Electronic Supplementary Material (ESI) for RSC Advances.

Supporting information

Nearly spherical CoP nanoparticle /carbon nanosheet hybrids: high-performance trifunctional electrocatalyst for oxygen reduction and water splitting

Wenjian Zou[a], Kunpeng Dou[b], Qi Jiang[a], Jiadong Xiang[a], Chao-Cheng Kaun[c], Hao Tang[a]*

[a] State Key Laboratory of Advanced Technology for Materials Synthesis and Processing, International School of Materials Science and Engineering, Wuhan University of Technology, Wuhan 430070, People's Republic of China

[b] College of Information Science and Engineering, Ocean University of China, Qingdao 266100, People's Republic of China

[c] Research Center for Applied Sciences, Academia Sinica, Taipei 11529

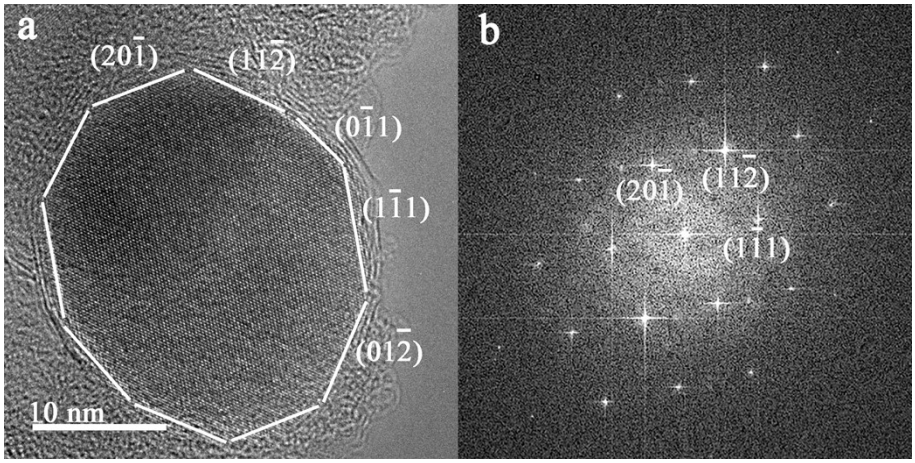

Figure S1. Structure of CoP nanoparticle. (a) HRTEM image of CoP nanocrystalline along [132] zone axis and; (b) corresponding FFT image of (a).

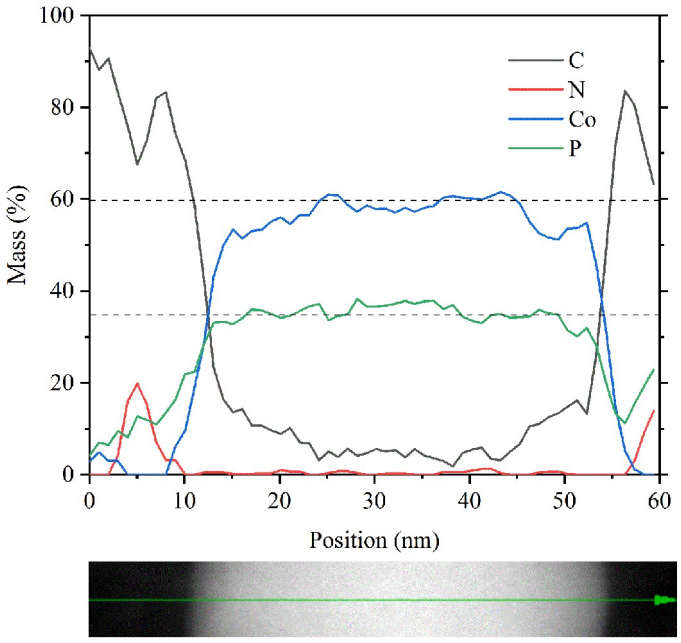

Figure S2. EDS linear scan result of the CoP NPs/CNSs.

