

## *Supplementary Information*

Hollow porous prismatic graphitic carbon nitride with nitrogen vacancies and oxygen  
doping: a high-performance visible light-driven catalyst for nitrogen fixation

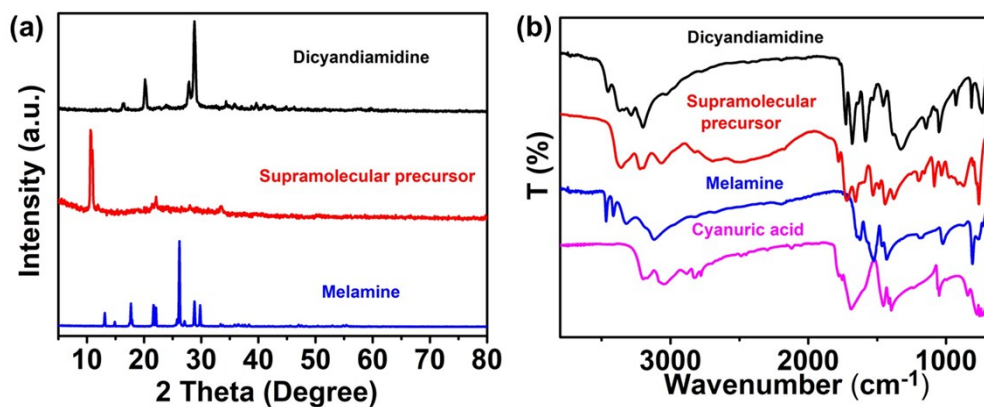
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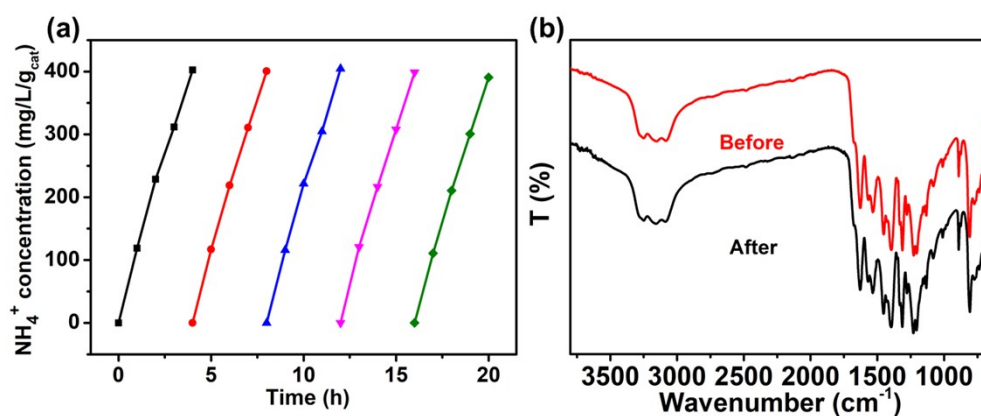
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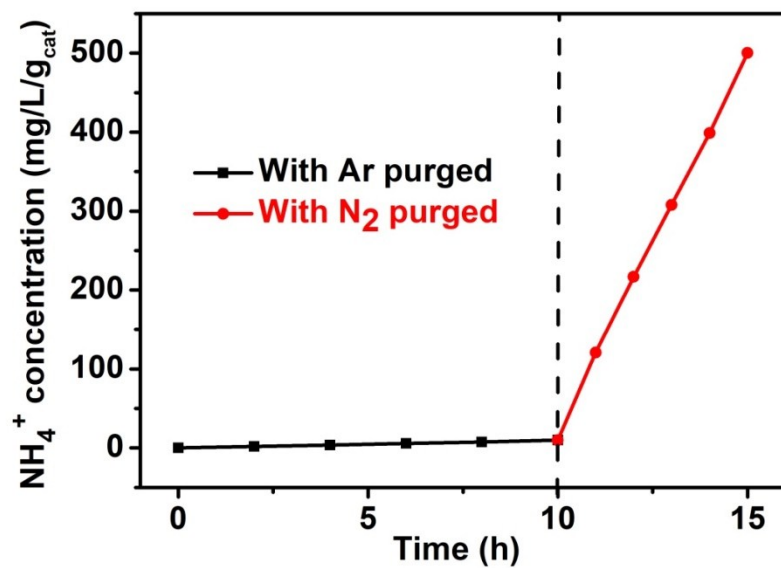
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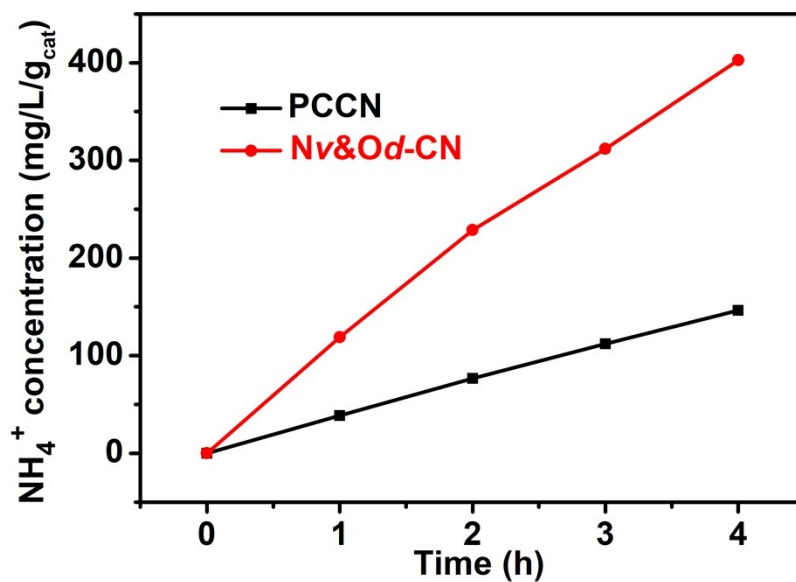
**Fig. S1** (a) X-ray diffraction (XRD) of the dicyandiamidine, supramolecular precursor, melamine and cyanuric acid. (b) FT-IR spectra of the dicyandiamidine, melamine and supramolecular precursor.



