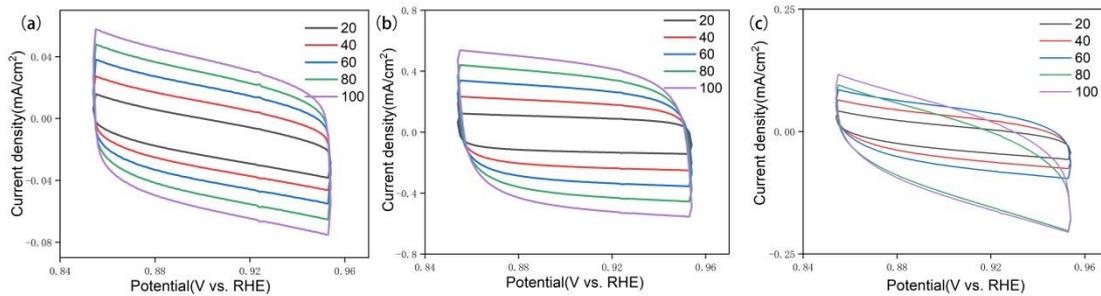
**Figure S7** XPS spectra of the bimetallic Ni-CN catalysts :  
 (a) survey spectrum, (b) C 1s (c) N 1s, and (d) Ni 2p.



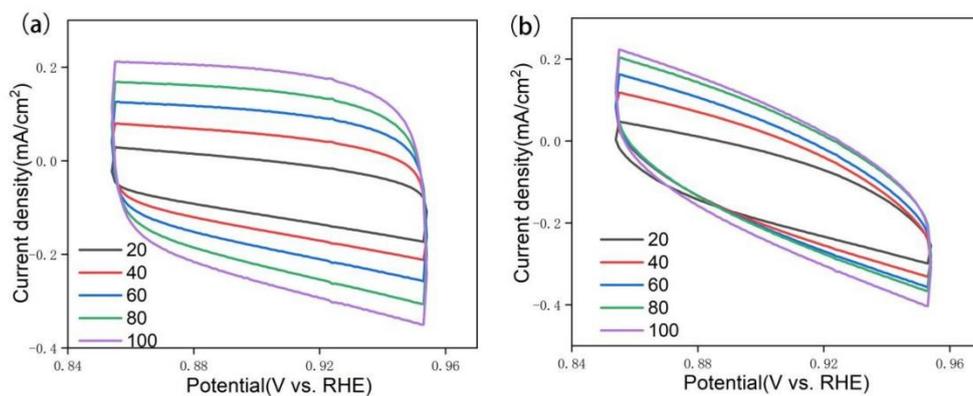
**Figure S8** XPS spectra of the bimetallic Mo-CN catalysts :  
 (a) survey spectrum, (b) C 1s (c) N 1s, and (d) Mo 3d.



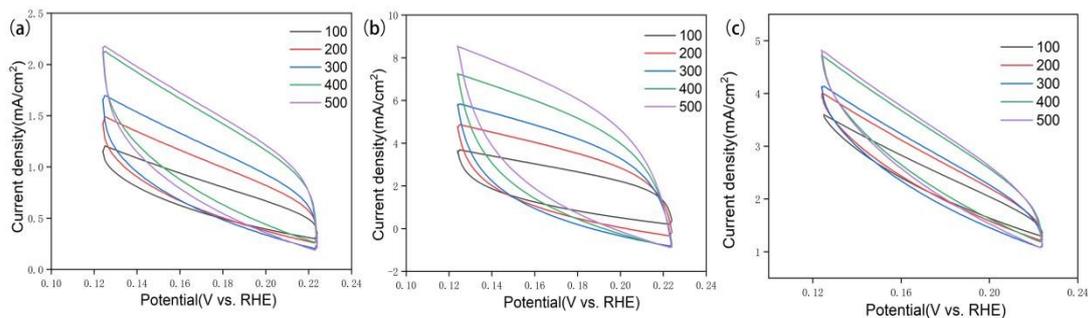
**Figure S9** Electrocatalytic activity in 1 M KOH (a) The polarization curves of OER,  
 (a) The polarization curves of HER



