Electronic Supplementary Information (ESI)

Electronic structure exquisite restructuring of cobalt phosphide via rationally controlling iron induction for water splitting at industrial condition

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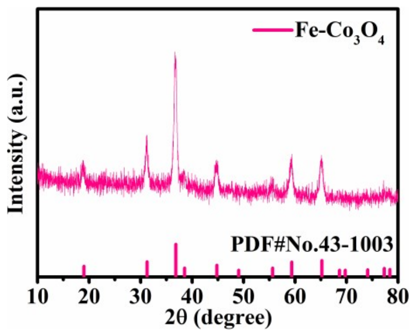

Fig. S1 XRD pattern of Fe-Co_3O_4 product.

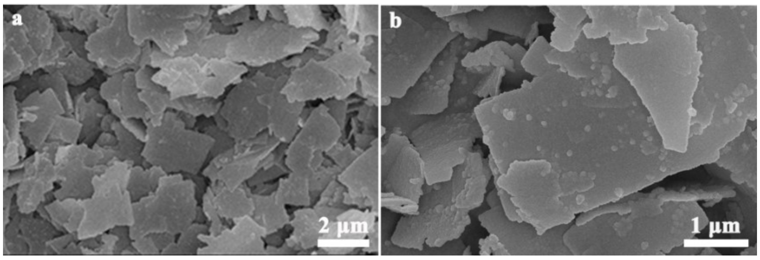

Fig. S2 (a, b) SEM images of CoP product.

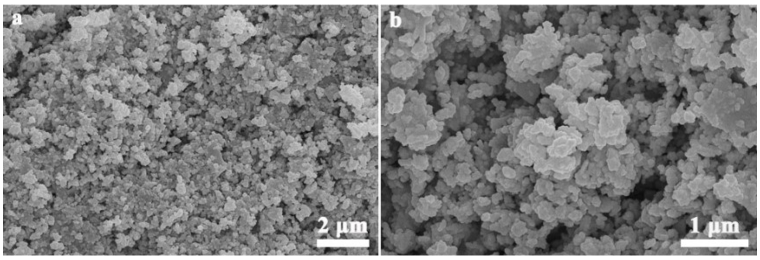

Fig. S3 (a, b) SEM images of CoP product prepared at 120 °C.

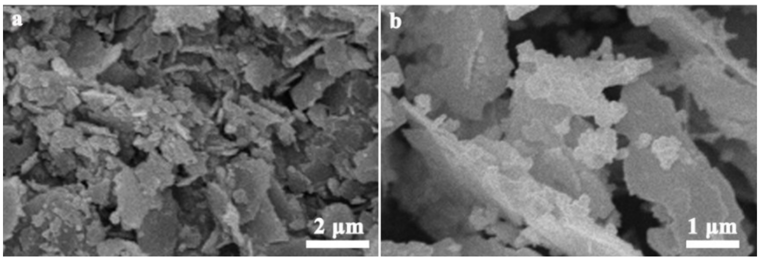

Fig. S4 (a, b) SEM images of CoP product prepared at 180 °C.

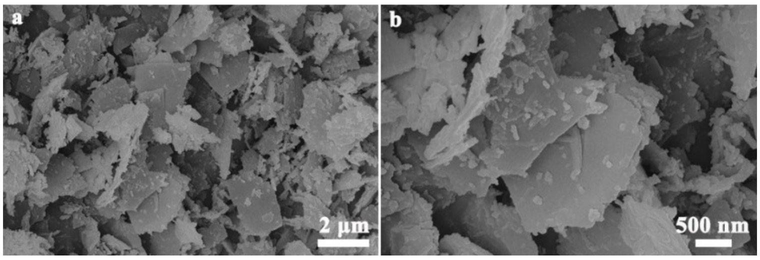

Fig. S5 (a, b) SEM images of CoP product prepared for 3.0 h.

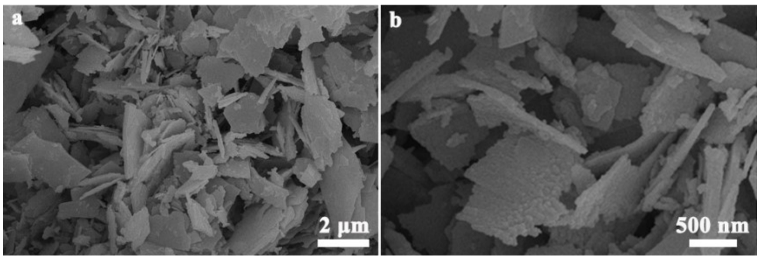

Fig. S6 (a, b) SEM images of CoP product prepared for 8.0 h.

