

Supporting information for

**Oxygenated P/N co-doped carbon for efficient $2e^-$ oxygen reduction
to H_2O_2**

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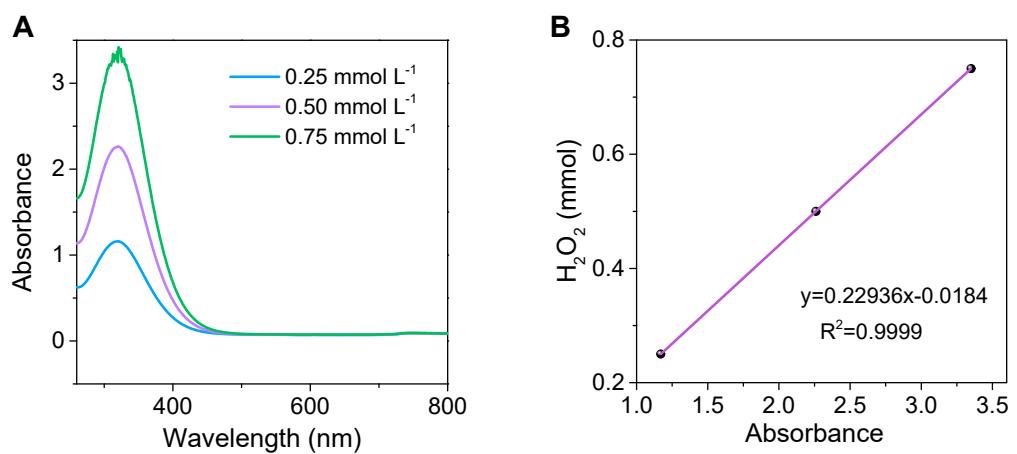


Figure S1. (A) UV-vis spectra of $\text{Ce}(\text{SO}_4)_2$ solution of different concentrations. (B) The standard curve of $\text{Ce}(\text{SO}_4)_2$ titration method

