Electronic Supplementary Material (ESI) for CrystEngComm.

Supporting Information

Facile formation of Fe-doped NiCoP hollow nanocage as bifunctional electrocatalysts for overall water splitting

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Table S1. HER performances comparison of recently reported representative electrocatalysts in alkaline medium (1.0 M KOH, at 10 mA cm^{-2})

catalyst	Overpotential (mV)	Reference
NiCoFeP	147	This work
MoS_2-NiS_2/NGF	172	[1]
Co/β-Mo_2C@NCNTs	170	[2]
EBP@NG	190	[3]
p-WCx NWs/CC	122	[4]
N-Ni_3S_2/NF	110	[5]
$Ni_{0.9}Fe_{0.1}PS_3$@MXene	196	[6]
amorphous CoP/NF	143	[7]
MoS_2/NiS	244	[8]
$Co(OH)_2$@NCNTs@NF	170	[9]
Mo-doped NiCoP	76	[10]
Ni_3S_2 nanosheet arrays/NF	223	[11]
Fe-Ni_2P/MoS_x/NF	112	[12]
Co@CNTs@DSCNCs	214	[13]
$Co(OH)_2$@P-NiCo-LDH	226	[14]
CFC-CNT-CoO_x/CoP	108	[15]

Table S2. OER performances comparison of recently reported representative eletrocatalysts in alkaline medium (1.0 M KOH, at 10 mA cm^{-2})

catalyst	Overpotential (mV)	Reference
NiCoFeP	235	This work
Ni_3N-NiMoN	277	[16]
FeCo-FeCoP@C@NCCs	280	[17]
amorphous CoP/NF	284	[7]
CP/CTs/Co-S	190	[18]
Ni_3S_2@NGCLs/NF	271	[19]
MoS_2-NiS_2/NGF	370	[1]
Ni_3S_2@MoS_2/FeOOH	260	[20]
Co_6W_6C@NC	286	[21]
CoS_2 HNSs	290	[22]
S-CoWP@(S,N)-C	280	[23]
FeNiB/FeNi foam-700	272	[24]
Ni_6Fe_2W-LDH@CC	264	[25]
$CoMoN_x$-500 NSAs/NF	231	[26]
CdP_2-CDs-CoP	285	[27]
CoFeP/CoP/CC	240	[28]

Table S3. Overall water splitting performances of our sample compared with recently reported representative electrocatalysts in alkaline electrolytes

catalyst	Potential (V) at 10 mA cm^{-2}	Reference
NiCoFeP	1.60	This work
$CoTe_2$@NCNTFs	1.67	[29]
MoS_2-NiS_2/NGF	1.64	[1]
Ni_3S_2@NGCLs/NF	1.55	[19]
NiS/Ni_2P	1.67	[30]
CoP/NCNHP	1.64	[31]
Fe–CoP HTPAs	1.59	[32]
CoTeNR/NF	1.64	[33]
A-$NiSe_2$|P	1.62	[34]
FeCo-FeCoP@C	1.64	[17]
CoxP	1.72	[35]
$CoNi_2S_4$/Ni_3S_2@NF	1.65	[36]
Co_9S_8/Cu_2S/CF	1.6	[37]
Fe-Ni_5P_4/NiFeOH	1.55	[38]
CuO@CoZn-LDH/CF	1.55	[39]