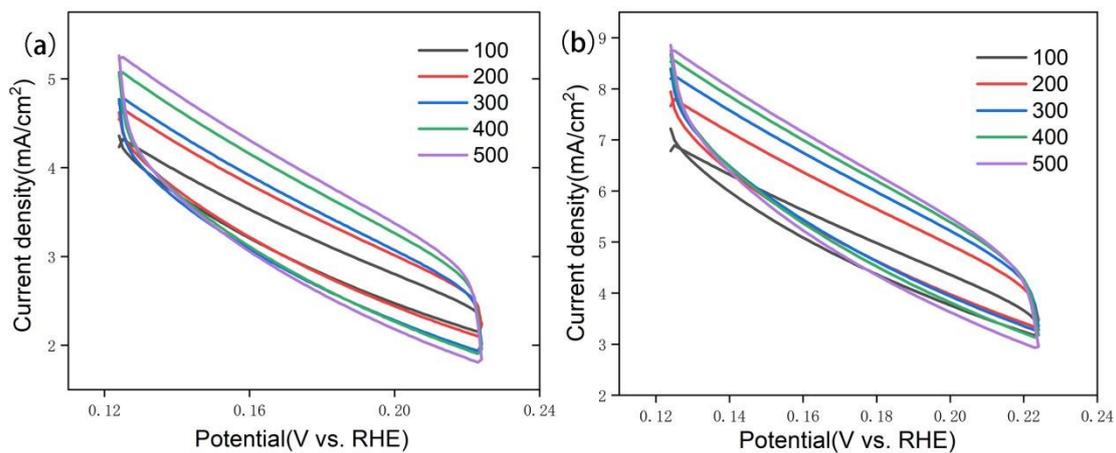
**Figure S10** Cyclic voltammograms with the scan rate from 20 to 100 mV/s for NiMoN-1, NiMoN-2, NiMoN-3 in 1 M KOH on electrocatalytic OER activity



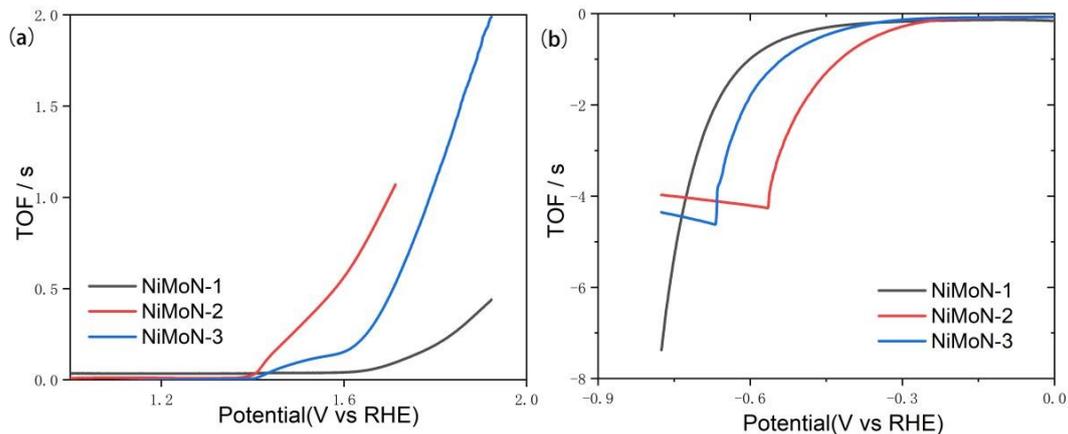
**Figure S11** Cyclic voltammograms with the scan rate from 20 to 100 mV/s for Ni-CN, Mo-CN in 1 M KOH on electrocatalytic OER activity



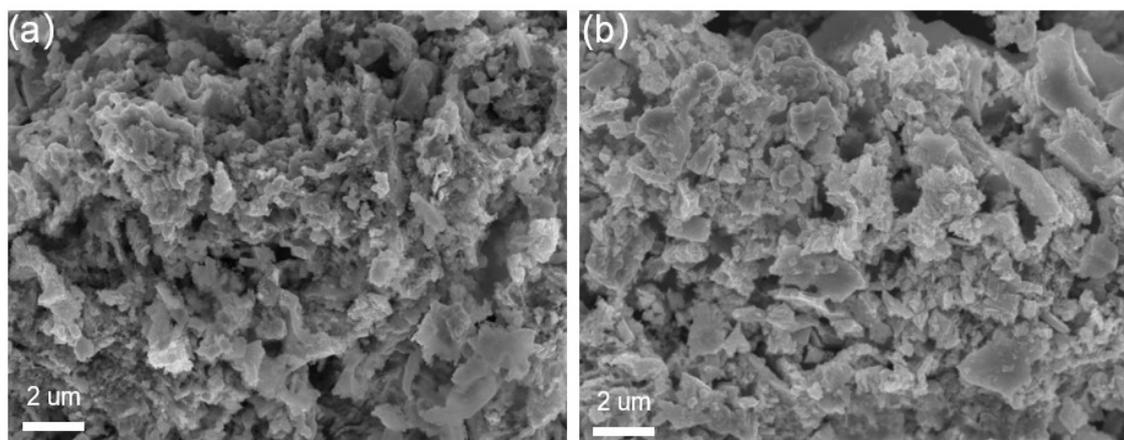
**Figure S12** Cyclic voltammograms with the scan rate from 20 to 100 mV/s for NiMoN-1, NiMoN-2, NiMoN-3 in 1 M KOH on electrocatalytic HER activity.