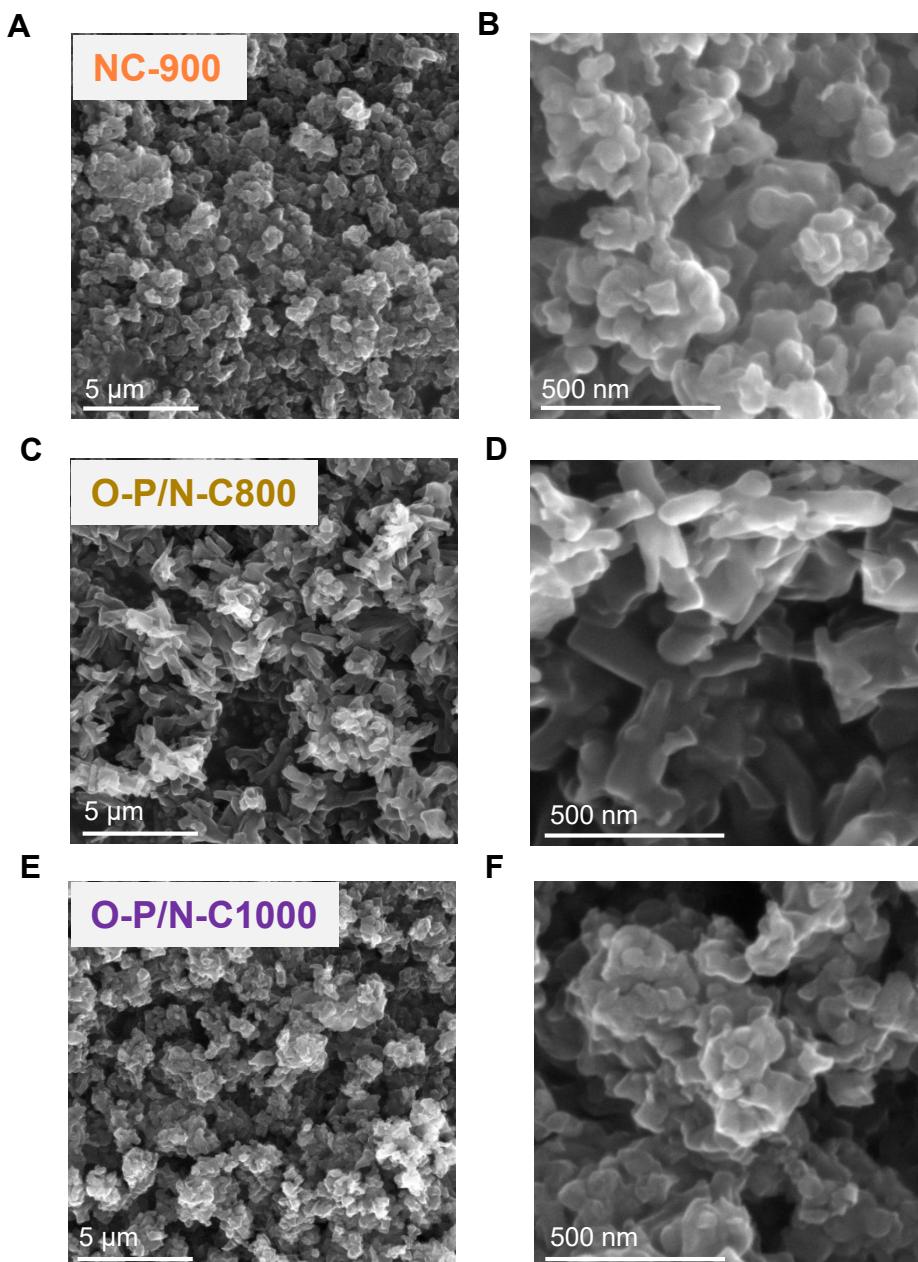


Figure S2. SEM images of (A-B) NC-900, (C-D) O-P/N-C800 and (E-F) O-P/N-C1000.