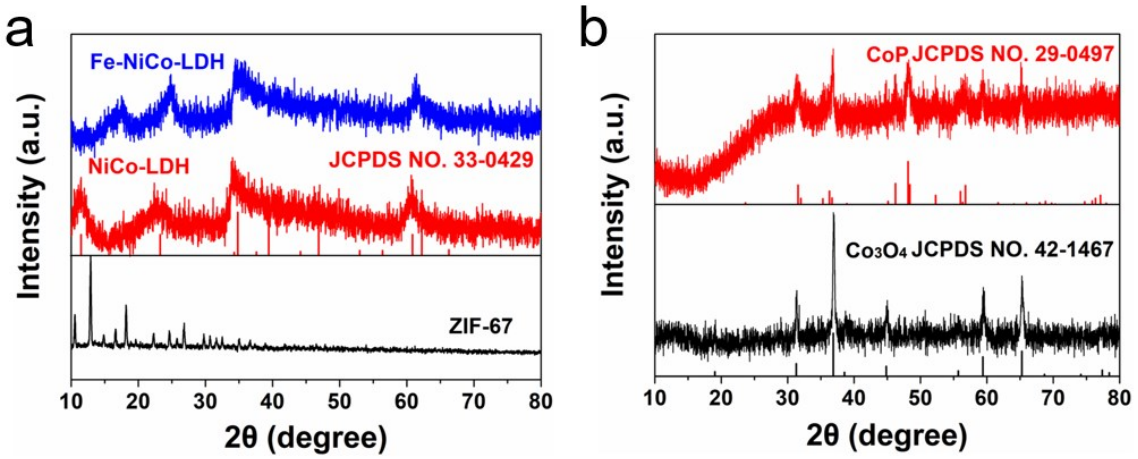

Fig. S1. (a) XRD pattern of the as-prepared ZIF-67, NiCo-LDH and Fe-NiCo-LDH samples; (b) XRD pattern of the as-prepared Co_3O_4 and CoP samples.

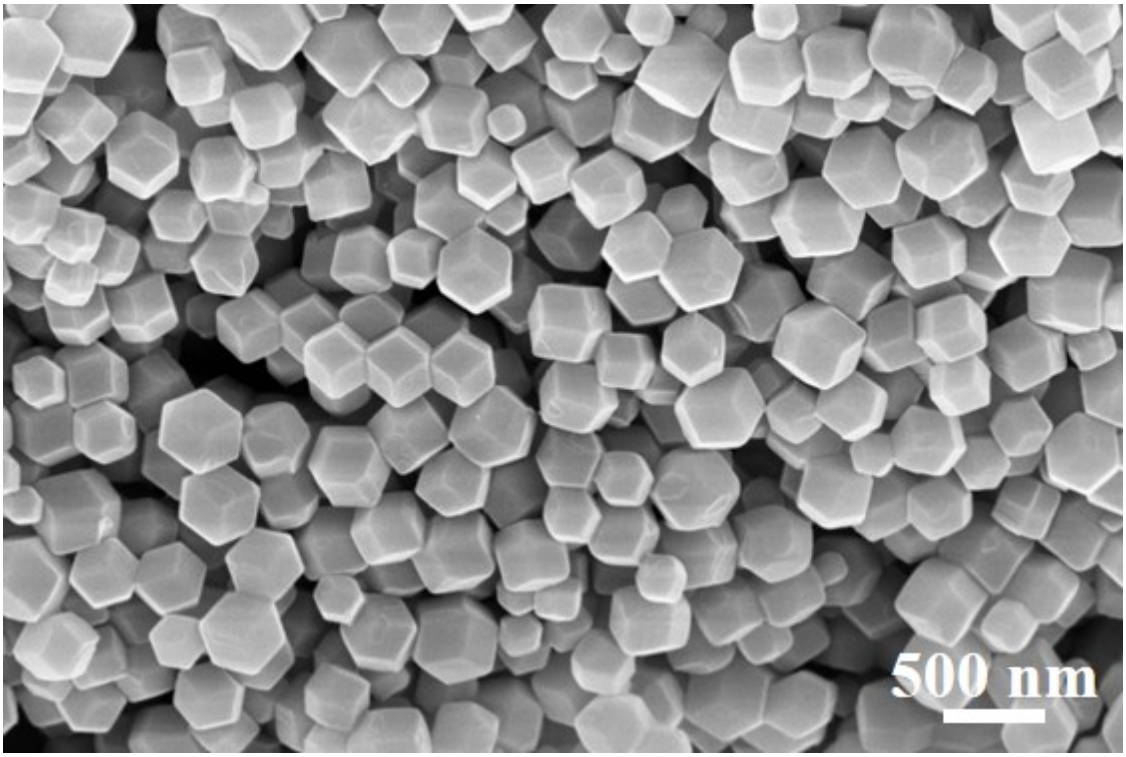

Fig. S2. SEM image of ZIF-67.