**Fig. S2** (a) The cycling testing of the photocatalytic activity over 20 h for Nv&Od-CN under the visible light irradiation ( $\lambda > 420$  nm), (b) FI-IR spectra of Nv&Od-CN before and after reaction.



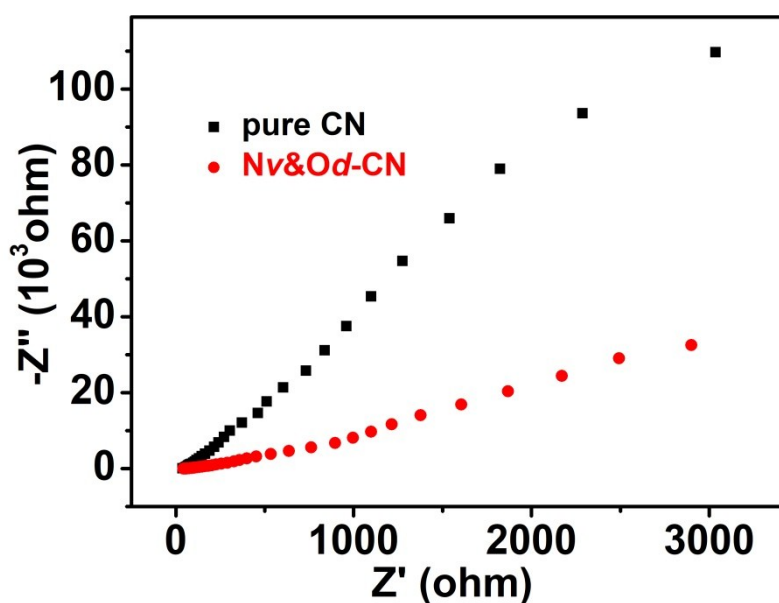
**Fig. S3** Photocatalytic nitrogen fixation for Nv&Od-CN under the visible light irradiation ( $\lambda > 420$  nm) with Ar purged or N<sub>2</sub> purged.



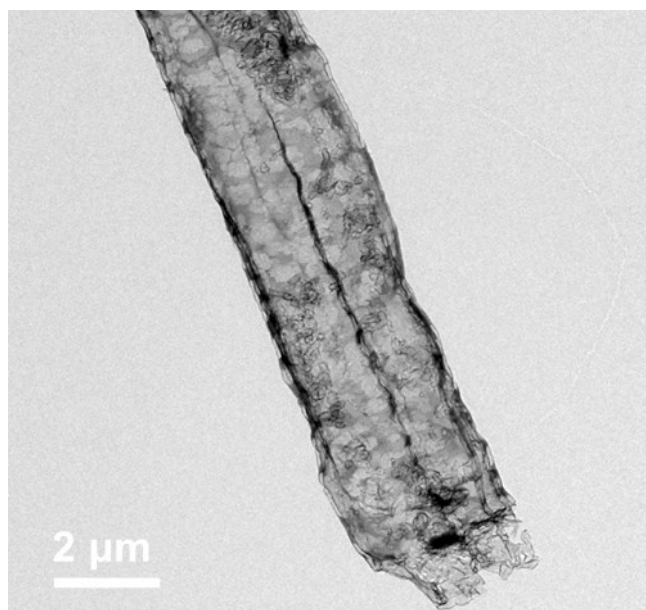
**Fig. S4** Photocatalytic nitrogen fixation for PCCN and Nv&Od-CN under the visible light irradiation ( $\lambda > 420$  nm).