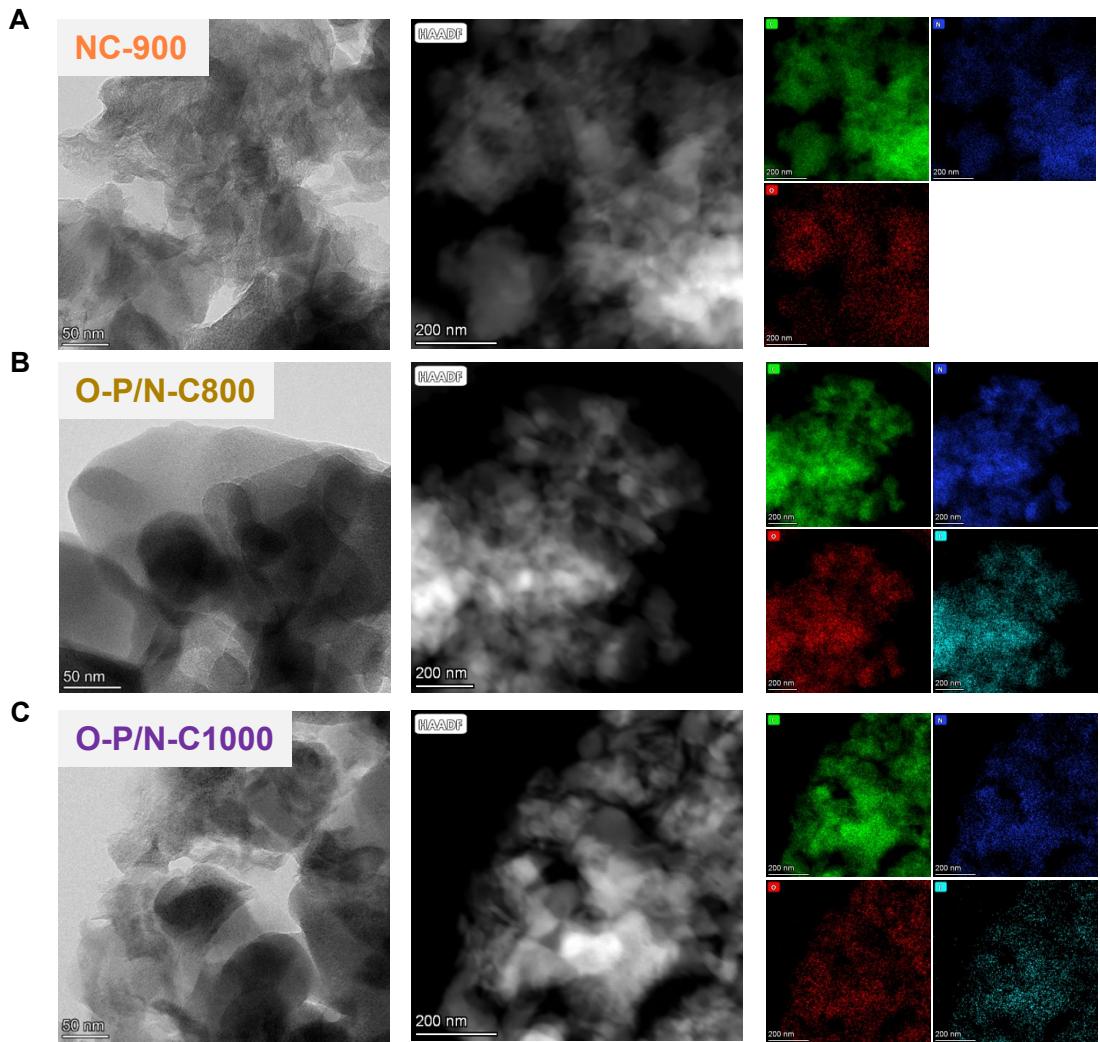


Figure S3. TEM images and HAADF-HRTEM EDS of (A) NC-900, (B) O-P/N-C800 and (C) O-P/N-C1000.

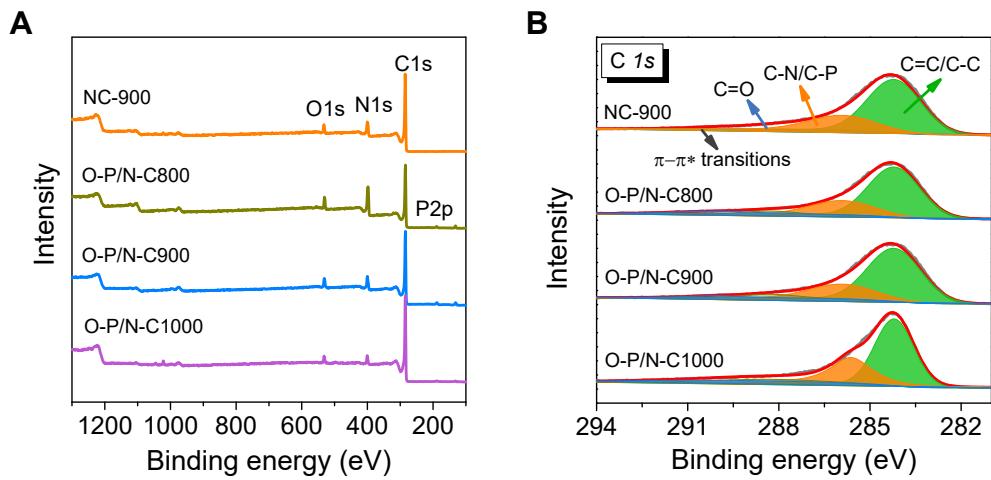


Figure S4. (A) XPS element survey, (B) C 1s spectra of NC-900, O-P/N-C800, O-P/N-C900 and O-P/N-C1000.