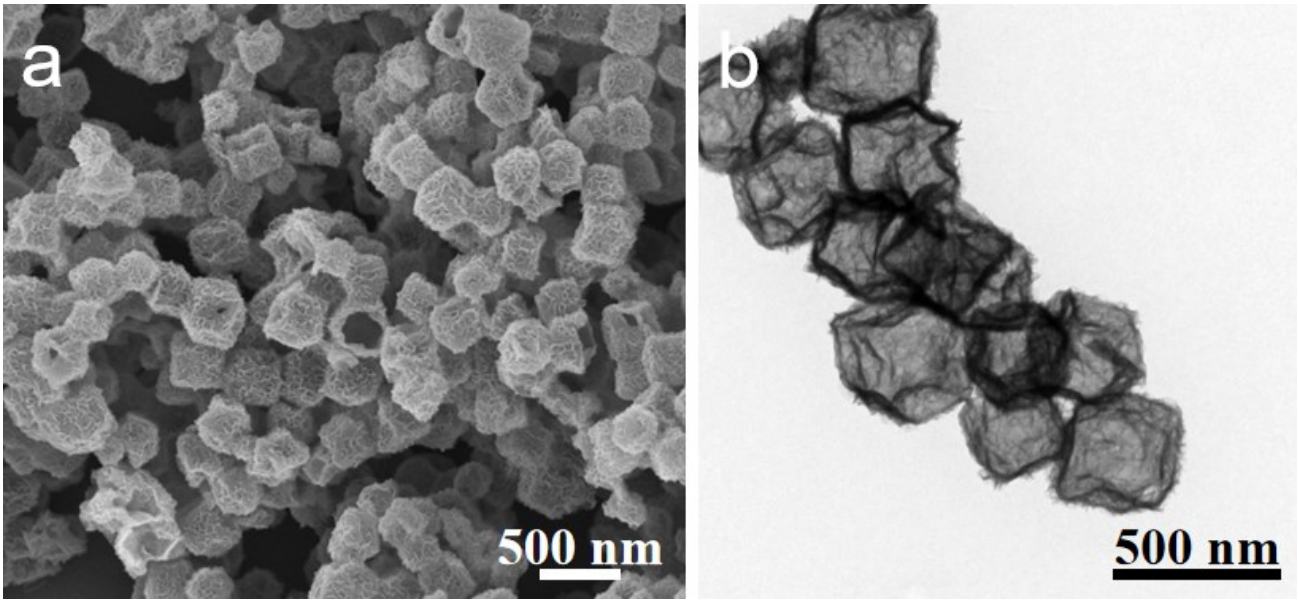

Fig. S3. (a, b) SEM and TEM images of NiCo-LDH.

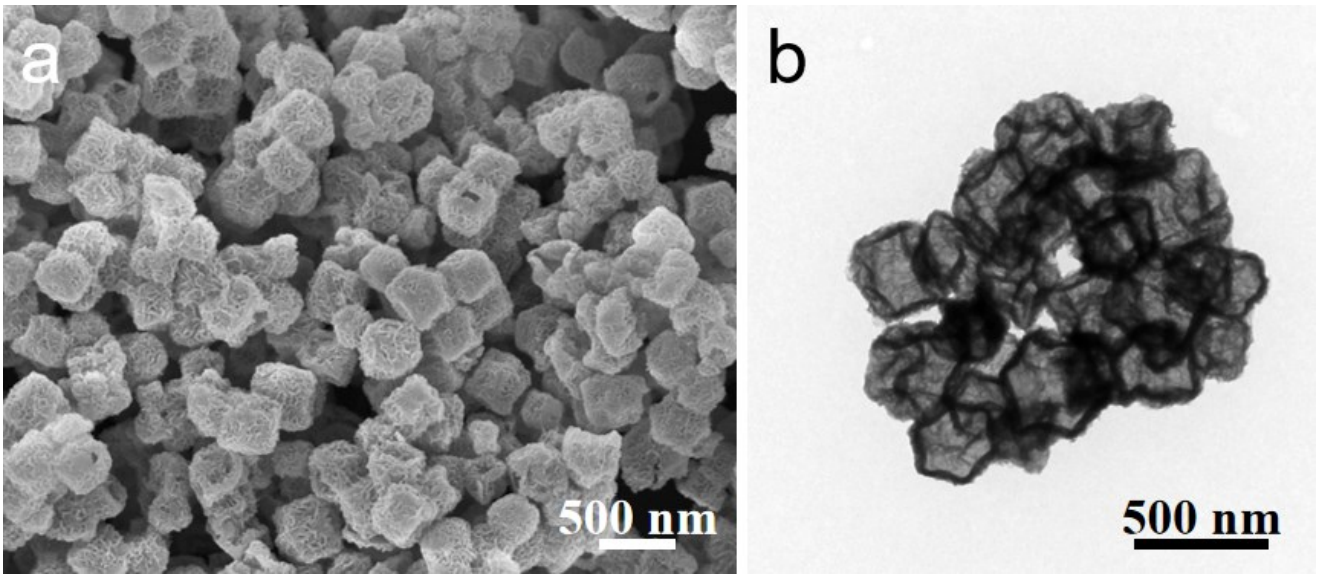

Fig. S4. (a, b) SEM and TEM images of Fe-NiCo-LDH.