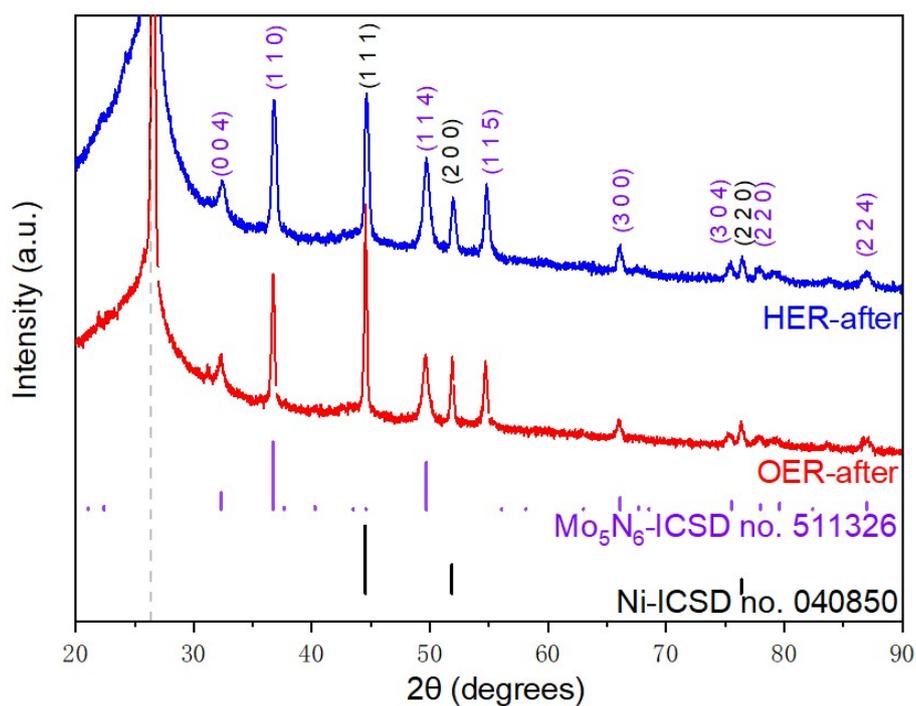
**Figure S13** Cyclic voltammograms with the scan rate from 20 to 100 mV/s for NiCN, Mo-CN in 1 M KOH on electrocatalytic HER activity.