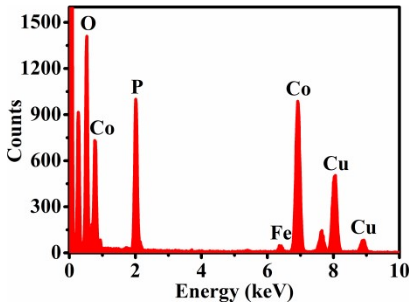

Fig. S7 EDX spectrum of Fe-CoP product.

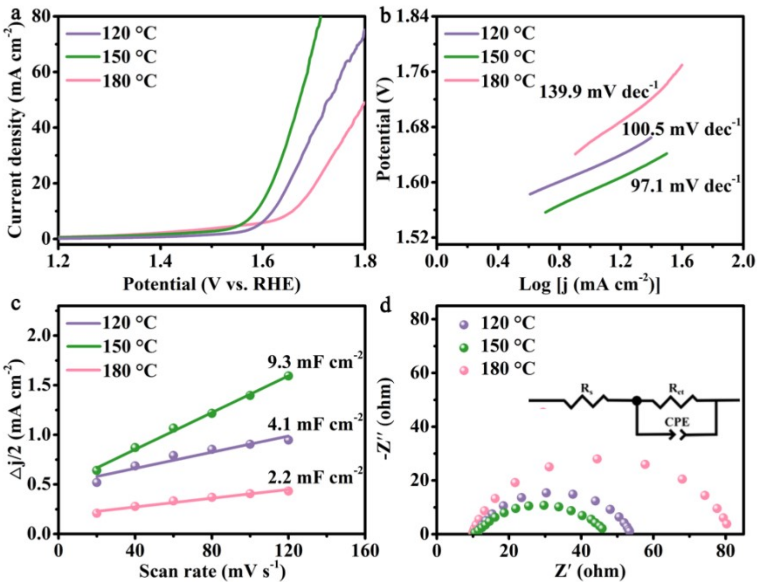

Fig. S8 OER performance of CoP products prepared at different reaction temperatures. (a) Polarization, (b) Tafel, (c) C_{dl} and (d) Nyquist curves.

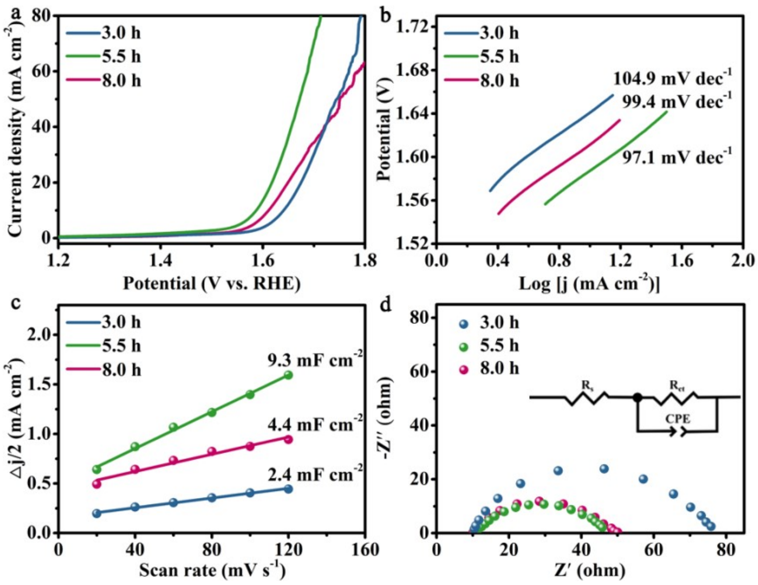

Fig. S9 OER performance of CoP products prepared for different reaction time. (a) Polarization, (b) Tafel, (c) C_{dl} and (d) Nyquist curves.

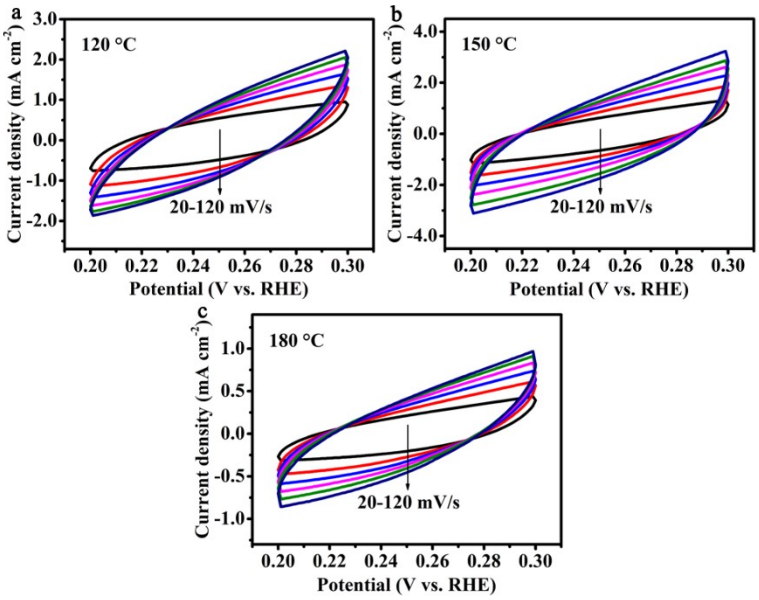

Fig. S10 OER cyclic voltammograms of CoP products prepared at different reaction temperatures.

