Supporting Information

Construction of Fe-doped CoP with hybrid nanostructures as a

bifunctional catalyst for overall water splitting

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Supplementary Figures and Tables



Fig. S1 (a) SEM and (b, c) TEM images of Co-PBA



Fig. S2 (a, b) TEM and (c) SEM images of HIP and (d) SEM image of CoP without doping of Fe^{3+}



Fig. S3 XRD pattern of Co-PBA, HIP and Fe_{0.25}-HIP



Fig. S4 The elemental composition and contents of Fe_{0.25}-CoP **Fig. S5** CV curves of (a) CoP, (b) Fe_{0.33}-CoP, (c) Fe_{0.25}-CoP and (d) Fe_{0.20}-CoP for HER



Fig. S6 CV curves of (a) CoP, (b) Fe_{0.33}-CoP, (c) Fe_{0.25}-CoP and (d) Fe_{0.20}-CoP for OER



Fig. S7 The electrochemical surface area (ECSA) of CoP, $Fe_{0.33}$ -CoP, $Fe_{0.25}$ -CoP and $Fe_{0.20}$ -CoP



Fig. S8 (a) TEM image and (b) polarization curves of the phosphide which was prepared without the addition of Co-PBA



Fig. S9 Polarization curves of HIP and Fe_{0.25}-HIP measured in 1.0 M KOH electrolyte



Fig. S10 (a) XRD pattern and SEM image (b) before and (c) after durability tests for $Fe_{0.25}$ -CoP



Fig. S11 XPS spectra of (a) survey, (b) Co 2p, (c) P 2p and (d) Fe 2p for $Fe_{0.25}$ -CoP after the water oxidation

Catalyst	Voltage at 10 mA·cm ⁻ ² (V)	Electrolyte	Reference
Fe _{0.25} -CoP	1.57	1.0 M KOH	[This work]
(Ni ₁₁ (HPO ₃) ₈ (OH) ₆	1.60	1.0 M KOH	1
Ni/NiS/NC	1.61	1.0 M KOH	2
C-(Fe-Ni)P@PC/(Ni- Co)P@CC	1.63	1.0 M KOH	3
MoS ₂ /LDH	1.57	1.0 M KOH	4
VOOH-3Fe	1.53	1.0 M KOH	5
E-Mo-NiCoP	1.61	1.0 M KOH	6
Co ₄ S ₃ /Mo ₂ C-NSC	1.62	1.0 M KOH	7
CoP NF	1.65	1.0 M KOH	8
P-CoS ₂ HNA/CC	1.56	1.0 M KOH	9
Ni/Ni(OH) ₂	1.59	1.0 M KOH	10

Table. S1 Comparison of the overall water splitting properties of Fe_{0.25}-CoP with some previously reported bifunctional catalysts

References

- P. W. Menezes, C. Panda, S. Loos, F. Bunschei-Bruns, C. Walter, M. Schwarze, X. Deng, H. Dau and M. Driess, *Energy Environ. Sci.*, 2018, 11, 1287-1298.
- 2. J. Ding, S. Ji, H. Wang, H. Gai, F. Liu, V. Linkov and R. Wang, *Int. J. Hydrog. Energy*, 2019, **44**, 2832-2840.
- 3. C.-N. Lv, L. Zhang, X.-H. Huang, Y.-X. Zhu, X. Zhang, J.-S. Hu and S.-Y. Lu, *Nano Energy*, 2019, **65**, 103995.
- P. Xiong, X. Zhang, H. Wan, S. Wang, Y. Zhao, J. Zhang, D. Zhou, W. Gao, R. Ma, T. Sasaki and G. Wang, *Nano Lett*, 2019, 19, 4518-4526.
- J. Zhang, R. Cui, C. Gao, L. Bian, Y. Pu, X. Zhu, X. Li and W. Huang, *Small*, 2019, 15, 1904688.
- 6. J. Lin, Y. Yan, C. Li, X. Si, H. Wang, J. Qi, J. Cao, Z. Zhong, W. Fei and J. Feng, *Nanomicro Lett*, 2019, **11**, 55.
- Y. Liu, X. Luo, C. Zhou, S. Du, D. Zhen, B. Chen, J. Li, Q. Wu, Y. Iru and D. Chen, *Appl. Catal. B*, 2020, 260, 118197.
- 8. L. Ji, J. Wang, X. Teng, T. J. Meyer and Z. Chen, *ACS Catal.*, 2019, **10**, 412-419.
- 9. Y. Li, Z. Mao, Q. Wang, D. Li, R. Wang, B. He, Y. Gong and H. Wang, *Chem. Eng. J.*, 2020, **390**.

10. L. Dai, Z. N. Chen, L. Li, P. Yin, Z. Liu and H. Zhang, *Adv Mater*, 2020, **32**, 1906915.