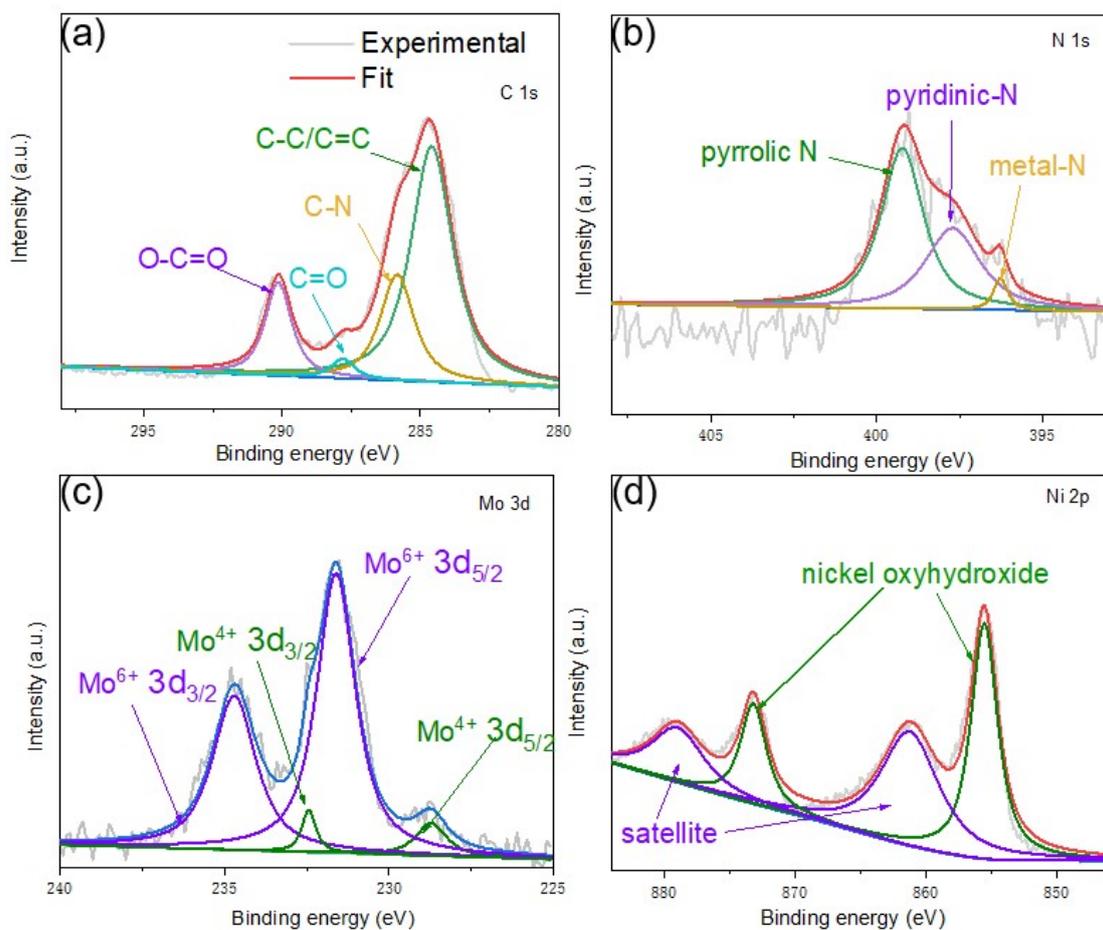
**Figure S14** (a) The OER-TOFs of the NiMoN-1, NiMoN-2, NiMoN-3 (b) The HER-TOFs of the NiMoN-1, NiMoN-2, NiMoN-3.



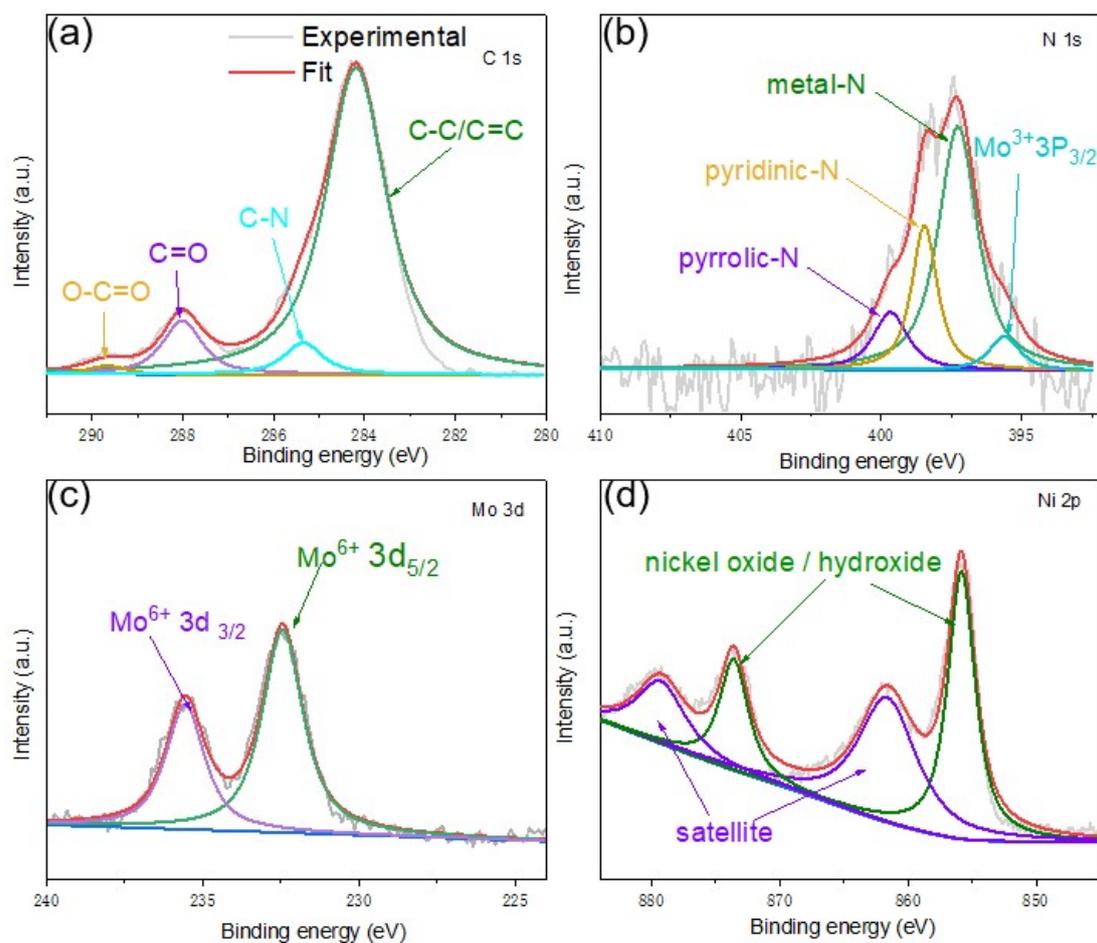
**Figure S15** SEM images of NiMoN-2 catalysts after (a) OER and (b) HER.