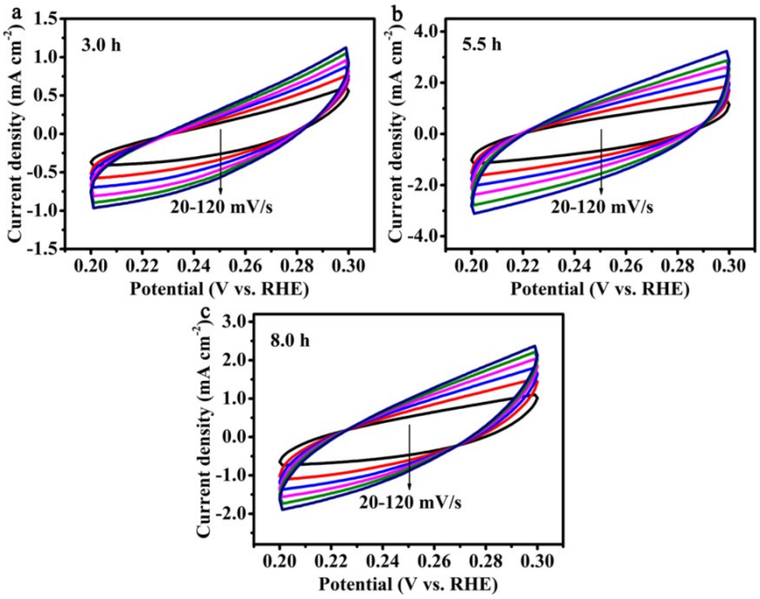

Fig. S11 OER cyclic voltammograms of CoP products prepared at different reaction time.

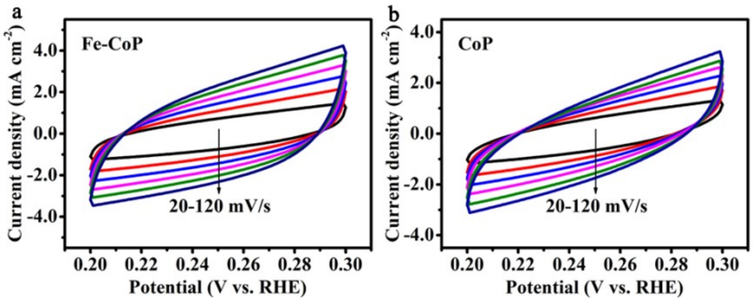

Fig. S12 OER cyclic voltammograms of (a) Fe-CoP and (b) CoP products at different scan rates.

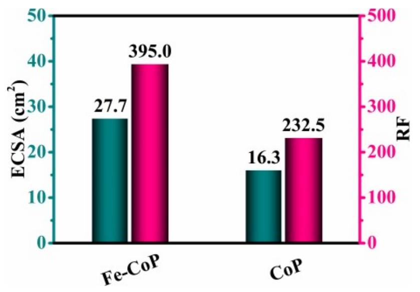

Fig. S13 OER ECSA and RF comparison of Fe-CoP and CoP products.

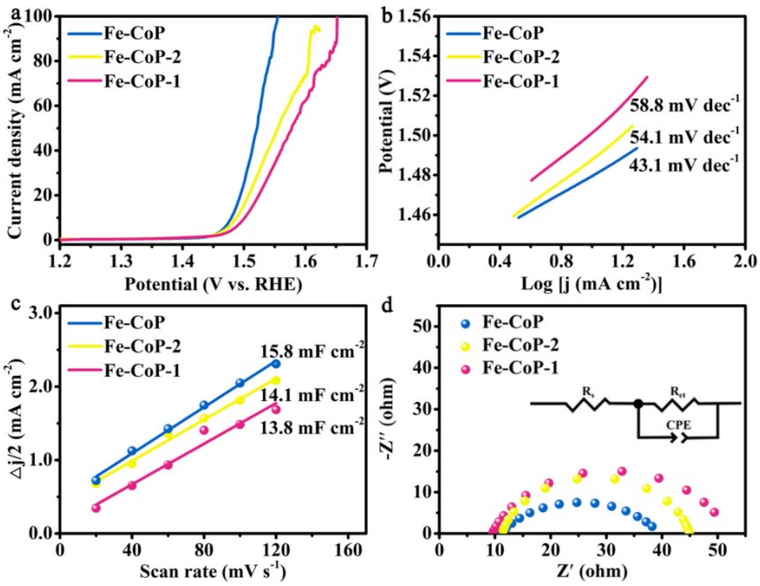

Fig. S14 OER performance of Fe-CoP products prepared with different Fe contents. (a) Polarization, (b) Tafel, (c) C_{dl} and (d) Nyquist curves.