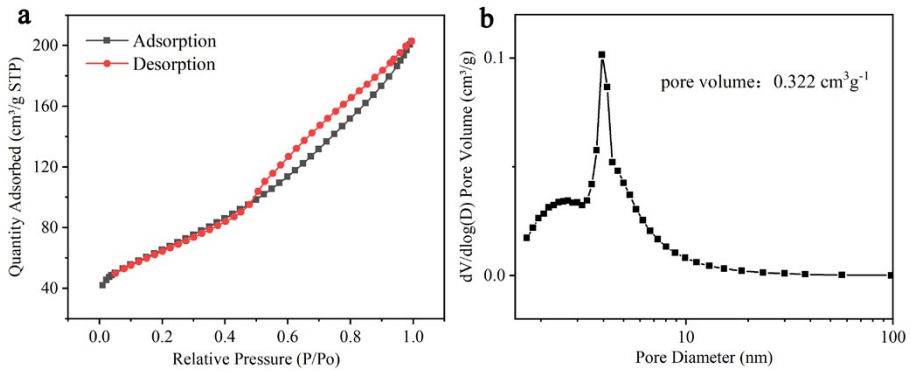

Figure S3. (a) Nitrogen adsorption desorption curve. (b) pore-diameter distribution.

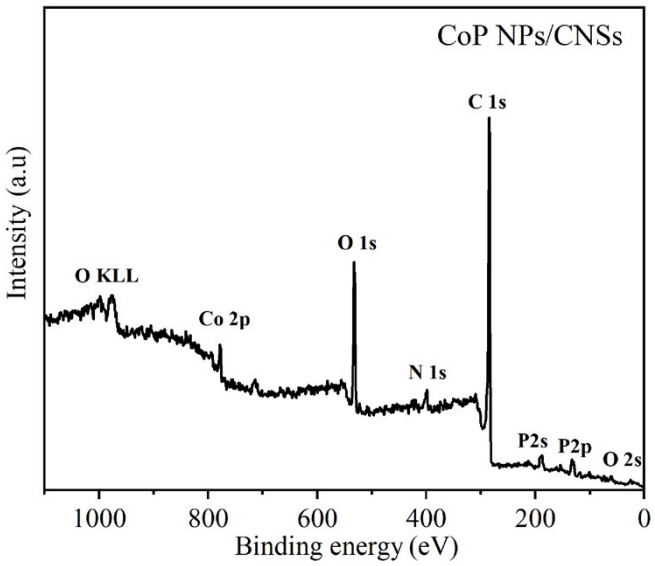

Figure S4. XPS spectra of CoP NPs/CNSs.

Table S1 The content ratio of each kind of nitrogen.

	Binding energy (eV)	Content (%)
Pyridinic-N	398.8	40.5
Pyrrolic-N	401.1	42.7
Graphite-N	402.2	11.1
Oxidized-N	404.8	5.7

