

Crystalline sulfur-doped poly(heptazine imide) for enhanced photocatalytic H₂ evolution under visible light irradiation

Cheng Cheng^a, Wenze Luo^b, Binjiang Zhai^b, Li Tian^b, Jinwen Shi^b, Zhifu Zhou^b, Fei Chen^{*a}, Xiangjiu Guan^{*b}

^a School of Chemical Engineering and Technology, Xi'an Jiaotong University (XJTU), 28 West Xianning Road, Xi'an 710049, China.

^b International Research Center for Renewable Energy (IRCRE), State Key Laboratory of Multiphase Flow in Power Engineering (MFPE), Xi'an Jiaotong University (XJTU), 28 West Xianning Road, Xi'an 710049, China.

* Corresponding authors. E-mail: xj-guan@mail.xjtu.edu.cn; feichen@xjtu.edu.cn

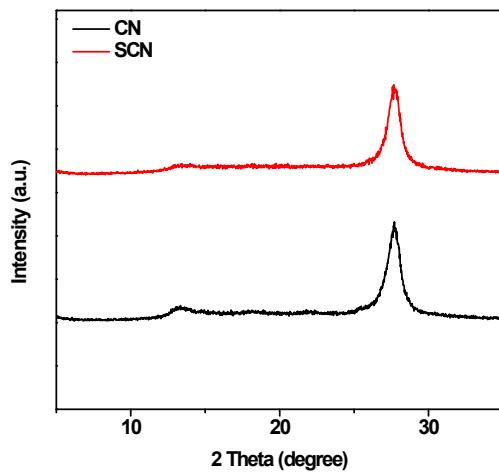


Figure S1. PXRD patterns of CN and SCN.

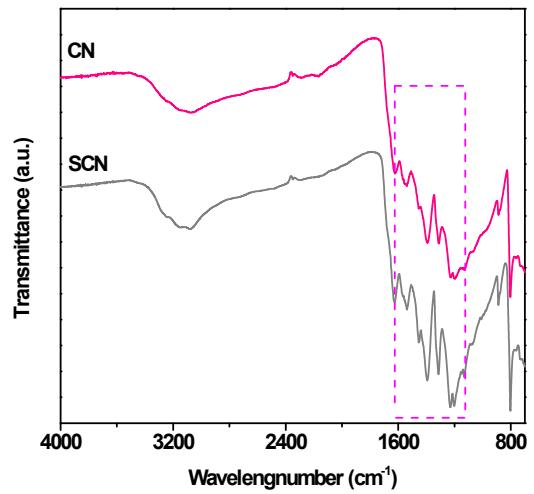


Figure S2. FTIR spectra of CN and SCN.

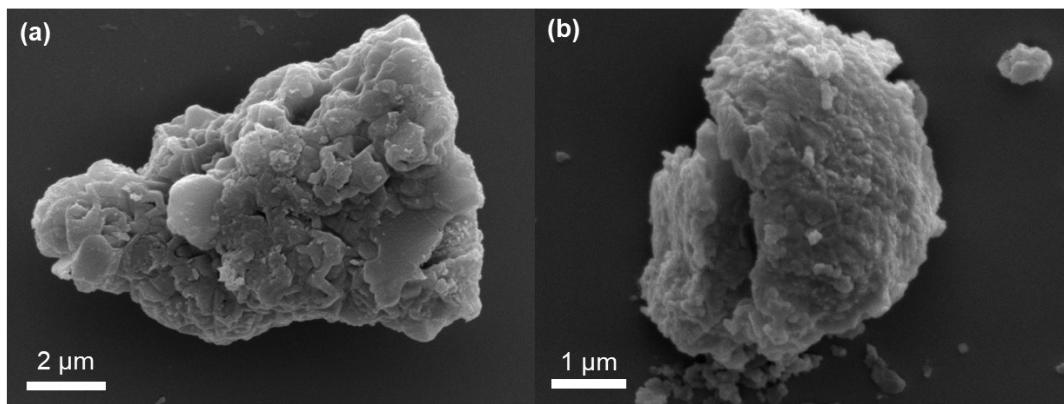


Figure S3. SEM images of (a) CN and (b) SCN.