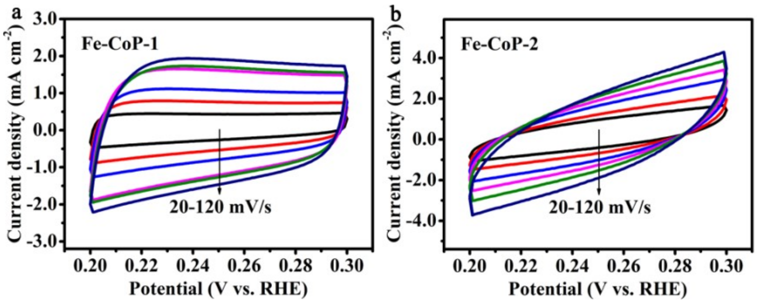

Fig. S15 OER cyclic voltammograms of Fe-CoP products prepared with different Fe contents.

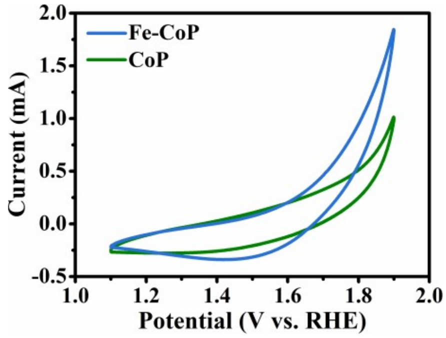

Fig. S16 OER cyclic voltammograms of Fe-CoP and CoP products in 1.0 M PBS with the scan rate of 100 mV s^{-1}.

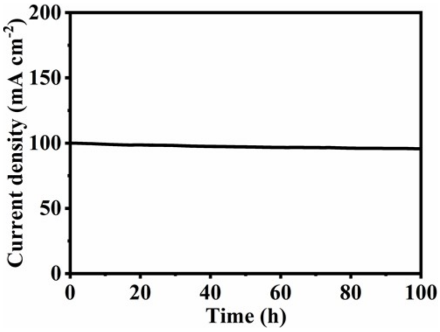

Fig. S17 I-t curve of Fe-CoP product at 100 mA cm^{-2}.

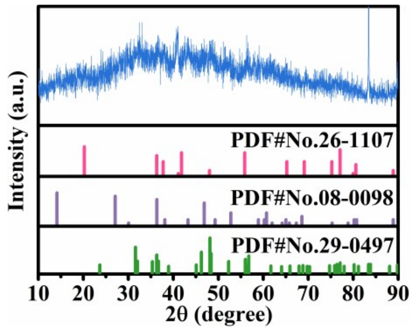

Fig. S18 XRD pattern of Fe-CoP after OER.

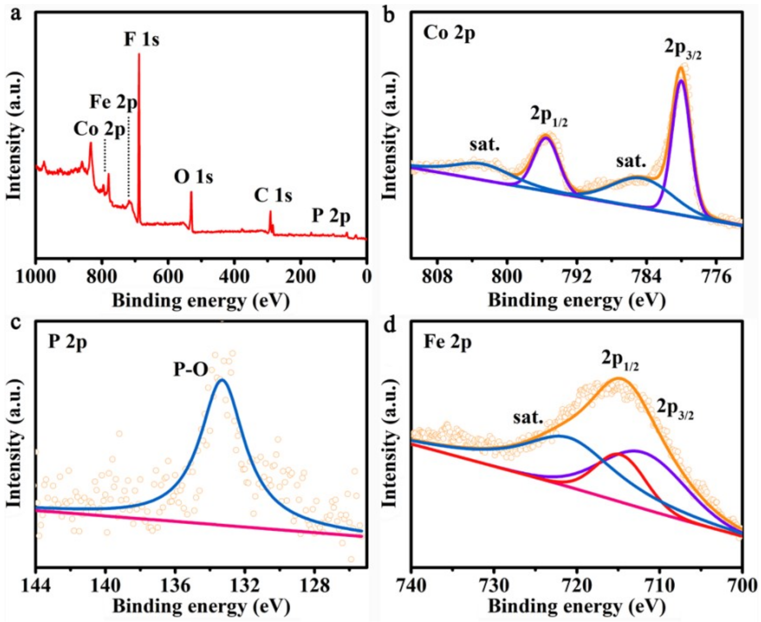

Fig. S19 XPS analysis of Fe-CoP after OER. (a) Survey spectrum, high resolution (b) Co 2p, (c) P 2p, (d) Fe 2p XPS spectra.