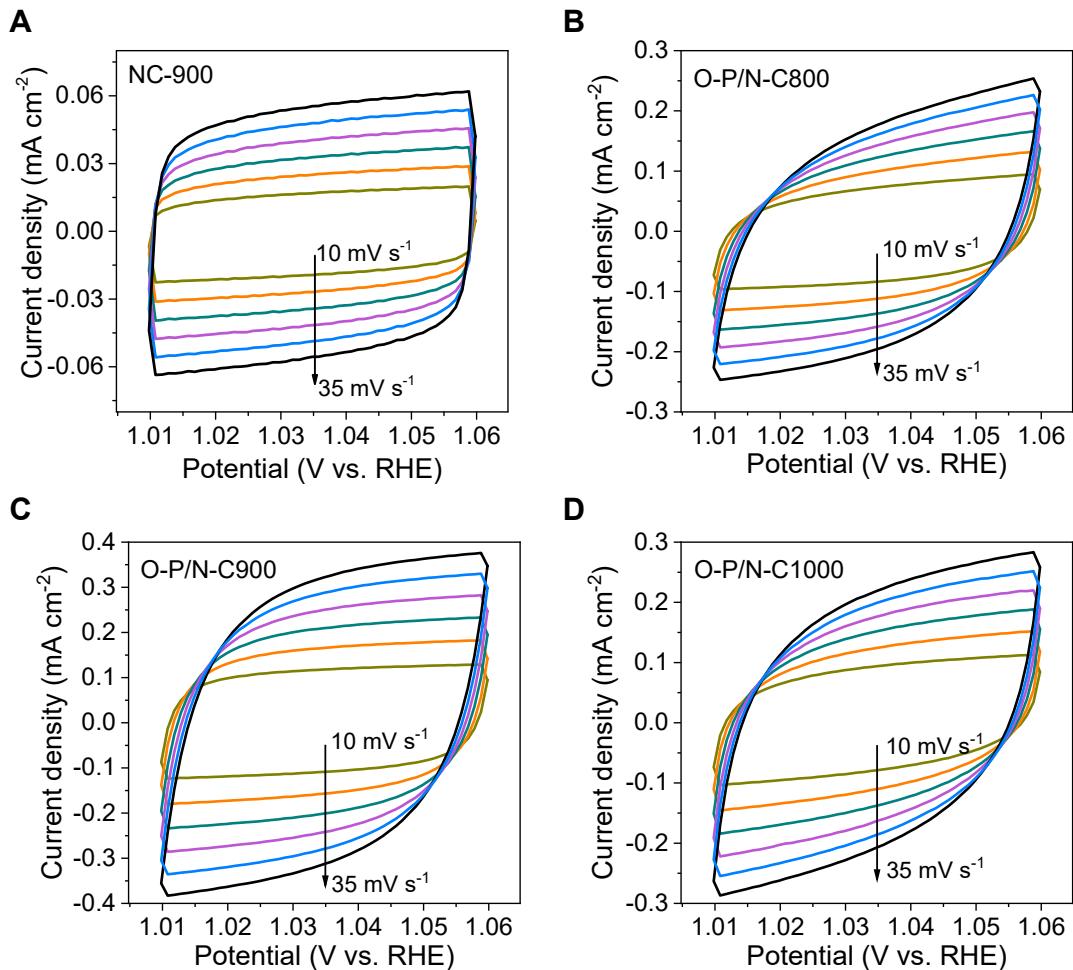


Figure S5. CV curves of (A) NC-900, (B) O-P/N-C800, (C) O-P/N-C900 and (D) O-P/N-C1000 at different scan rates in the potential range of 1.01-1.06 V (vs. RHE).

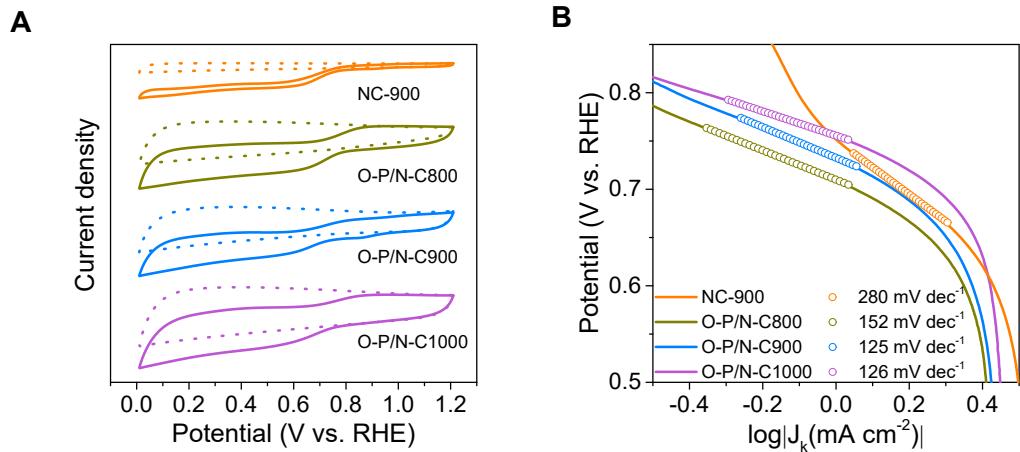


Figure S6. (A) CV curves (The dotted and solid lines represent N₂- and O₂-saturated electrolytes, respectively), and (B) Tafel slopes of NC-900, O-P/N-C800, O-P/N-C900 and O-P/N-C1000.