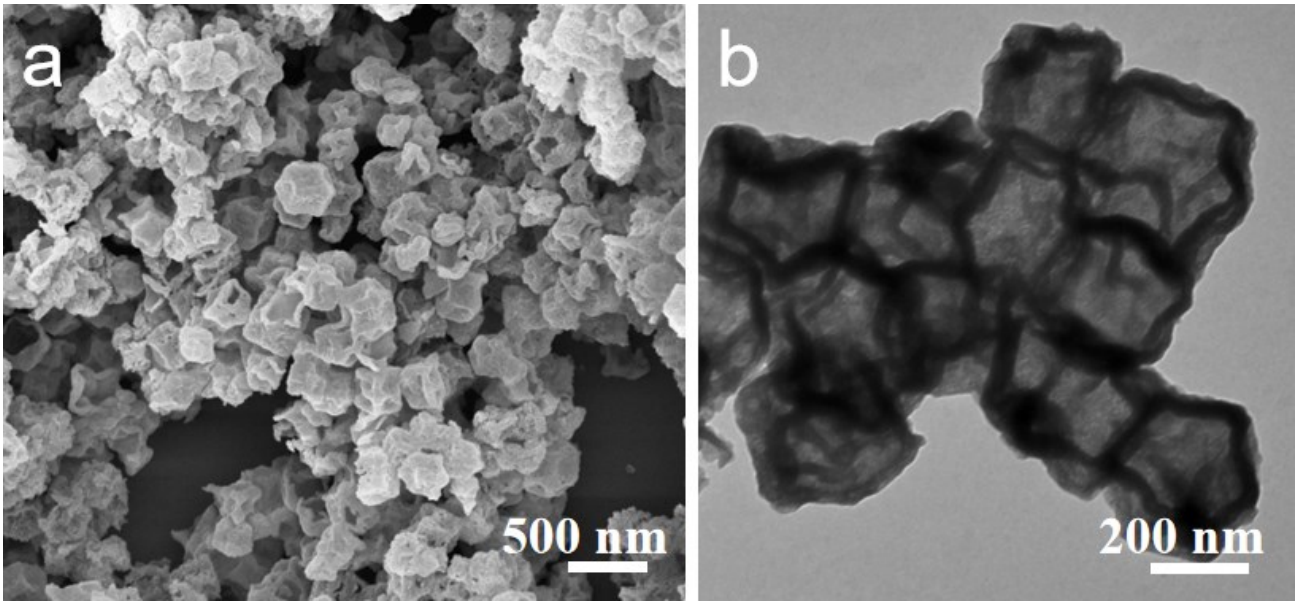

Fig. S5. (a, b) SEM and TEM images of NiCoP.