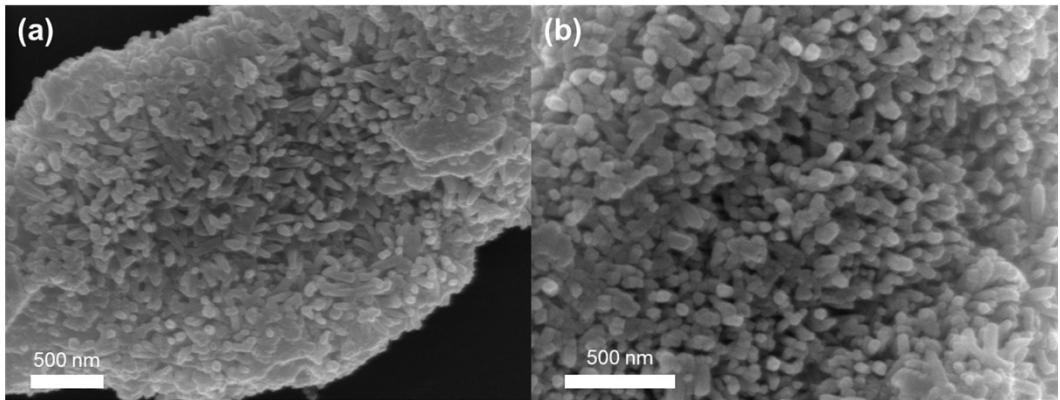


Figure S4. (a and b) SEM images of PHI.

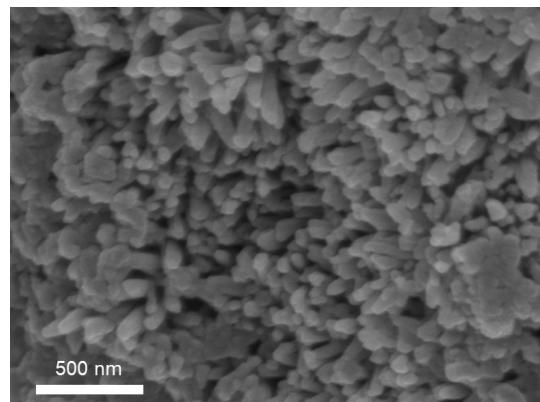


Figure S5. SEM image of S-PHI.

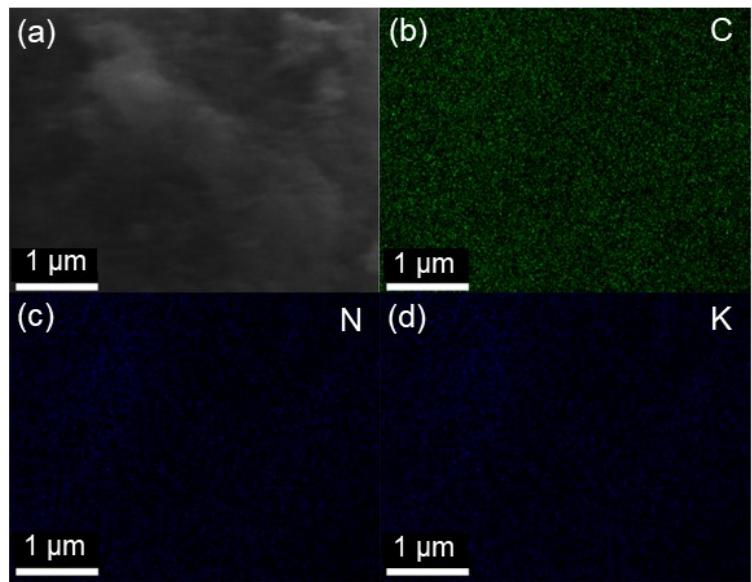


Figure S6. (a) SEM image, corresponding EDX mapping images of (b) C, (c) N and (d) K elements of PHI.

