Electronic supplementary information (ESI)

Oxygen vacancy rich Cu_2O based composite material with nitrogen doped carbon as matrix for photocatalytic H_2 production and organic pollutant removal

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X-Ray crystallography

Suitable single crystal of **CuCP** was carefully selected under an optical microscope and glued on a glass fiber. Structural measurement was performed on a Bruker AXS SMART APEX II CCD diffractometer at 293 K. The structure was solved with the direct method and refined by the full-matrix least-squares method on F^2 using the SHELXTL crystallographic software package. Anisotropic thermal parameters were used to refine all non-hydrogen atoms. Carbon-bound hydrogen atoms were placed in geometrically calculated positions; Oxygen-bound hydrogen atoms were located in the difference Fourier maps, kept in that position and refined with isotropic temperature factors. The details have been deposited to the Cambridge Crystallographic Data Centre (CCDC 1812937). The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif

Table S1. Crystal data and structure refinement results for **CuCP**

Empirical formula	$C_{20}H_{18}CuN_2O_5$
Formula weight	429.90
Space group	Monoclinic
Crystal system	C2/c
Z	4
a (Å)	5.6629(3)
b (Å)	19.4888(10)
c (Å)	17.2426(8)
β(˚)	99.1860(10)
Volume (Å^3)	1878.54(16)
F(000)	884
Reflections collected	6850
Reflections unique	2326
R(int)	0.0197
Goodness-of-fit	0.884
R_1	0.0262
wR_2	0.0971
R_1 (all data)	0.0299
wR2 (all data)	0.1029

Note. $R_1 = \Sigma||F_o|-|F_c||/\Sigma|F_o|$; $wR_2 = \Sigma[w(F_o^2-F_c^2)^2]/\Sigma[w(F_o^2)^2]^{1/2}$

Table S2. Selected bond lengths and angles of **CuCP**

Cu(1)-O(1)#1	1.9538(11)	Cu(1)-O(1)	1.9538(11)
Cu(1)-N(1)	1.9932(13)	Cu(1)-N(1)#1	1.9932(13)
O(1)#1-Cu(1)-O(1)	93.00(7)	O(1)#1-Cu(1)-N(1)#1	93.83(5)
O(1)-Cu(1)-N(1)	93.83(5)	O(1)-Cu(1)-N(1)#1	167.88(5)
O(1)#1-Cu(1)-N(1)	167.88(5)	N(1)-Cu(1)-N(1)#1	81.31(7)

Symmetry transformations used to generate equivalent atoms: #1 -x, y, -z+1/2.

Table S3 Comparison of photocatalytic H_2 production rate reported in the literature with Cu_2O based composite photocatalysts and our works.

Photocatalyst	Catalyst dose (g)	H_2 Production ($\mu mol \cdot h^{-1} \cdot g^{-1}$)	Ref.
NPs/Cu_2O	0.003	47.0	S1
C_3N_4/Pd/Cu_2O	0.015	32.5	S2
g-C_3N_4/Cu_2O	0.300	265.0	S3
NCs/Cu_2O	0.150	132.7	S4
HD-Au-NR/Cu_2O	0.005	80.2	S5
HD-Au-NR/TiO_2/Cu_2O	0.005	105.1	
Cu_2O	0.100	29.78	S6
NCs/Cu_2O	0.025	15.0	S7
Cu/Cu_2O@NC(A)	**0.020**	**379.6**	**Our work**

Table 4 The contents of Cu, C, N and H in **Cu/Cu_2O@NC**.

	Cu/Cu_2O@NC(A)	**Cu/Cu_2O@NC(B)**	**Cu/Cu_2O@NC(C)**
Cu (%)	4.5	4.4	4.2
C (%)	89.2	89.5	89.9
N (%)	3.0	2.9	2.8
H (%)	1.1	1.3	1.1