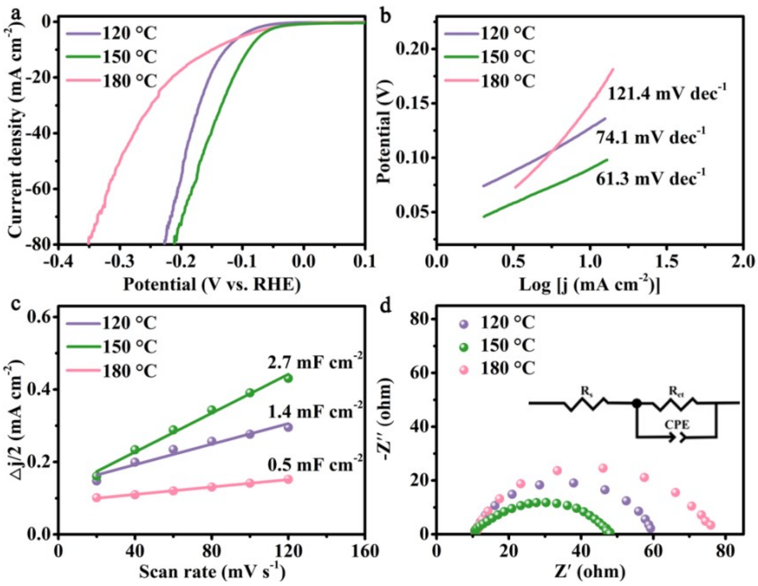

Fig. S20 HER performance of CoP products prepared at different reaction temperatures. (a) Polarization, (b) Tafel, (c) C_{dl} and (d) Nyquist curves.

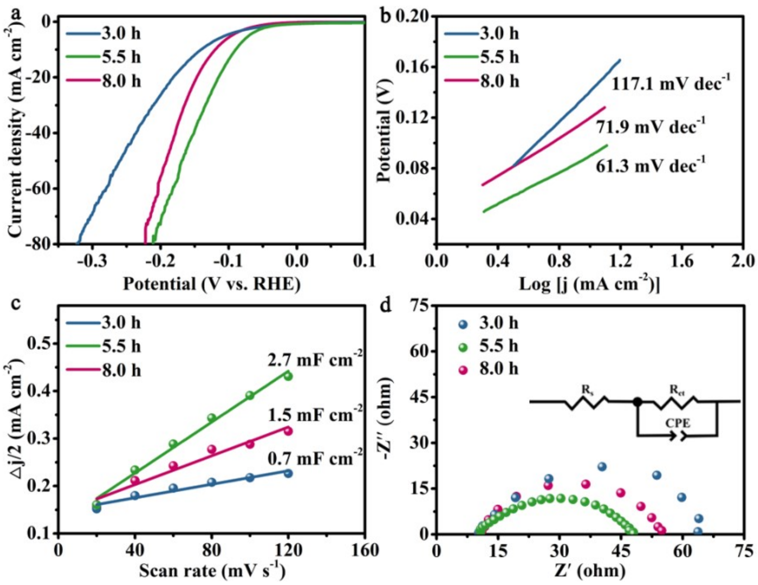

Fig. S21 HER performance of CoP products prepared for different reaction time. (a) Polarization, (b) Tafel, (c) C_{dl} and (d) Nyquist curves.

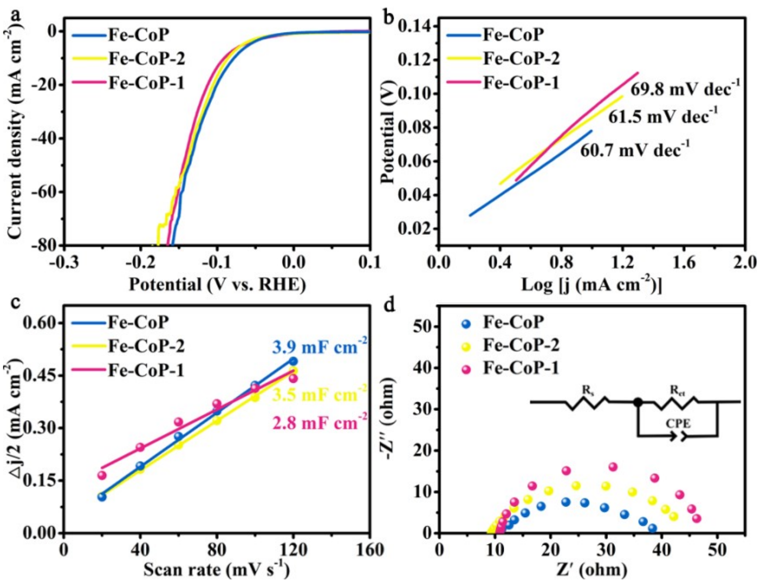

Fig. S22 HER performance of Fe-CoP products prepared with different Fe contents. (a) Polarization, (b) Tafel, (c) C_{dl} and (d) Nyquist curves.