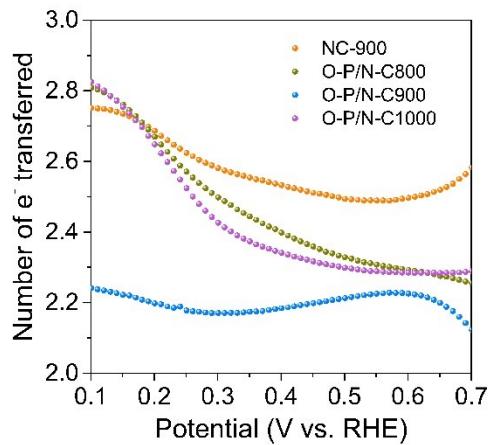


Figure S7. Calculated curves of transfer electron number (n) of NC-900, O-P/N-C800, O-P/N-C900 and O-P/N-C1000 samples.

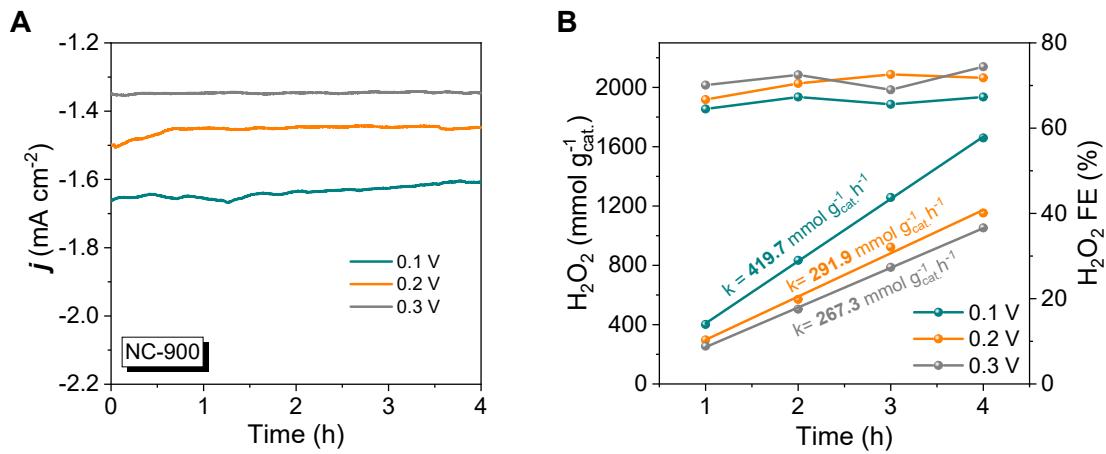


Figure S8. (A) Current stability and (B) H₂O₂ production rate and faradaic efficiency (FE, %) of O-P/N-C900 at 0.1, 0.2, and 0.3 V (vs. RHE) with the catalyst loading amount of 1 mg cm⁻².