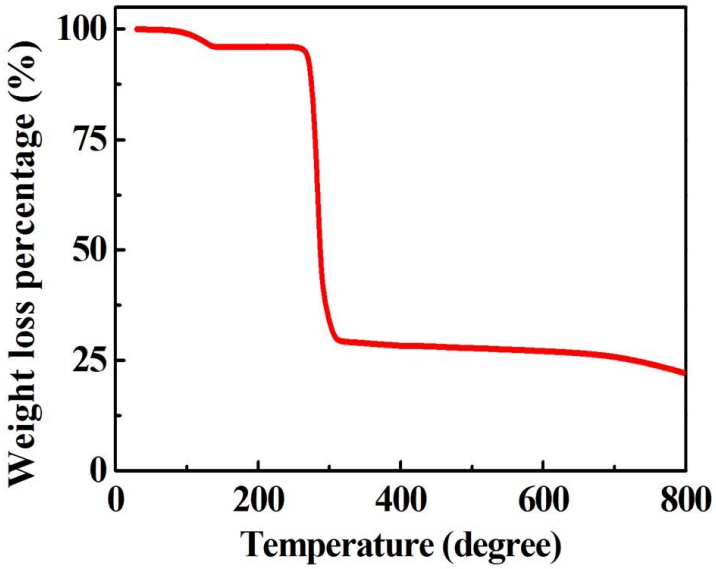

Fig. S1 TGA of **CuCP**

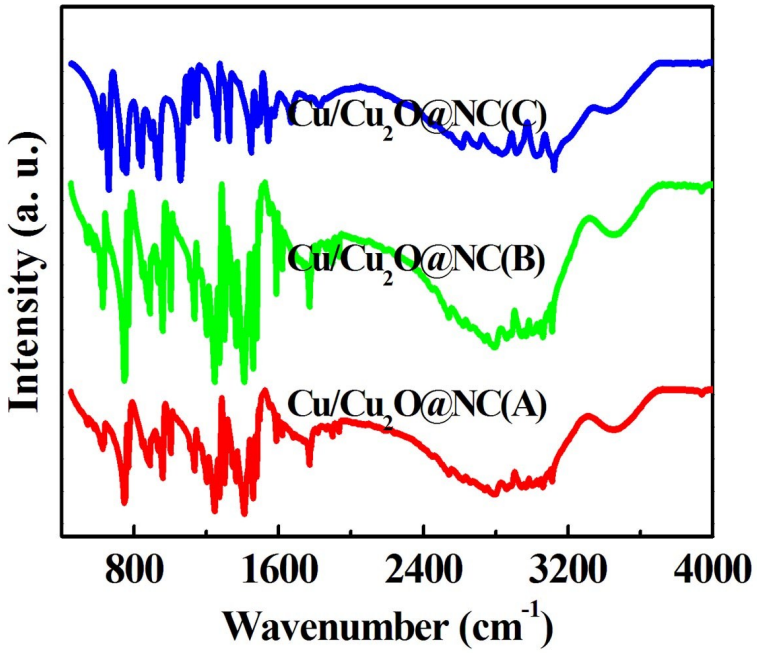

Fig. S2 FTIR of **Cu/Cu_2O@NC**

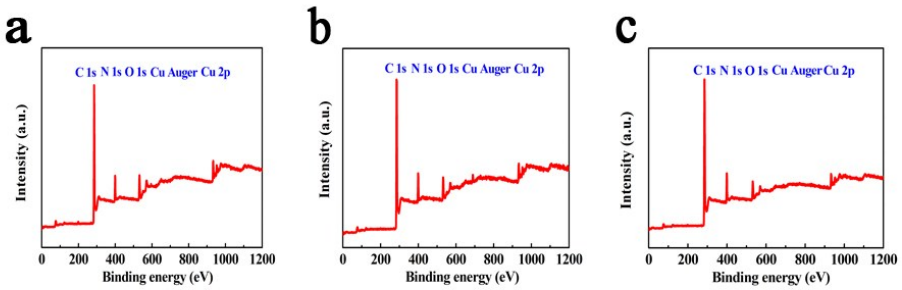

Fig. S3 XPS survey of (a) **Cu/Cu_2O@NC(A)**; (b) **Cu/Cu_2O@NC(B)**; (c) **Cu/Cu_2O@NC(C)**.