The porous crimped graphitic carbon nitride (PCCN) with a large specific surface area

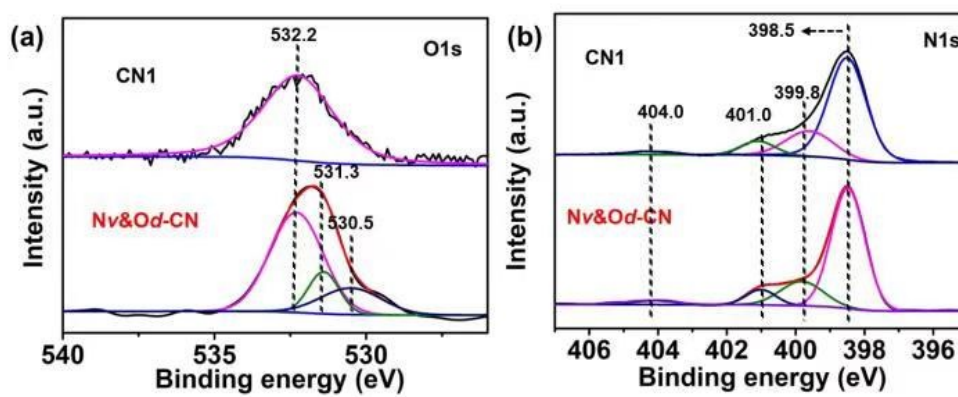
(146.14 m<sup>2</sup> g<sup>-1</sup>) was prepared based on our previous work (*Appl. Surf. Sci.* 2019, 480: 888–895) and was used as the contrast sample, which has neither nitrogen vacancies nor oxygen doping for the PCCN. The photocatalytic nitrogen fixation performances over the Nv&Od-CN and PCCN have been carried out under visible-light irradiation at room temperature and the results are shown in Fig. S4. It is noteworthy that although both the PCCN and Nv&Od-CN possess large specific surface area, the nitrogen fixation rate of PCCN is obviously lower than that of Nv&Od-CN, indicating that the change of specific surface area is not a mainly factor for improving photocatalytic nitrogen fixation performance.



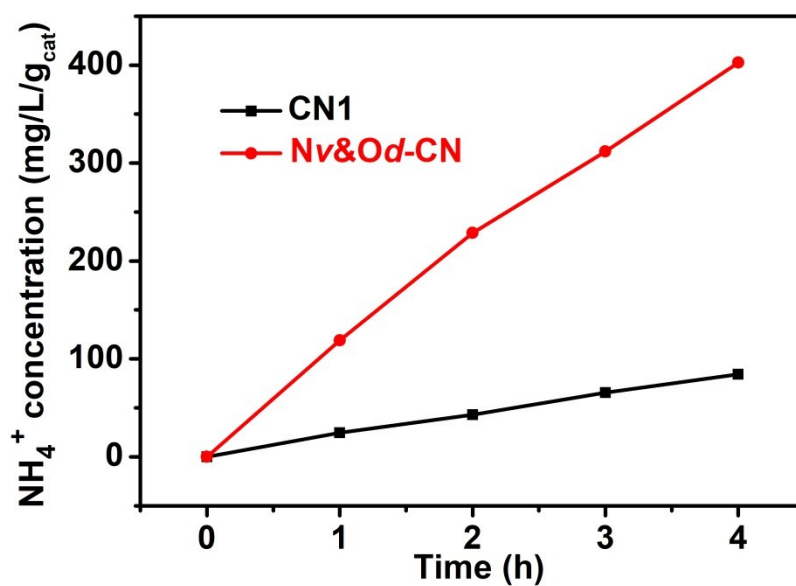
**Fig. S5** EIS Nyquist plots of the pure CN and Nv&Od-CN.



**Fig. S6** TEM images of CN1.



**Fig. S7** (a) XPS high resolution O 1s and (b) N 1s spectra for CN1 and Nv&Od-CN.



**Fig. S8** Photocatalytic nitrogen fixation for CN1 and Nv&Od-CN under the visible light irradiation ( $\lambda > 420$  nm).

**Table S1** Elemental analysis of the pure CN and Nv&Od-CN.

Samples	N (wt.%)	C (wt.%)	H (wt.%)	O (wt.%)
Pure CN	55.31	42.18	2.37	0.17
Nv&Od-CN	51.76	41.08	1.93	5.23

**Table S2** The peak areas of N species of the pure CN and Nv&Od-CN.

Samples	N <sub>2C</sub> area	N <sub>3C</sub> area	N <sub>NHx</sub> area
Pure CN	35713	11702	3423
Nv&Od-CN	33048	8553	3697

## References

- 1 T. Huang, Y.S. Fu, Q. Peng, C.Y. Yu, J.W. Zhu, A.P. Yu and X. Wang, *Appl. Surf. Sci.*, 2019, **480**, 888–895.