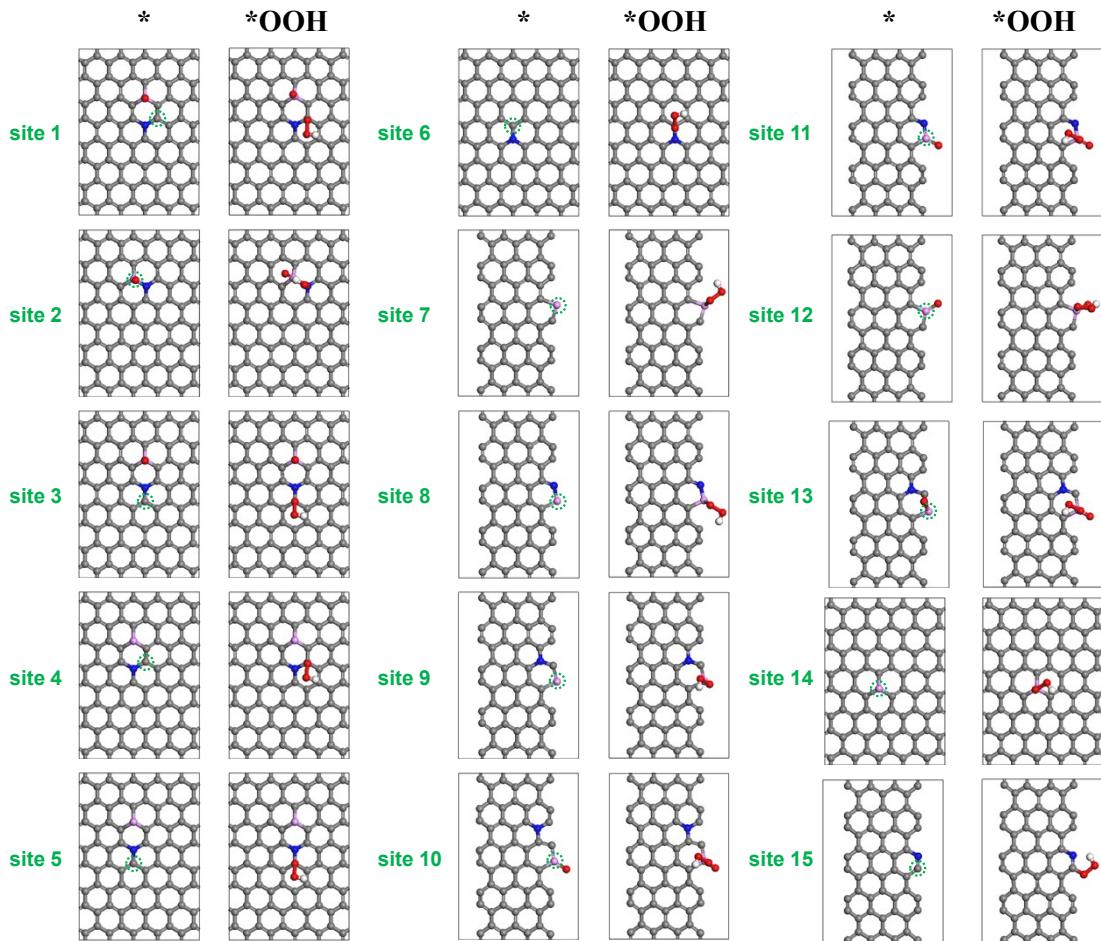


Figure S9. The atomic structures of the examined oxygen functional groups. Color code: carbon, gray; oxygen, red; hydrogen, white; nitrogen, blue; phosphorus, pink. The corresponding examined active sites are marked with a dashed green circle in each model structure.

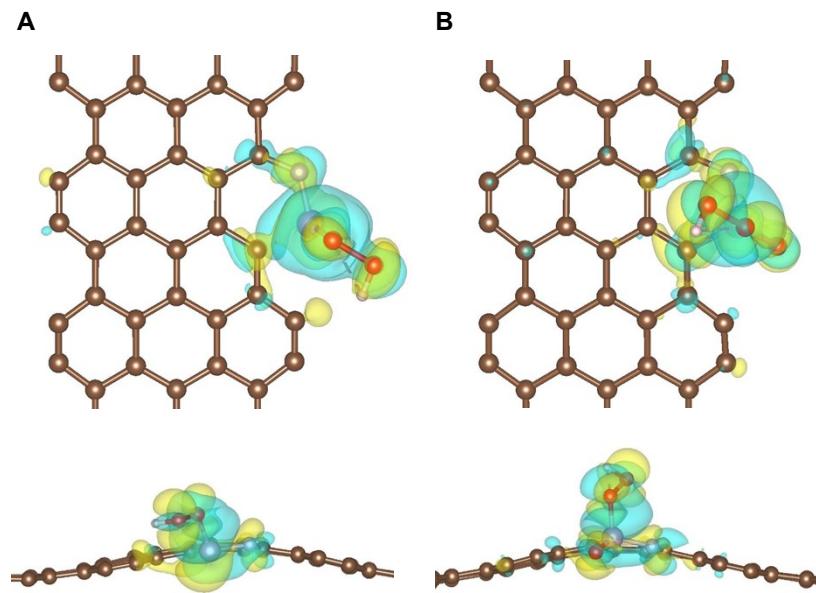


Figure S10. Differential charge distribution of (A) site 8 (edged N-P) and (B) site 11 (edged N-P=O) after absorbing OOH species.

Table S1. XPS element contents of NC-900 and O-P/N-C samples.