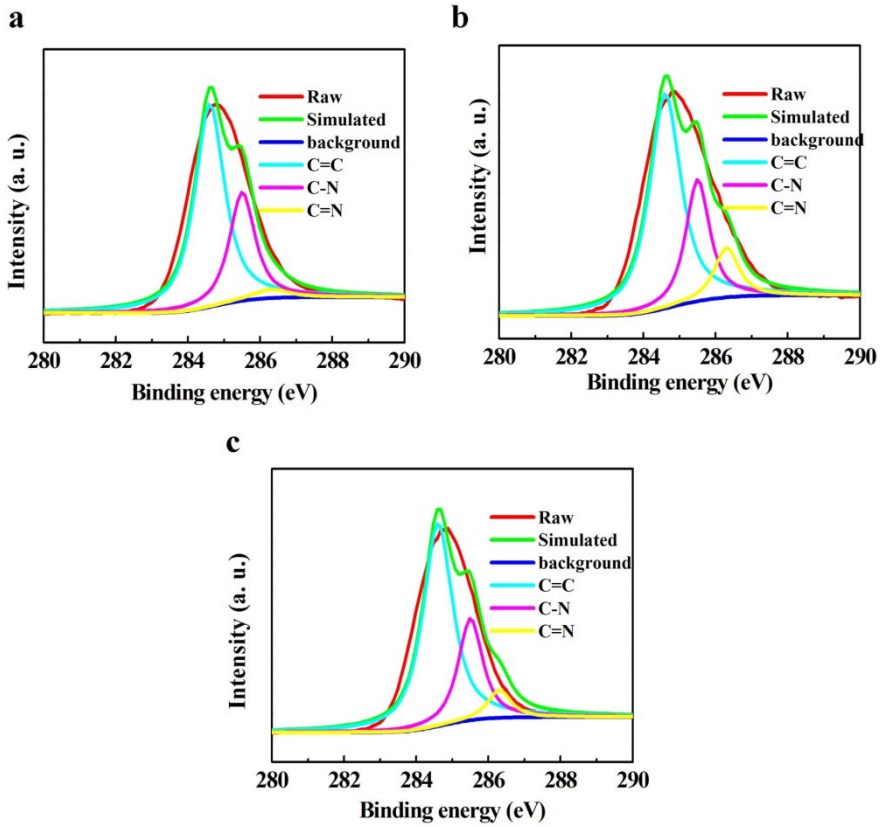

Fig. S4 C1s of (a) **Cu/Cu_2O@NC(A)**; (b) **Cu/Cu_2O@NC(B)**; (c) **Cu/Cu_2O@NC(C)**.

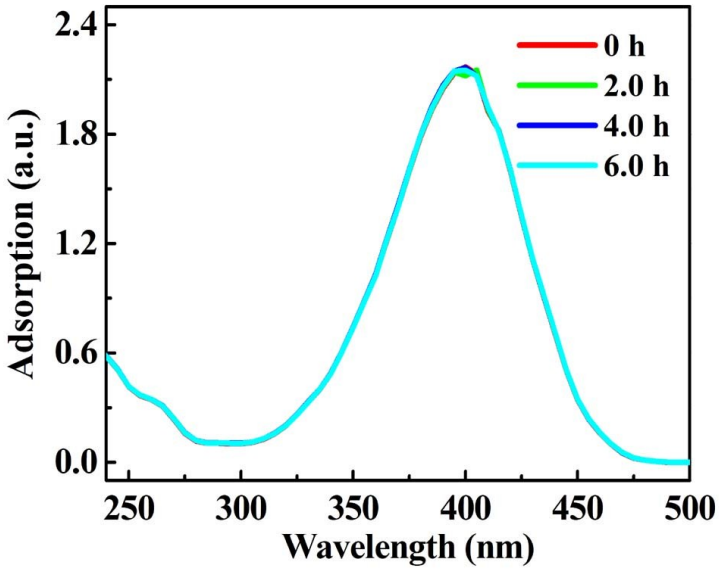

Fig. S5 UV-vis spectra of 4-nitrophenol without **Cu/Cu_2O@NC**.

References

(S1) D. Mateo, I. Esteve-Adell, J. Albero, A. Primo and H. García, *Appl. Catal. B: Environ.,* 2017, **201**,582-590.

(S2) W.J. Yin, L.J. Bai, Y.Z. Zhu, S.X. Zhong, L.H. Zhao, Z.Q. Li and S. Bai, *ACS Appl. Mater. Interfaces,* 2016, **8**, 23133-23142.

(S3) L. Liu, Y.H. Qi, J.S. Hu, Y.H. Liang and W.Q. Cui, *Appl. Surf. Sci.,* 2015, **351**, 1146-1154.

(S4) F. Wang, Y.T. Zhao, F. Feng, C.L. Li, F. Cao and W.F. Shangguan, *J. Alloys Compd.,* 2016, **688**, 632-638.

(S5) X.J. Yu, F.Z. Liu, J.L. Bi, B. Wang and S.C. Yang, *Nano Energy,* 2017, **33**, 469-475.

(S6) Z.Y. Lin, L.H. Li, Li.L. Yu, W.J. Li and G.W. Yang, *Phys. Chem. Chem. Phys.,* 2017, **19**, 8356-8362.

(S7) S. Kumar, C.M.A. Parlett, M.A. Isaacs, D.V. Jowett, R.E. Douthwaite, M.C.R. Cockett and A.F. Lee, *Appl. Catal. B: Environ.,* 2016, **189**, 226-232.