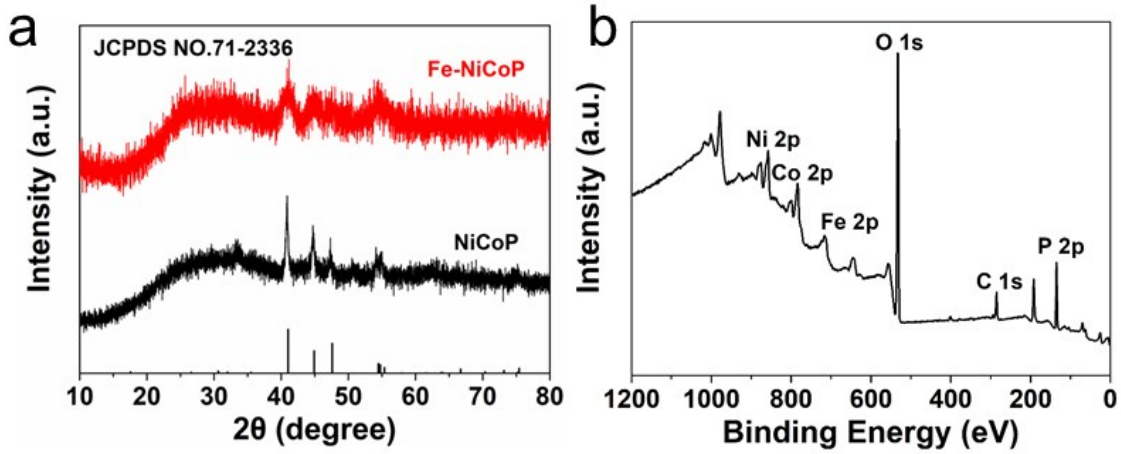

Fig. S6. (a) XRD pattern of the as-prepared NiCoP and Fe-NiCoP samples; (b) XPS survey spectra of Fe-NiCoP sample.

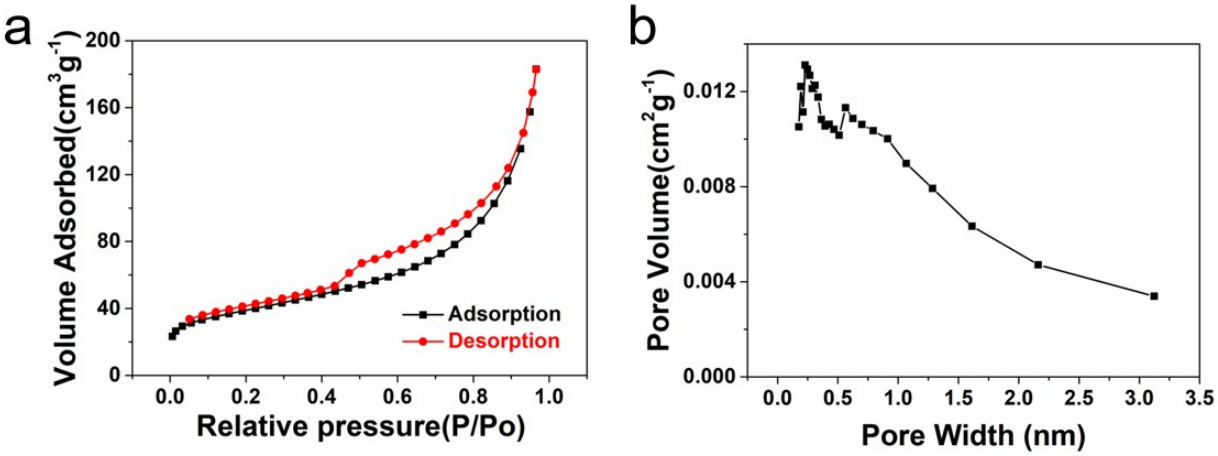

Fig. S7. (a,b) N_2 adsorption-desorption isotherms and pore size distribution of the as-prepared Fe-NiCoP.