Sample	C	N	O	P
NC-900	81.44	13.59	4.97	—
O-P/N-C800	68.19	23.87	6.18	1.76
O-P/N-C900	80.74	11.56	5.21	2.49
O-P/N-C1000	88.46	6.92	3.99	0.63

Table S2. Comparison of H₂O₂ production on various electrocatalysts in H-type cells.

Catalyst	Electrolyte	Production rate	Reference
Oxo-G/NH₃	0.1 M KOH	224.8 mmol g ⁻¹ h ⁻¹	1
Co-SAs NC	0.1 M KOH	38.1 mmol g ⁻¹ h ⁻¹	2
BNTO	1 M KOH	208 mmol g ⁻¹ h ⁻¹	3
CNO-glu-H	0.1 M KOH	200 mmol g ⁻¹ h ⁻¹	4
DGLC	0.1 M KOH	355 mmol g ⁻¹ h ⁻¹	5
Fe₂O_{3-x}	0.1 M KOH	454 mmol g ⁻¹ h ⁻¹	6
NCMK3IL50	0.1 M KOH	561.7 mmol g ⁻¹ h ⁻¹	7
Ni-MOF NS	0.1 M KOH	80 mmol g ⁻¹ h ⁻¹	8
Ni-NPs BC	0.1 M KOH	162.7 mmol g ⁻¹ h ⁻¹	9
NOC-6M	0.1 M KOH	548.8 mmol g ⁻¹ h ⁻¹	10

SA ZnO₃C	0.1 M KOH	350 mmol g ⁻¹ h ⁻¹	11
O-P/N-C900	0.1 M KOH	698.4 mmol g⁻¹ h⁻¹	This work

References

1. L. Han, Y. Sun, S. Li, C. Cheng, C. E. Halbig, P. Feicht, J. L. Hübner, P. Strasser and S. Eigler, *ACS Catal.*, 2019, **9**, 1283-1288.
2. 54. H. Xu, S. Zhang, J. Geng, G. Wang and H. Zhang, *Inorg. Chem. Front.*, 2021, **8**, 2829-2834.
3. Z. Zhang, Q. Dong, P. Li, S. L. Fereja, J. Guo, Z. Fang, X. Zhang, K. Liu, Z. Chen and W. Chen, *J. Phys. Chem. C*, 2021, **125**, 24814-24822.
4. H. Shao, Q. Zhuang, H. Gao, Y. Wang, L. Ji, X. Wang, T. Zhang, L. Duan, J. Bai, Z. Niu and J. Liu, *Inorg. Chem. Front.*, 2021, **8**, 173-181.
5. C. Zhang, J. Zhang, J. Zhang, M. Song, X. Huang, W. Liu, M. Xiong, Y. Chen, S. Xia, H. Yang and D. Wang, *ACS Sustainable Chem. Eng.*, 2021, **9**, 9369-9375.
6. R. Gao, L. Pan, Z. Li, C. Shi, Y. Yao, X. Zhang and J. J. Zou, *Adv. Funct. Mater.*, 2020, **30**, 1910539.
7. Y. Sun, I. Sinev, W. Ju, A. Bergmann, S. Dresp, S. Kühl, C. Spöri, H. Schmies, H. Wang, D. Bernsmeier, B. Paul, R. Schmack, R. Krahnert, B. Roldan Cuenya and P. Strasser, *ACS Catal.*, 2018, **8**, 2844-2856.
8. M. Wang, X. Dong, Z. Meng, Z. Hu, Y. G. Lin, C. K. Peng, H. Wang, C. W. Pao, S. Ding, Y. Li, Q. Shao and X. Huang, *Angew. Chem., Int. Ed.*, 2021, **60**, 11190-11195.
9. H. Xu, M. Jin, J. Geng, S. Zhang and H. Zhang, *Sci. China Mater.*, 2021, **65**, 721-731.
10. C. Zhang, G. Liu, B. Ning, S. Qian, D. Zheng and L. Wang, *Int. J. Hydrogen Energy*, 2021, **46**, 14277-14287.
11. Y. Jia, Z. Xue, J. Yang, Q. Liu, J. Xian, Y. Zhong, Y. Sun, X. Zhang, Q. Liu, D. Yao and G. Li, *Angew. Chem., Int. Ed.*, 2022, **61**, 202110838.