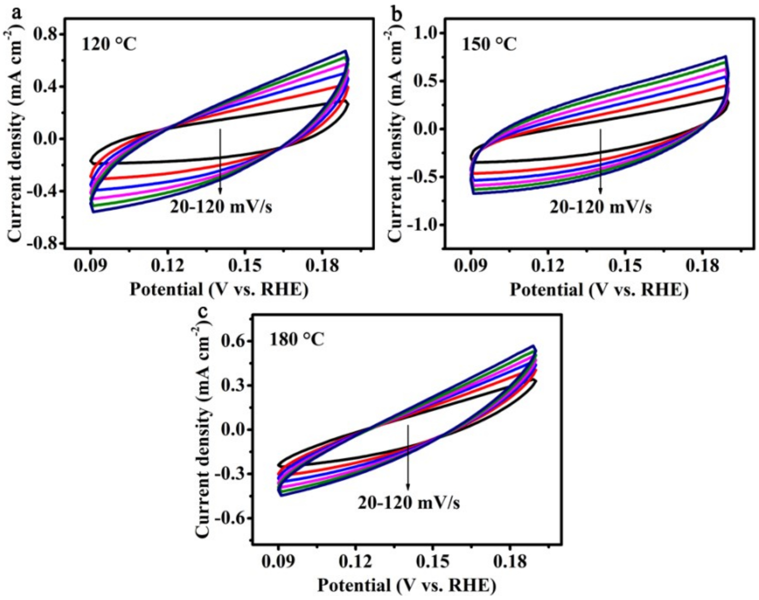

Fig. S23 HER cyclic voltammograms of CoP products prepared at different reaction temperatures.

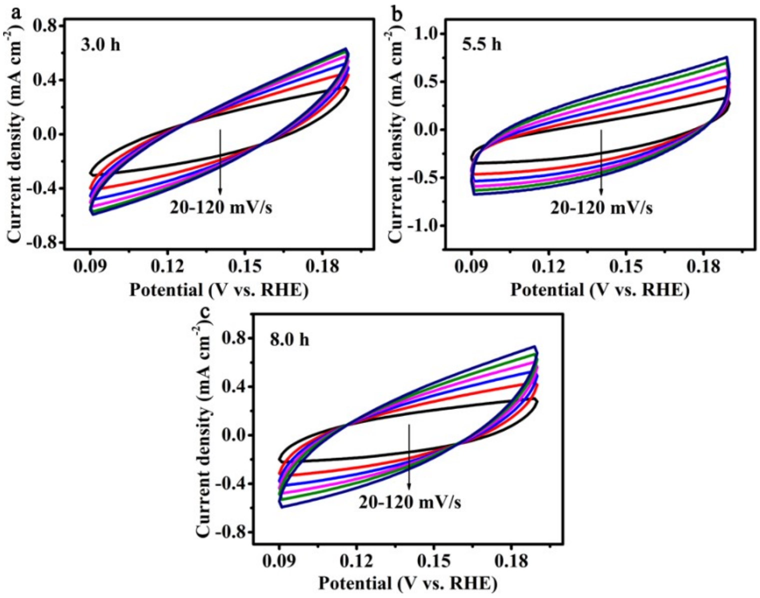

Fig. S24 HER cyclic voltammograms of CoP products prepared at different reaction time.

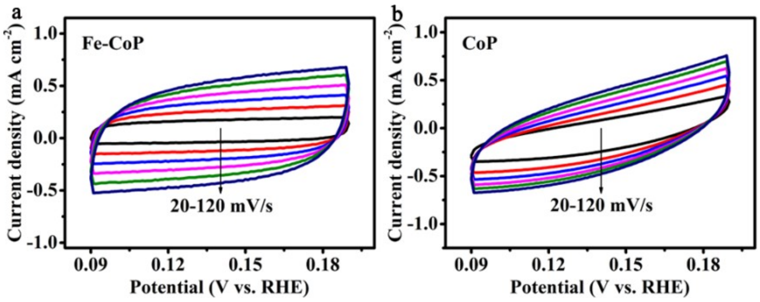

Fig. S25 HER cyclic voltammograms of (a) Fe-CoP and (b) CoP products at different scan rates.

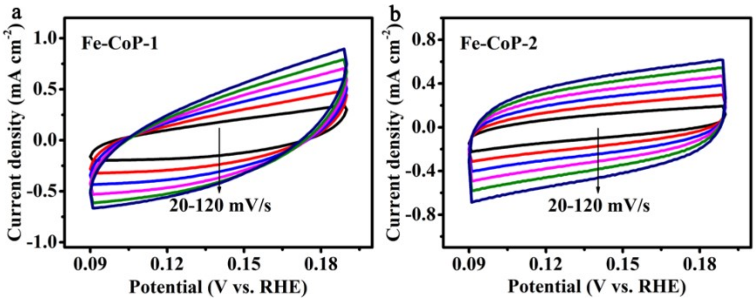

Fig. S26 HER cyclic voltammograms of Fe-CoP products prepared with different Fe contents.