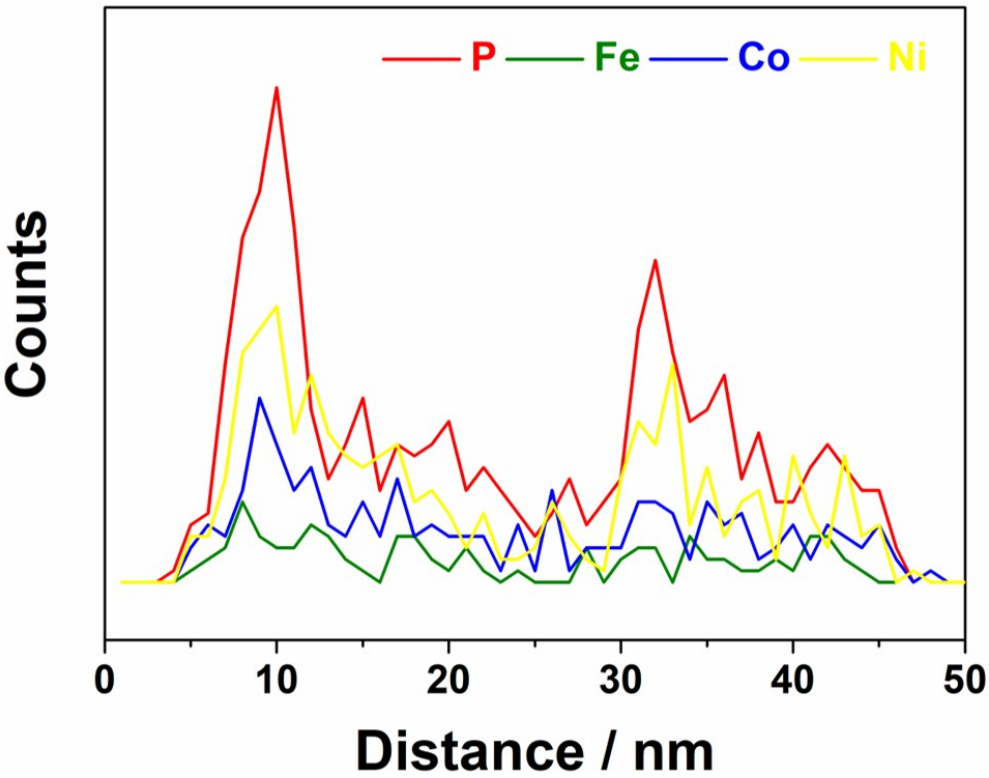

Fig. S8. EDX cross-sectional line scan profiles of the Fe-NiCoP sample.

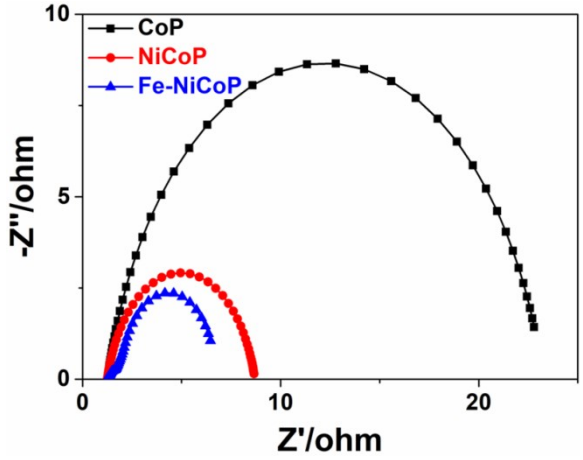

Fig. S9. Nyquist plots of CoP, NiCoP, and Fe-NiCoP samples.

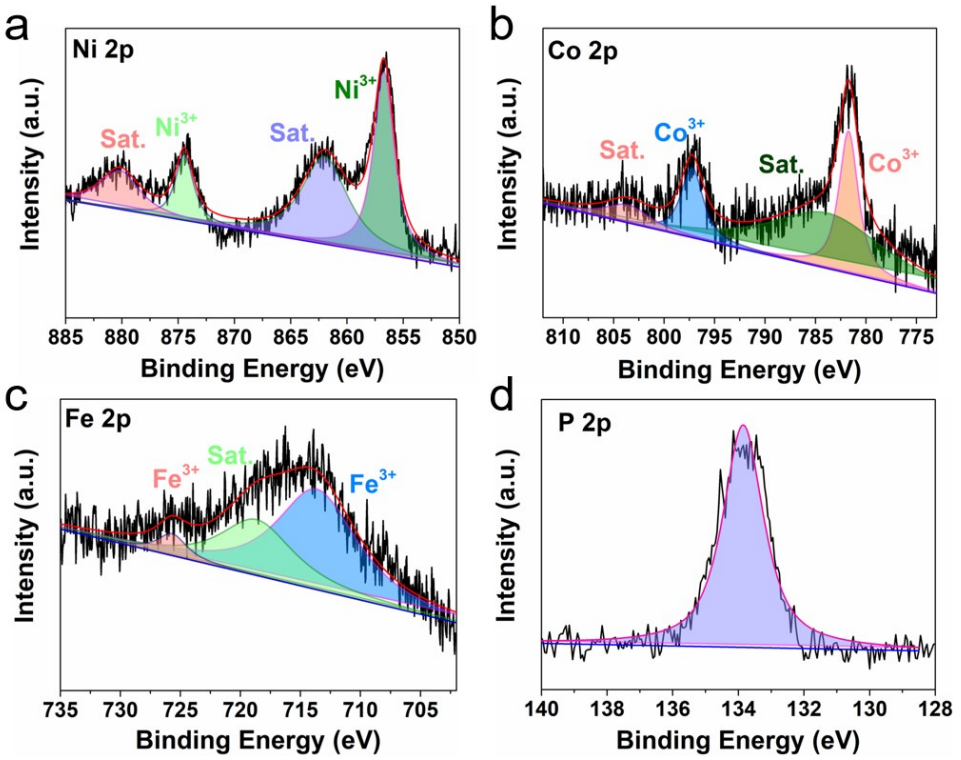

Fig. S10. XPS spectra of the Fe-NiCoP after OER test: (a) Ni 2p, (b) Co 2p, (c) Fe 2p, and (d) P 2p.