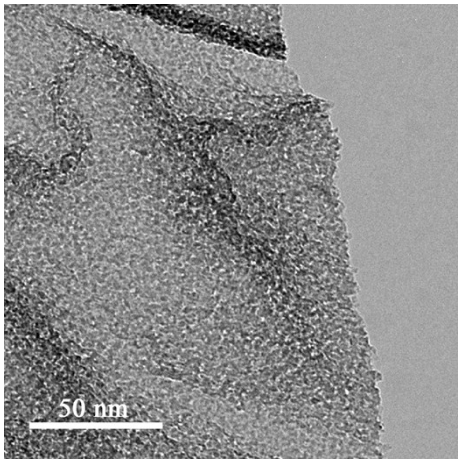

Figure S5. HRTEM image of CNSs

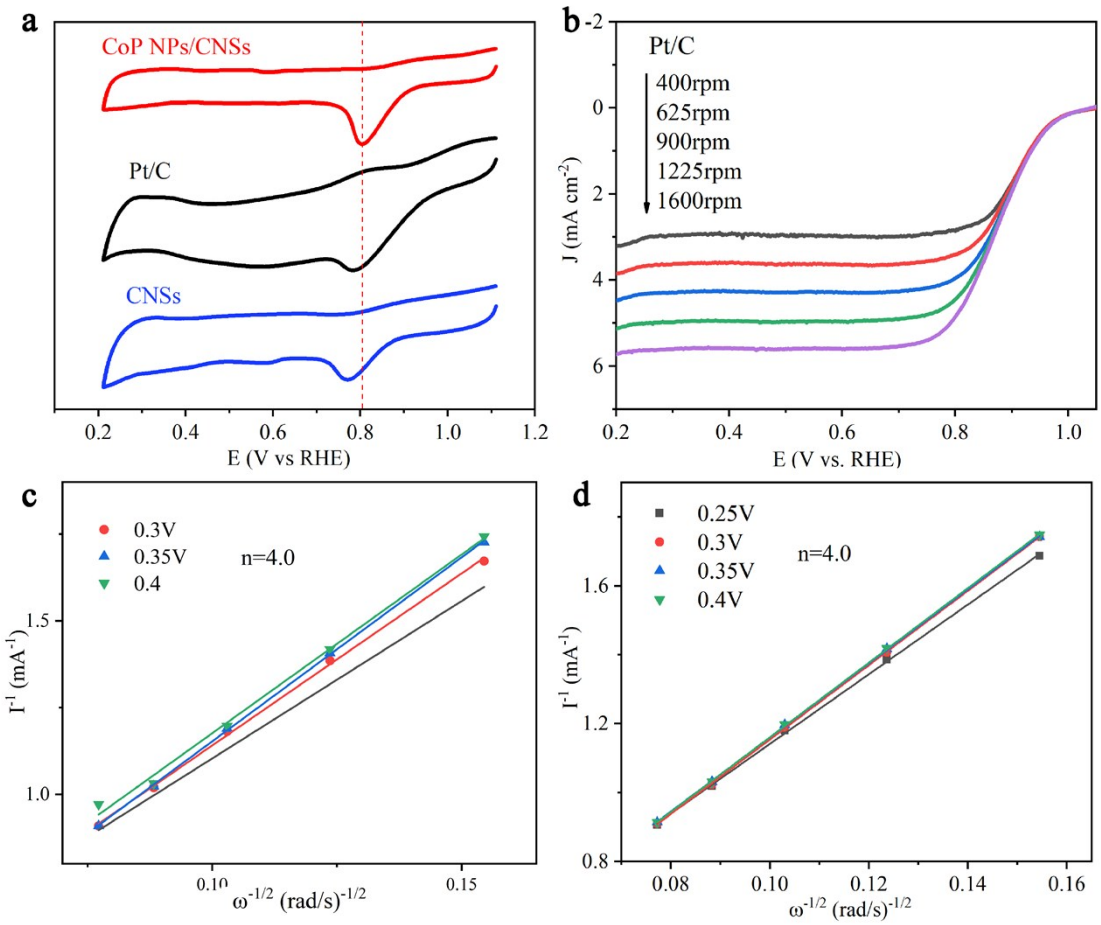

Figure S6. Electrocatalytic properties of the electrodes. (a) CV curves of CoP NPs/CNSs, CNSs and Pt/C catalyst in O_2-saturated 0.1 M KOH. (b) LSV curves of Pt/C at different rotation rates in rpm. (c)K-L plot of CoP NPs/CNSs. (d) K-L plot of Pt/C

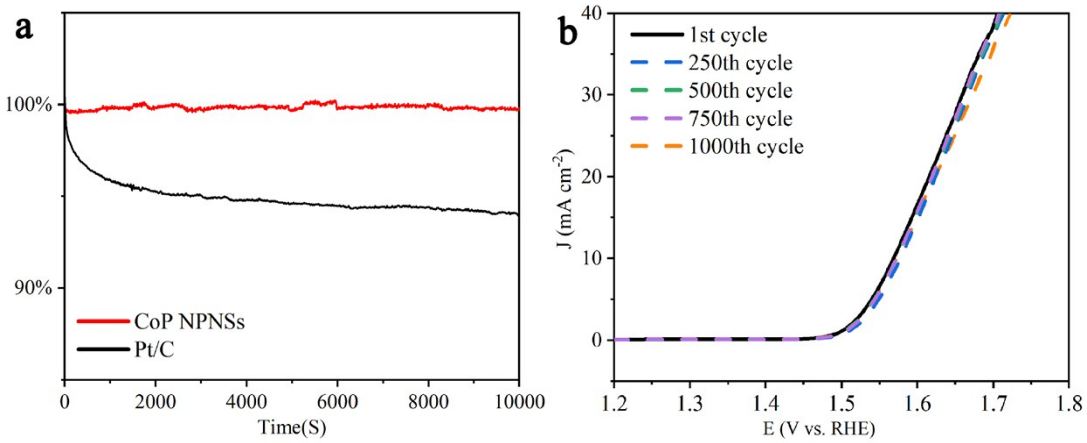

Figure S7. Stability of the catalysts. (a) I-T curve of CoP NPs/CNSs. (b) LSV curve of CoP NPs/CNSs before and after 1000 potential cycles under 1 M KOH