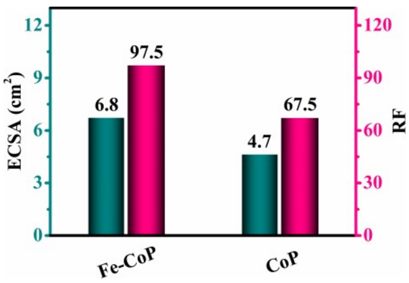

Fig. S27 HER ECSA and RF comparison of Fe-CoP and CoP products.

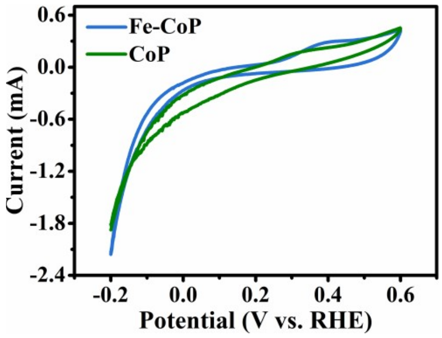

Fig. S28 HER cyclic voltammograms of Fe-CoP and CoP products in 1.0 M PBS with the scan rate of 100 mV s^{-1}.

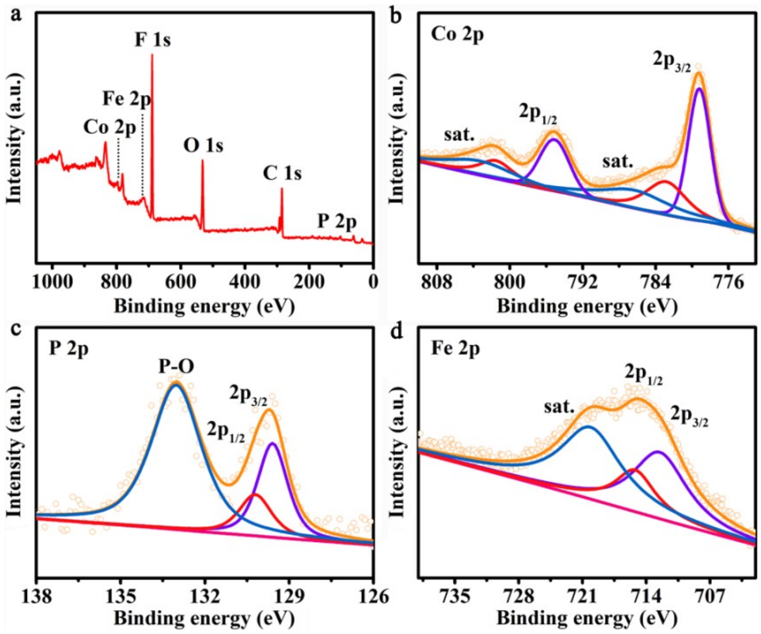

Fig. S29 XPS analysis of Fe-CoP after HER. (a) Survey spectrum, high resolution (b) Co 2p, (c) P 2p, (d) Fe 2p XPS spectra.

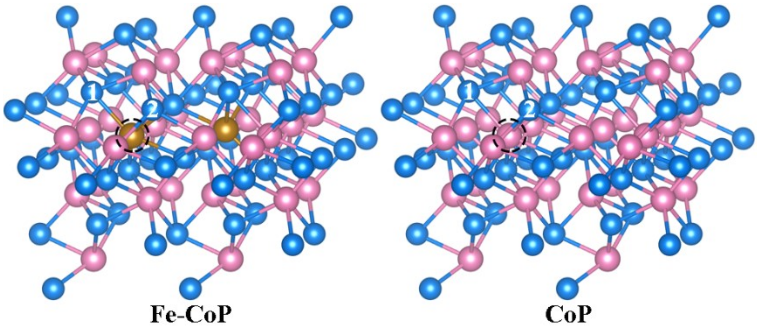

Fig. S30 Charge density distribution diagrams of Fe-CoP and CoP.

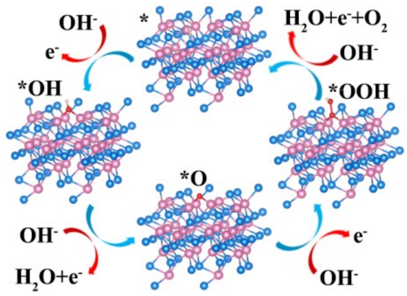

Fig. S31 Evolution step and adsorbent model of CoP for OER.

