

Supporting Information

K-intercalated polymeric carbon nitride with nitrogen defects for efficient photocatalytic H₂O₂ production

Qinyuan Wang ^a, Lulu Bai ^a, Qiang Wu ^{a*}, Weifeng Yao ^{a,b,c*}

^a Shanghai Key Laboratory of Materials Protection and Advanced Materials in Electric Power, College of Environmental & Chemical Engineering, Shanghai University of Electric Power, Shanghai, P. R. China.

^b Shanghai Institute of Pollution Control and Ecological Security, Shanghai, PR China.

^c Shanghai Engineering Research Center of Heat-exchange System and Energy Saving, Shanghai University of Electric Power, Shanghai, PR China

*Corresponding author E-mail address: yaoweifeng@shiep.edu.cn;

qiangwu@shiep.edu.cn

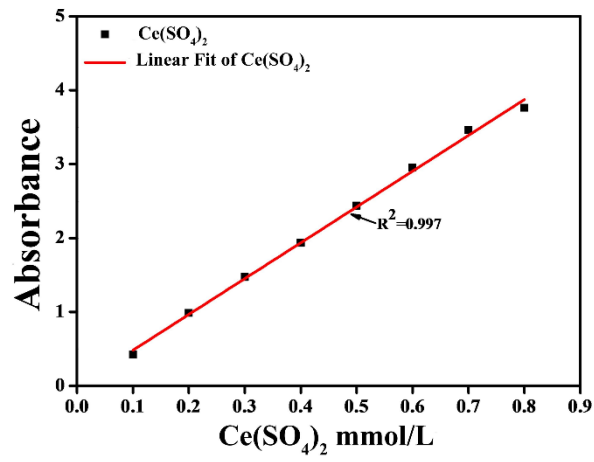


Fig. S1. $\text{Ce}(\text{SO}_4)_2$ standard curve for concentration

