Ultrafine CoPS nanoparticles encapsulated in N, P, S tri-doped porous carbon as an efficient bifunctional water splitting electrocatalyst in both acid and alkaline solution

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Figure S1 SEM images of Co-MOF@XC-72 (A, B) and CoPS@NPS-C (C, D).



Figure S2 TEM images of pure XC-72.



Figure S3 TEM images of CoPS@NPS-C.



Figure S4 Raman spectra of pure Co-MOF, pure XC-72, Co-MOF@XC-72 and CoPS@NPS-C (4 wt.%).



Figure S5 (A) Nitrogen adsorption/desorption isotherm of CoPS@NPS-C (4 wt.%), (B) The corresponding pore diameter distribution.



Figure S6 Comparison of the over-potentials for different catalysts at 10 mA cm⁻²



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Figure S7 The LSV curves of overall water splitting with CoPS@NPS-C (4 wt.%) used as both anode and cathode (CoPS@NPS-C (4 wt.%))|CoPS@NPS-C (4 wt.%)), XC-72-PS as both anode and cathode (XC-72-PS)|XC-72-PS), and IrO₂ as anode and commercial Pt/C as cathode (Pt/C||IrO₂) in a two-electrode configuration at a scan rate of 5 mV s⁻¹ in 1.0 M KOH.

Catalysts	Mass loading/mg cm ⁻²	Overpotential ηj=10 mA cm ⁻² / mV	Acid	Alkaline	Reference
CoPS@NPS- C (4 wt.%)	0.35	93 (Acid) 191 (Alkaline)	R	Ð	This work
PNC/Co	0.35	298		B	1
rGO-few- layer NiPS ₃	0.16	178 (Acid) 281 (Alkaline)	R	R	2
Ni-Co-P NP	0.158	180		B	3
CoSe ₂ /CC	N.A.	190		B	4
CoS ₂ NWs	N.A.	145		B	5
CoeNeP- CNFs	0.229	0.248		Ð	6
Polymorphic CoSe ₂	N.A.	150	R		7
CoP/CNT	0.285	122	B		8
Porous CoP concave polyhedron	0.35	133	P		9
$CoSe_2 NP$	0.28	139	R		10
Mo ₂ C/NPCN Fs	~0.4	134	R		11
CoS ₂ /MoS ₂ /R GO	0.35	160	R		12

 Table S1.
 Comparison of electrochemical activity of CoPS@NPS-C (4 wt.%) to the other reported HER catalysts

 Table S2.
 Comparison of electrochemical activity of CoPS@NPS-C (4 wt.%) to the other reported OER catalysts in alkaline electrolyte.

Catalysts	Mass loading/mg cm ⁻²	Overpotential η _j =10 mA cm ⁻² / mV	Reference
CoPS@NPS-C (4 wt.%)	0.35	326	This work
CoP NP/C	0.71	320	13
CoOx@CN	1	260	14
Co/N-CNTs-700	0.20	390	15
Co-P film	N.A.	345	16
sea-urchin-like (Co _{0.54} Fe _{0.46}) ₂ P	0.2	370	17
Co-UTSA-16	0.35	408	18
Co ₂ V ₂ O ₇ nanosheet	0.28	340	19

- 1 X. Li, Z. Niu, J. Jiang and L. Ai, J. Mater. Chem. A, 2016, 4, 3204-3209.
- 2 R. N. Jenjeti, M. P. Austeria and S. Sampath, *Chemelectrochem*, 2016, **3**, 1392-1399.
- 3 J. A. Vigil, T. N. Lambert and B. T. Christensen, J. Mater. Chem. A, 2016, 4, 7549-7554.
- 4 P. Chen, K. Xu, S. Tao, T. Zhou, Y. Tong, H. Ding, L. Zhang, W. Chu, C. Wu and Y. Xie, *Adv. Mater.*, 2016, **28**, 7527-7532.
- 5 M. S. Faber, R. Dziedzic, M. A. Lukowski, N. S. Kaiser, Q. Ding and S. Jin, *J. Am. Chem. Soc.*, 2014, **136**, 10053-10061.
- 6 Z. Wang, P. Zuo, L. Fan, J. Han, Y. Xiong and G. Yin, *J. Power Sources*, 2016, **311**, 68-80.
- 7 H. Zhang, B. Yang, X. Wu, Z. Li, L. Lei and X. Zhang, ACS Appl. Mater. Inter., 2015, 7, 1772-1779.
- 8 Q. Liu, J. Tian, W. Cui, P. Jiang, N. Cheng, A. M. Asiri and X. Sun, *Angew. Chem. Int. Ed.*, 2014, **53**, 6710-6714.
- 9 M. Xu, L. Han, Y. Han, Y. Yu, J. Zhai and S. Dong, J. Mater. Chem. A, 2015, **3**, 21471-21477.
- 10 D. Kong, H. Wang, Z. Lu and Y. Cui, J. Am. Chem. Soc., 2014, 136, 4897-4900.
- 11 H. Wang, C. Sun, Y. Cao, J. Zhu, Y. Chen, J. Guo, J. Zhao, Y. Sun and G. Zou, *Carbon*, 2017, **114**, 628-634.
- 12 Y.-R. Liu, X. Shang, W.-K. Gao, B. Dong, J.-Q. Chi, X. Li, K.-L. Yan, Y.-M. Chai, Y.-Q. Liu and C.-G. Liu, *Appl. Surf. Sci.*, 2017, **412**, 138-145.
- 13 J. Chang, Y. Xiao, M. Xiao, J. Ge, C. Liu and W. Xing, ACS Catal., 2015, 5, 6874-6878.
- 14 H. Jin, J. Wang, D. Su, Z. Wei, Z. Pang and Y. Wang, J. Am. Chem. Soc., 2015, 137, 2688-2694.
- 15 Y. Liu, H. Jiang, Y. Zhu, X. Yang and C. Li, *J. Mater. Chem. A*, 2016, **4**, 1694-1701.
- 16 N. Jiang, B. You, M. Sheng and Y. Sun, *Angew. Chem. Int. Ed.*, 2015, **54**, 6251.
- 17 A. Mendoza-Garcia, H. Zhu, Y. Yu, Q. Li, L. Zhou, D. Su, M. J. Kramer and S. Sun, *Angew. Chem. Int. Ed.*, 2015, **54**, 9642-9645.
- 18 J. Jiang, L. Huang, X. Liu and L. Ai, ACS Appl. Mater. Inter., 2017, 9, 7193-7201.
- 19 X. Peng, L. Wang, L. Hu, Y. Li, B. Gao, H. Song, C. Huang, X. Zhang, J. Fu and K. Huo, *Nano Energy*, 2017, **34**, 1-7.