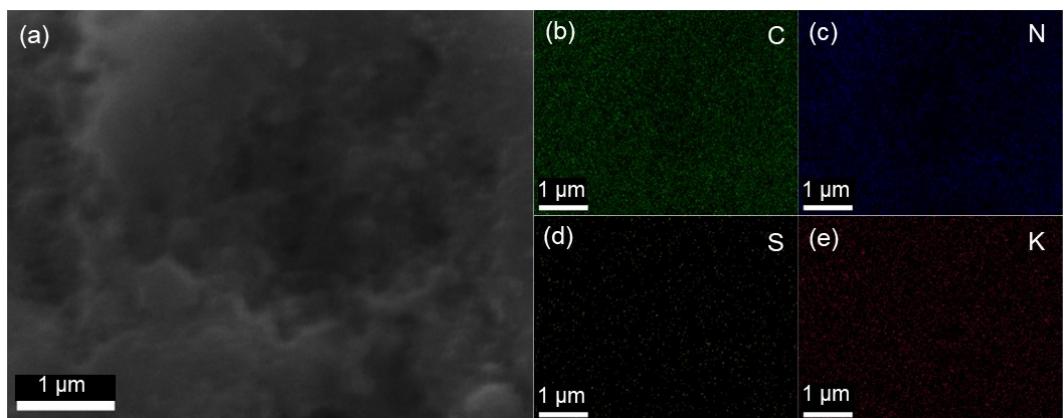


Figure S7. (a) SEM image, corresponding EDX mapping images of (b) C, (c) N, (d) S and (e) K elements.

Table S1. Elemental compositions measured by EA for PHI and S-PHI.

Sample	C (wt%)	N (wt%)	H (wt%)	S (wt%)	C/N (mol%)
PHI	26.71	45.04	1.94	0	0.69
S-PHI	26.57	44.34	2.48	1.29	0.70

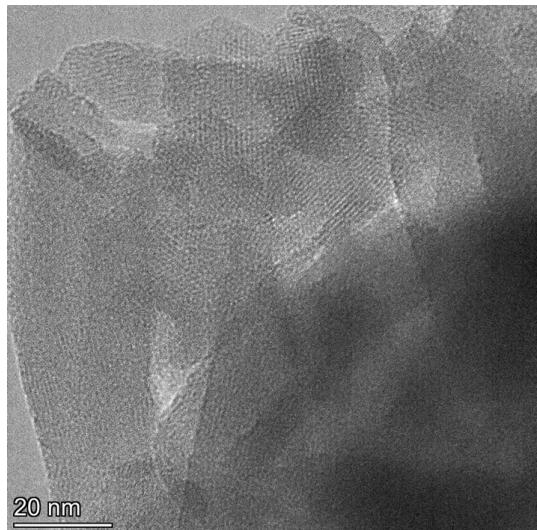


Figure S8. TEM image of PHI.

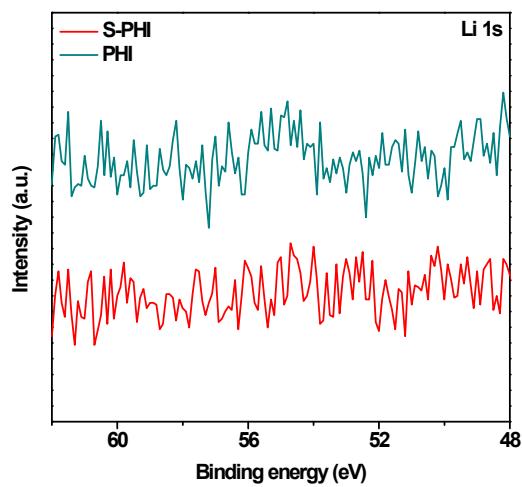


Figure S9. High-resolution XPS spectra of Li 1s for PHI and S-PHI.