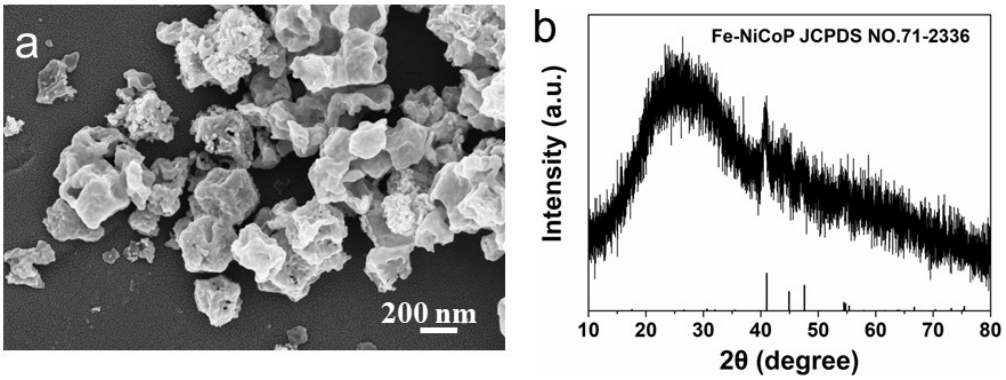

Fig. S11. (a) SEM and (b) XRD pattern for Fe-NiCoP after HER test.

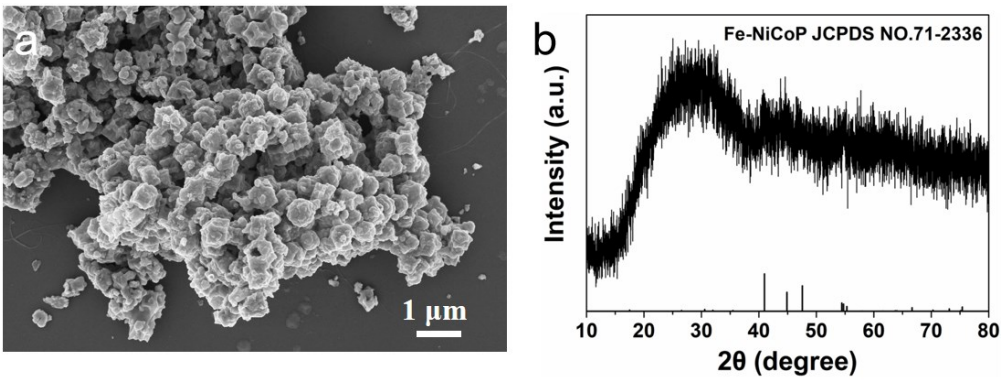

Fig. S12. (a) SEM and (b) XRD pattern for Fe-NiCoP after OER test.

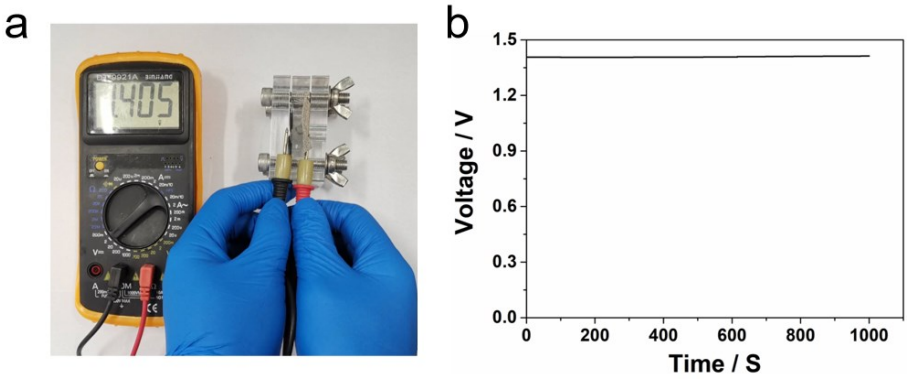

Fig. S13. (a,b) Open-circuit voltage plot of the Fe-NiCoP + Pt/C based Zn-air battery.

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