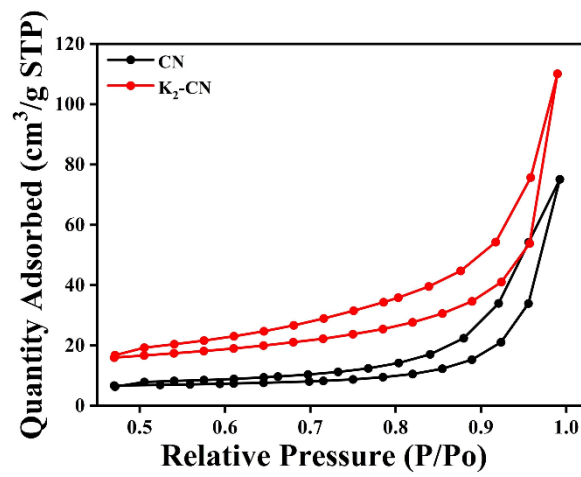


Fig. S2. N_2 adsorption-desorption isotherm curves of as-prepared sample

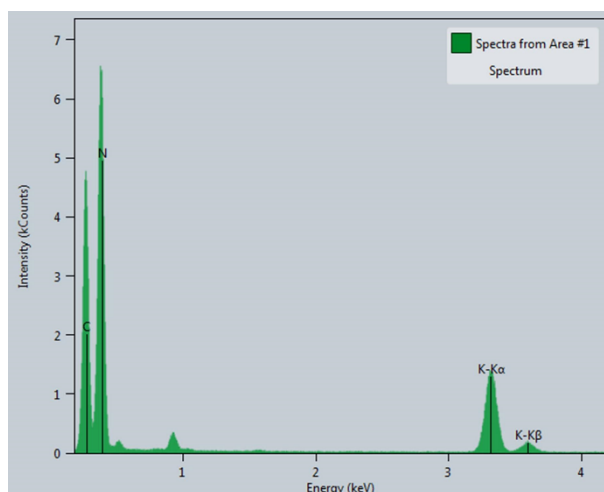


Fig.S3. EDS spectrum of K_2 -CN

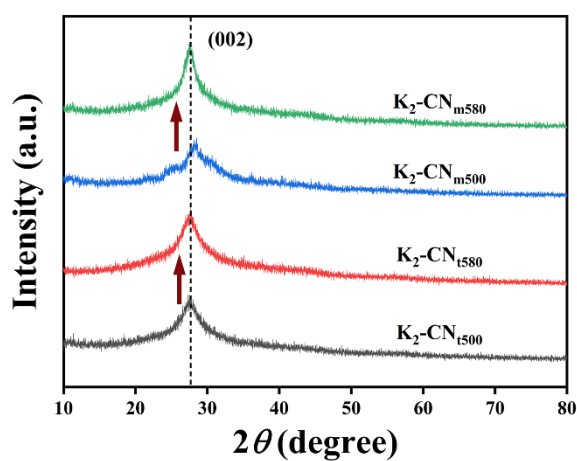


Fig. S4. XRD patterns of K_2 -CN_{t580}, K_2 -CN_{m580}, K_2 -CN_{t500}

Table. S1. Elemental Composition and the N/C Atomic Ratios of the K_2 -CN_{m500} and K_2 -CN_{t500}

Catalyst	C (wt %)	N (wt %)	N/C (mol/mol)	Weight (mg)
K_2 -CN _{m500}	26.92	45.05	1.67	2.00
K_2 -CN _{t500}	26.01	43.08	1.65	2.00
K_2 -CN _{m580}	25.21	41.05	1.63	2.00
K_2 -CN _{t580}	26.62	43.13	1.62	2.00

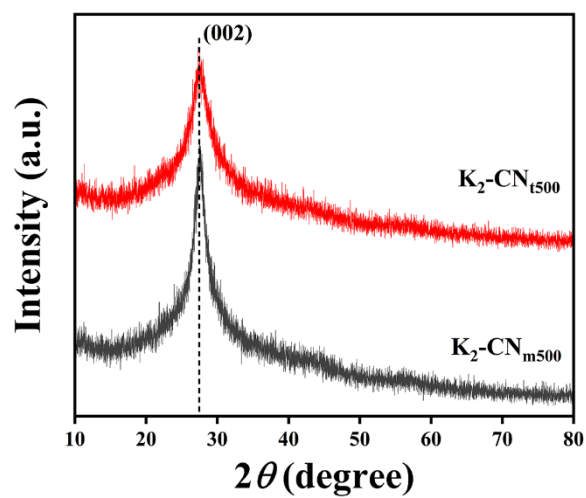


Fig. S5. XRD patterns of K_2-CN_{t500} and K_2-CN_{m500}

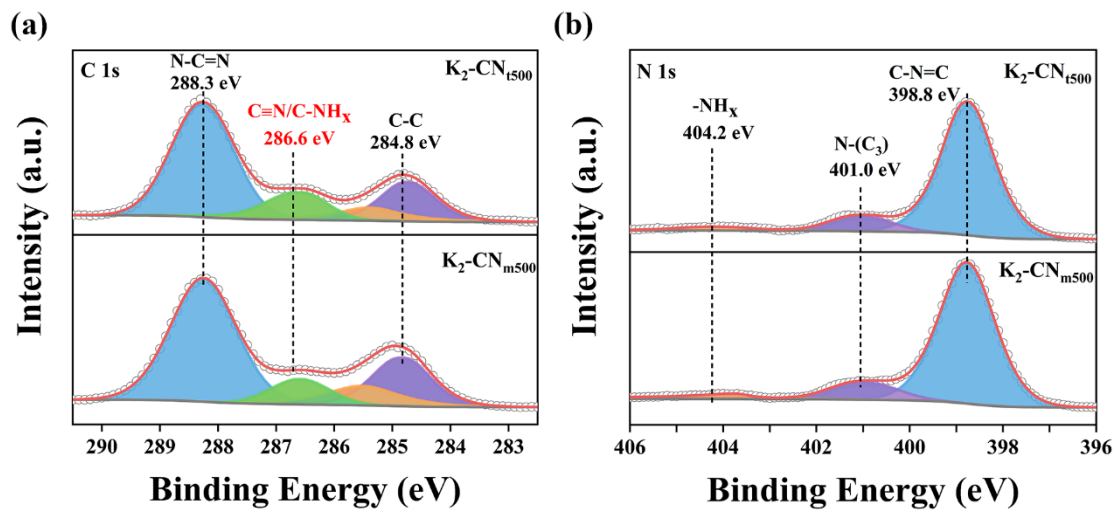


Fig. S6. (a) C 1s XPS spectra and (b) N 1s XPS spectra of K_2-CN_{t500} and K_2-CN_{m500} photocatalysts.