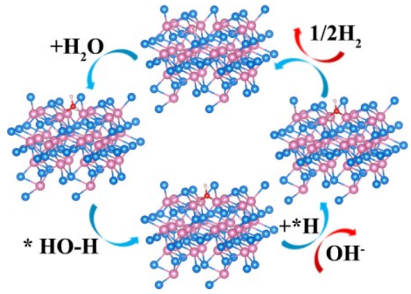

Fig. S32 Evolution step and adsorbent model of CoP for HER.

Table S1 Comparison of OER performance for Fe-CoP with recently reported electrocatalysts.

Catalysts	Overpotential (mV)	Ref.
Fe-CoP	249	This work
$Zn_{0.1}$-CoP	290	J. Alloys Compd. 2023, 934, 167828
Co_2P-FeP@C-15	260	J. Colloid Interface Sci. 2024, 653, 857-866
MoP@NPC	313	J. Mater. Chem. A 2024, 12, 1243
MoP/$CoMoP_2$@NPC	284	
Fe-CoP	269	Int. J. Hydrogen Energy 2024, 90, 1401-1410
Hf-XO-CoP	292	Inorg. Chem. 2024, 63, 13093-13099
CoP	388	
Fe-CoP NFs	255	Energy Environ. Mater. 2024, 7, e12747
Fe-CoP NCs	300	
CoP/Ni_2P@NHPC	275	J. Electroanal. Chem. 2024, 961, 118224
MoCoFeP	250	RSC Adv. 2024, 14, 10182-10190
Fe-CoP/NCNF-350	292	Int. J. Hydrogen Energy 2024, 63, 556-565
CN/Fe-CoS_2	304	ACS Appl. Nano Mater. 2024, 7, 9685-9695
H-Fe_3O_4	287	J. Colloid Interface Sci. 2024, 657, 684-694

Table S2 Comparison of HER performance for Fe-CoP with recently reported electrocatalysts.

Catalysts	Overpotential (mV)	Ref.
Fe-CoP	78.5	This work
NF/Ni_2P/CoP-NN	90	Electrochim. Acta 2022, 426, 140768
NF/Ni_2P	172	
Ni_2P/CoP@C-NSG	145	Mater. Today Sustainablity 2024, 25, 100677
V-CoP	98	Nanoscale Adv. 2023, 5, 4133-4139
CoP	149	
$Fe_{1.5}$-CoP	115	Ionic 2022, 28, 2301-2307
Fe_1-CoP	142	
O-CoP	125	Chem. Eur. J. 2023, 29, e202301252
B-CoP/NC	158	New J. Chem. 2023, 47, 17333
CoP@$NCDs_{0.5}$/NF	103	J. Cryst. Growth 2023, 624, 127430
CoP/NF	137	
Ni-CoP/Co_2P	125	J. Solid State Chem. 2021, 301, 122299
CoP/Co_2P	204	
Mo-CoP/$Ti_3C_2T_x$	117	ChemistrySelect 2022, 7, e202200254

Table S3 Comparison of overall water splitting performance for Fe-CoP with recently reported electrolyzers.

Catalysts	Voltage (V)	Ref.
Fe-CoP	1.50	This work
Mn-W-CoP/NF	1.57	Int. J. Hydrogen Energy 2024, 51, 276-284
CoP/CNTs/CC	1.54	J. Colloid Interface Sci. 2023, 651, 172-181
CoFe-P/NF-1	1.57	ACS Appl. Nano Mater. 2021, 4, 12083-12090
CoO-CoP-NC	1.53	J. Mater. Chem. A 2023, 11, 3136
$NiSe_2/Ni_2P$@FeP	1.554	J. Power Source 2020, 445, 227294
H-Fe_3O_4@FeP@NC	1.69	J. Colloid Interface Sci. 2024, 657, 684-694
N, Ce-NiCoP/NF	1.54	Nano Res. 2024, 17, 282-289
Ni_2P-MoP@NC	1.54	J. Mater. Chem. A 2023, 11, 15033
$Co_3Mo_3N/Co_4N/Co$	1.58	Angew. Chem. Int. Ed. 2024, 63, e202319239
Co_2P-NCS	1.69	Small 2024, 20, 2308956
Co-N-BP-CNTs/NF	1.52	J. Alloys Compd. 2024, 980, 173647
Ir_n-$CoMoPO_x$	1.53	ACS Appl. Mater. Interfaces 2024, 16, 7141-7151
CoP_2/Co_2P@CNT-CC	1.55	ACS Appl. Mater. Interfaces 2022, 14, 56847-56855
V-CoP	1.59	Adv. Energy Mater. 2021, 11, 2101758

Table S4 Charge density distribution analysis and their diversities to purely ionic models (ΔQ).

Catalysts	Atoms	Charge	ΔQ
CoP	P_1	5.18	0.18
	P_2	5.18	0.18
	Co	8.84	-0.16
Fe-CoP	P_1	5.21	0.21
	P_2	5.21	0.21
	Fe	7.73	-0.27