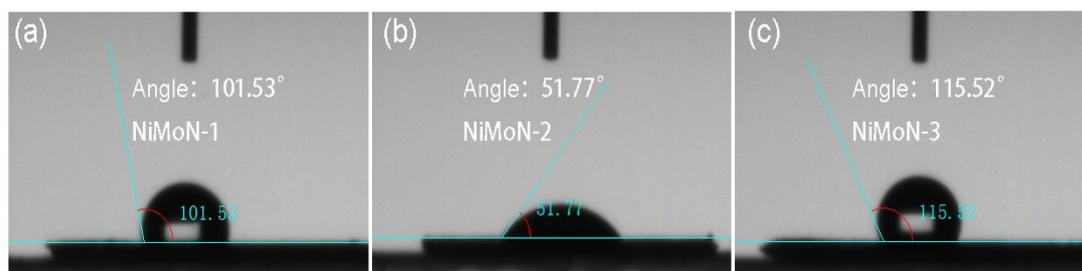
**Figure S16** XRD pattern of NiMoN-2 after OER and HER.



**Figure S17** XPS spectra of NiMoN-2 after OER.



**Figure S18** XPS spectra of NiMoN-2 after HER.



**Figure S19** Contact angles of (a) NiMoN-1, (b) NiMoN-2, and (c) NiMoN-3.

**Table S1.** Comparison of the  $R_{CT}$  values of the prepared materials .

Sample	$R_{CT}$ (Ohm)-OER	$R_{CT}$ (Ohm)-HER
NiMoN-1	1.74	1.57
NiMoN-2	1.51	1.42
NiMoN-3	1.86	1.63
Ni-CN	2.42	1.97
Mo-CN	3.37	2.85

**Table S2.** Comparison of the catalytic activities of OER on NiMoN-2 with recently reported catalysts in the  $1.0 \text{ mol}\cdot\text{L}^{-1}$  KOH medium ( $\text{pH} = 14$ )

Catalyst	$\eta$ /mV vs. RHE	Ref.
NiMoN-2	202	This work
Co-NiMoN-400	294	[6]
$\text{Ni}_{0.69}\text{Co}_{0.31}\text{P}$	266	[17]
Ni-Fe-MoN NTs	228	[18]
$\text{Ni}_3\text{FeS}$	223	[19]
NiMoN-550	295	[20]
NiMoC/NC-100	328	[25]
CoNiMo-O/H <sub>2</sub> -450	279	[27]
NiMoNS	260	[32]
Ni-NiO/HGF-1.5h	308	[36]
$\text{Ni}_3\text{FeN-NPs}$	280	[43]
$\text{Fe}^{3+}\text{NiCo}_2\text{O}_4$	210	[44]
Ni-BDC@NiFe-LDH-2	272	[46]
$\text{Ni}_3\text{N/NiMoN-5}$	277	[47]

Note:  $\eta$  is the overpotential measured at  $10 \text{ mA}\cdot\text{cm}^{-2}$ .

**Table S3.** Bifunctional electrocatalyst for overall water splitting in 1.0 M KOH solution.

Catalyst	<i>Voltage / V</i>	Ref.
NiMoN-2	1.58	This work
b-NiMoO <sub>4</sub> /NF	1.55	[2]
Co-NiMoN-400	1.57	[6]
Ni <sub>0.69</sub> Co <sub>0.31</sub> P	1.59	[17]
Ni-Fe-MoN NTs	1.513	[18]
NiMoN-550	1.596	[20]
Ni <sub>3</sub> FeS	1.57	[19]
NiMoC/NC-100	1.72	[25]
CoNiMo-O/H <sub>2</sub> -450	1.59	[27]