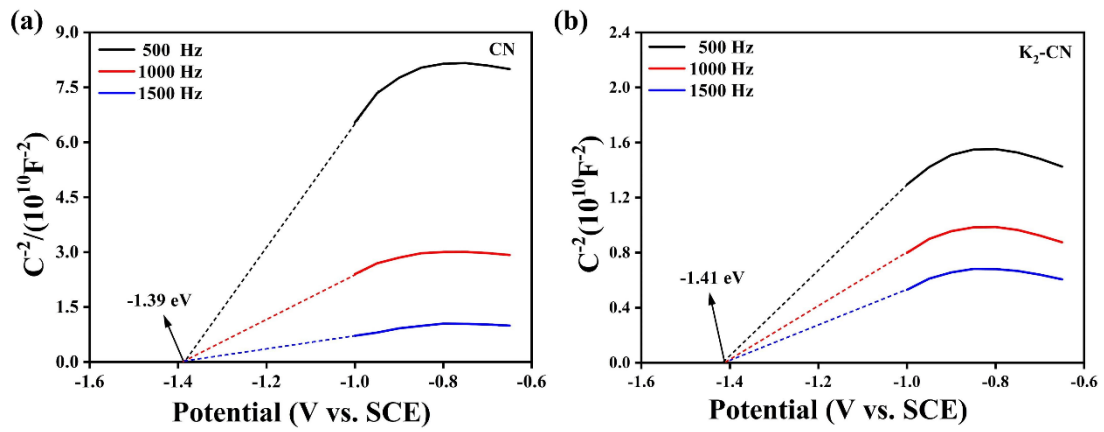


Fig. S7. Model-Schottky curves of plots (potential vs. SCE) of (a) CN and (b) $\text{K}_2\text{-CN}$ at 500 Hz, 1000 Hz and 1500 Hz

The Calculation of Apparent Quantum Efficiency:

$$AQE = \frac{N_e}{N_p} = \frac{\text{number of consumed electrons}}{\text{number of incoming photons}} = \frac{10^9 * (v * N_A * K) * (h * c)}{I * A * \lambda} * 100\% \quad (1)$$

N_e : number of consumed electrons; N_p : number of incoming photons; v : the reaction rate; N_A : Avogadro's number ($6.02 * 10^{23} \text{ mol}^{-1}$); K : number of electrons transferred by the reaction; h : Planck constant ($6.62 * 10^{-34} \text{ J}\cdot\text{s}$); c : the speed of light ($3.0 * 10^8 \text{ m}\cdot\text{s}^{-1}$); I : optical functional density ($\text{W}\cdot\text{m}^{-2}$); A : incident illumination area (m^2); λ : wavelength of incident light ($\lambda=420\text{nm}$). In this work, " I " is $9.02 \text{ mV}\cdot\text{cm}^{-2}$, the calculated AQE is 15.37%.

The Koutecky-Levich Equation:

$$j^{-1} = j_k^{-1} + B^{-1} \Omega^{-1/2} \quad (2)$$

$$B = 0.2nFv^{-1/6}CD^{-2/3} \quad (3)$$

The j , j_k , Ω , n , F , v , C and D respectively represent the current density; kinetic current density; rotational speed; Faraday's constant; the kinetic viscosity of water; the volumetric concentration of oxygen and the diffusion coefficient of oxygen.

Table. S2. Summary of the photocatalytic H₂O₂ production with modified g-C₃N₄ photocatalysts