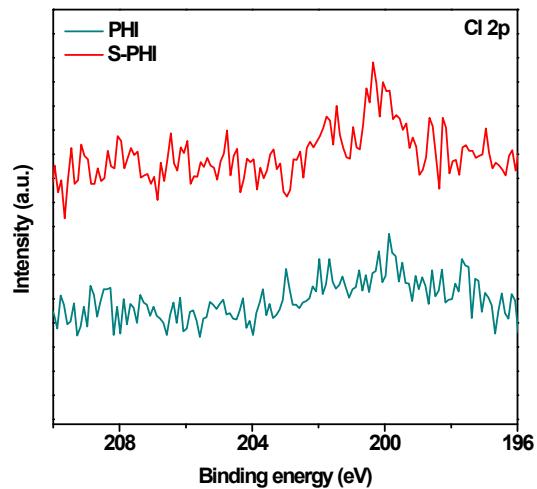


Figure S10. High-resolution XPS spectra of Cl 2p for PHI and S-PHI.

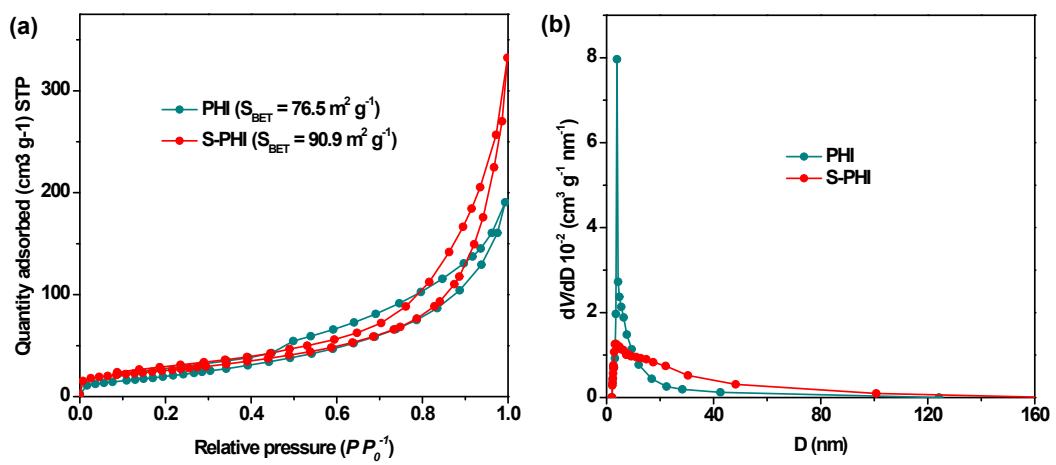


Figure S11. (a) N₂ adsorption-desorption isotherms and (d) pore-size distributions of PHI and S-PHI.

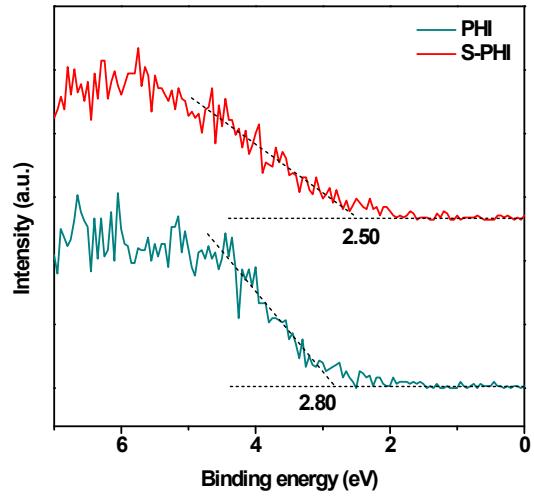


Figure S12. VB XPS spectra of PHI and S-PHI.

Table S2. The fitting details of TR-PL data for PHI and S-PHI.