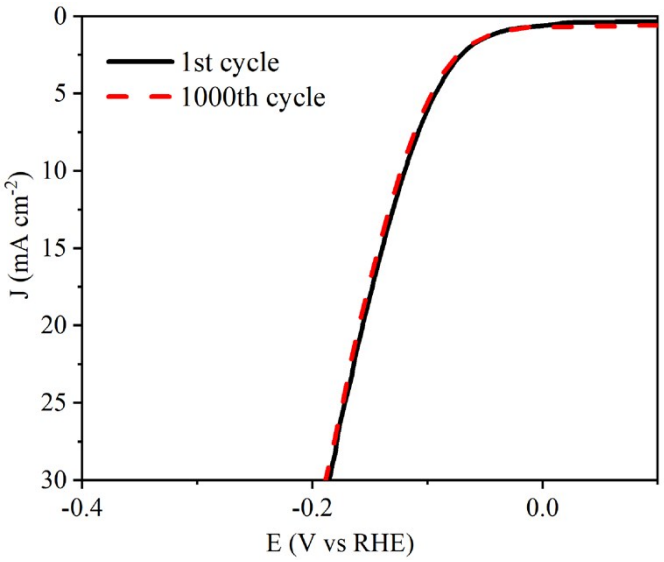

Figure S8. LSV curve of CoP NPs/CNSs before and after 1000 potential cycles under 1 M KOH

Table S2 OER, ORR and HER properties of CoP nanoparticles in alkaline condition reported in previous studies and our work.

Properties \ Facets		CoP(CoP-DC) with (111) and (101) facets[12]	colloidal CoP nanocrystals with (211 facets [9]	CoP nanocrystals with (011) facets [7]	CoP nanowire with (200) facets [8]	Ultrathin CoP nanosheet (011) and (111) facets [6]	This work
ORR properties	electrolyte	0.1M KOH	0.1M KOH	0.1M KOH	/	/	0.1M KOH
	Onset potential (V)	0.81	0.92	0.8	/	/	0.92
	Half wave potential (V)	0.76	0.858	0.7	/	/	0.88
	Tafel plot	/	72.1	51	/	/	89
	Diffusion current (mA cm^{-2})	5.3	4.64	4.5	/	/	5.4
OER properties	electrolyte	0.1 KOH	1M KOH	/	1M KOH	/	1M KOH
	Overpotential (mV)	320@10mA	280@10mA (Co_2P)	/	248@10mA 300@100mA		340@10mA
	Tafel plot (mV dec^{-1})	52.5	/	/	78	/	102.1
	ΔE (V)	0.76	/	/	/	/	0.84
HER properties	electrolyte	/	1M KOH	/	/	1M KOH	1M KOH
	Overpotential (10mA)	/	62.5	/	/	154	115
	Overpotential (20mA)	/	/	/	150	181	150
	Overpotential (100mA)	/	/	/	240	/	290
	Tafel plot (mV dec^{-1})	/	/	/	105	72	90

Table S3 Calculated Gibbs free energy for various surfaces of CoP during OER.

Facets	ΔG_1^0 (eV)	ΔG_2^0 (eV)	ΔG_3^0 (eV)	ΔG_4^0 (eV)
101	0.253	1.689	1.787	1.794
111	-0.531	0.836	3.317	1.901
112	0.530	-0.037	3.957	1.073
201	0.736	0.582	2.629	1.576
210	-0.120	1.284	2.675	1.684
012	1.612	0.098	2.502	1.312
311	-0.387	1.029	2.577	2.304
011	3.327	-2.751	3.337	1.610

Table S4 Calculated Gibbs free energy of Co-Co bridge sites, P top sites and Co-P bridge sites for various CoP surfaces during HER.

Active sites	Facets	G_0 (eV)	G_1 (eV)	G_2 (eV)	G_3 (eV)
Co-Co bridge	101	0	0.375	0.051	0
	111	0	0.002	-0.466	0
	112	0	0.084	0.187	0
	201	0	-0.873	-0.513	0
	210	0	0.605	-0.300	0
	012	0	1.061	0.347	0
	311	0	-0.105	-0.284	0
	011	0	0.350	0.461	0
P top	101	0	0.344	0.179	0
	111	0	-0.450	0.409	0
	112	0	0.498	0.029	0
	201	0	-0.509	-0.199	0
	210	0	0.945	0.530	0
	012	0	0.380	0.356	0
	311	0	0.096	-0.253	0
	011	0	0.027	0.135	0
Co-P bridge	101	0	0.615	0.181	0
	111	0	-0.394	0.230	0
	112	0	0.832	0.296	0
	201	0	0.555	-0.200	0
	210	0	-0.013	0.363	0
	012	0	0.658	0.054	0
	311	0	-0.122	0.425	0
	011	0	0.028	0.135	0