Material	Sacrificial Reagent	Concentration of photocatalyst	pH	Irradiation conditions	H₂O₂ yields	AQE	Rate multiples of raw materials	Ref.
CoP/g-C ₃ N ₄	ethanol	1 mg/mL	7	420 nm	140 μmol/L, 2h	----	1.35 times	1
OCN-NBS	isopropanol	1 mg/mL	3	325 nm	892 μmol/L, 1h	----	2.0 times	2
Au/C ₃ N ₄ -500	isopropanol	1 mg/mL	3	420 nm	330 μmol/L, 1h	----	2.3 times	3
OCN8	isopropanol	1.2 mg/mL	7	λ ≥ 420 nm	1965 μmol/L, 1h	----	2.6 times	4
Au/BiVO ₄ -CN	isopropanol	1 mg/mL	3	385 nm	675.89 μmol/L, 1h	6.7 %	2.65 times	5
ac-g-c ₃ n ₄	ethanol	0.67 mg/mL	7	420 nm	530 μmol/L, 1h	----	3.0 times	6
CN4	isopropanol	0.2 mg/mL	7	420 nm	287 μmol/L, 1h	27.8 %	3.3 times	7
g-C ₃ N ₄ /BDI	----	0.6 mg/mL	7	λ > 420 nm	9.6 μmol/L, 1h	----	4.0 times	8
NVCNS	isopropanol	0.2 mg/mL	7	420 nm	4413.1 μmol/g, 1h	3.0 %	4.6 times	9
PI _x -NCN	----	1 mg/mL	7	420 nm	120 μmol/L, 2h	3.2 %	6.0 times	10
PCN-5/CS	AgNO ₃	1 mg/mL	9	450 nm	826 μmol/g, 1h	18.1 %	6.55 times	11
P-CN	isopropanol	1 mg/mL	7	> 420 nm	1500 μmol/L, 3h	----	6.6 times	12
TC/CN	ethanol	1 mg/mL	7	420 nm	600 μmol/L, 1h	4.62 %	9.3 times	13
CN _{QDS} @MA-Ag	isopropanol	1 mg/mL	7	420 nm	39.82 μmol/L, 1h	----	10.0 times	14
PCNHS-17	isopropanol	0.5 mg/mL	7	λ > 420 nm	90 μmol/L, 1h	----	11.2 times	15
K ₂ -CN	isopropanol	1 mg/mL	7	λ > 420 nm	19663 μmol/L, 1h	15.37 %	14.0 times	This work

References

1. Y. Peng, L. Wang, Y. Liu, H. Chen, J. Lei and J. Zhang, *Eur. J. Inorg. Chem.*, 2017, **2017**, 4797-4802.
2. F. Farzin, M. K. Rofouei, M. Mousavi and J. B. Ghasemi, *J. Phys. Chem. Solids*, 2022, **163**.
3. X. Chang, J. Yang, D. Han, B. Zhang, X. Xiang and J. He, *Catalysts*, 2018, **8**.
4. Y. Zhang, L. Zhang, D. Zeng, W. Wang, J. Wang, W. Wang and W. Wang, *Chinese Journal of Catalysis*, 2022, **43**, 2690-2698.
5. H. Shi, Y. Li, X. Wang, H. Yu and J. Yu, *Appl. Catal., B*, 2021, **297**.
6. Q. Hu, Y. Dong, K. Ma, X. Meng and Y. Ding, *J. Catal.*, 2022, **413**, 321-330.
7. C. Feng, L. Tang, Y. Deng, J. Wang, J. Luo, Y. Liu, X. Ouyang, H. Yang, J. Yu and J. Wang, *Adv. Funct. Mater.*, 2020, **30**.
8. Y. Kofuji, S. Ohkita, Y. Shiraishi, H. Sakamoto, S. Tanaka, S. Ichikawa and T. Hirai, *ACS Catalysis*, 2016, **6**, 7021-7029.
9. Y. Zheng, Y. Luo, Q. Ruan, J. Yu, X. Guo, W. Zhang, H. Xie, Z. Zhang, J. Zhao and Y. Huang, *J. Colloid Interface Sci.*, 2022, **609**, 75-85.
10. L. Yang, G. Dong, D. L. Jacobs, Y. Wang, L. Zang and C. Wang, *J. Catal.*, 2017, **352**, 274-281.
11. H. Zhang and X. Bai, *J. Colloid Interface Sci.*, 2022, **627**, 541-553.
12. L. Xue, H. Sun, Q. Wu and W. Yao, *J. Colloid Interface Sci.*, 2022, **615**, 87-94.
13. S. Lin, N. Zhang, F. Wang, J. Lei, L. Zhou, Y. Liu and J. Zhang, *ACS Sustain. Chem. Eng.*, 2020, **9**, 481-488.
14. M. Yin, X. Chen, Y. Wan, W. Zhang, L. Feng, L. Zhang and H. Wang, *ChemCatChem*, 2020, **12**, 1512-1518.
15. X. Dang, R. Yang, Z. Wang, S. Wu and H. Zhao, *Journal of Materials Chemistry A*, 2020, **8**, 22720-22727.