Sample	τ_1 (ns)	A_1	τ_2 (ns)	A_2	τ_3 (ns)	A_3	τ_{avg} (ns)
PHI	3.07	0.20	12.92	0.01	0.96	8.38	1.28
S-PHI	0.75	25.2	8.2	0.02	2.22	0.36	0.87

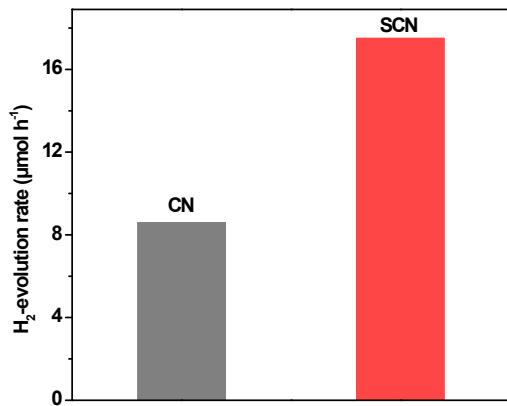


Figure S13. Photocatalytic H_2 -evolution rates of CN and SCN under visible-light irradiation

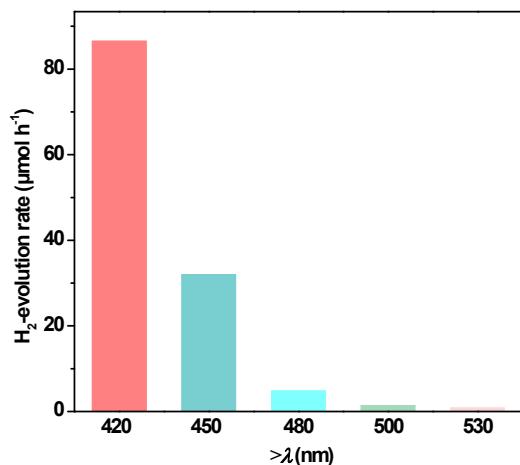


Figure S14. Photocatalytic H_2 -evolution activities for PHI under different light-spectrum irradiation.

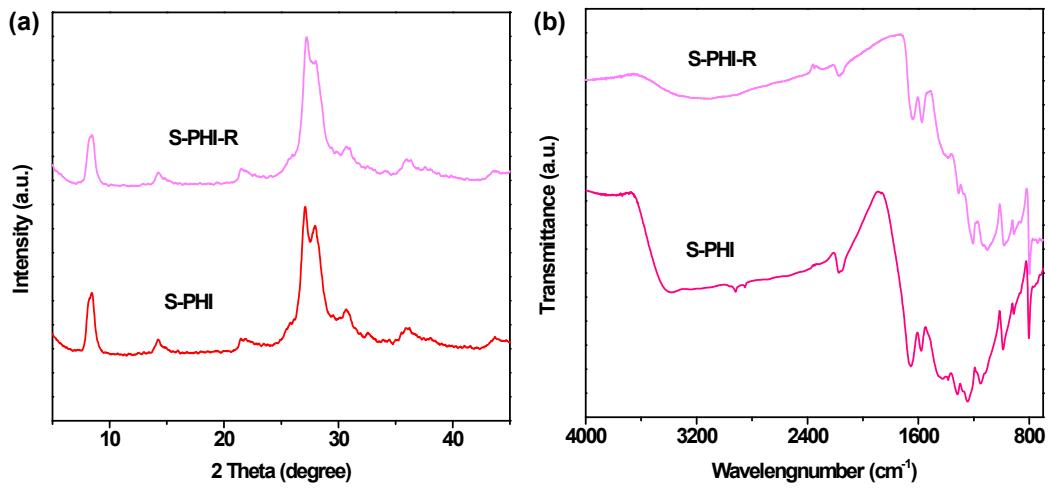


Figure S15. (a) PXRD patterns, (b) FTIR spectra of S-PHI and S-PHI-R.