Electronic Supplementary Information

Hydrogen peroxide-assisted synthesis of oxygen-doped carbon nitride nanorods for enhanced photocatalytic hydrogen evolution

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Density Functional Theory (DFT) Calculations: DFT calculations were performed using CASTEP module in Material Studio software package. Geometry optimization and single energy calculations was carried out by the generalized gradient approximation (GGA) with the Perdew–Burke–Ernzerhof (PBE) exchange-correlation functional. The energy cutoff was set to be 500 eV and Monkhorst-Pack k-point mesh of $5 \times 5 \times 1$ was used. A two-dimensional melon sheet was constructed to represent the incomplete polycondensation of melon, with a large vacuum space of 15 Å to separate two neighboring melon sheets. The convergences of energy, maximum displacement, and maximum force were set as 5.0×10^{-6} eV atom^{-1}, 5.0×10^{-4} Å, and 0.01 eV Å^{-1}, respectively.

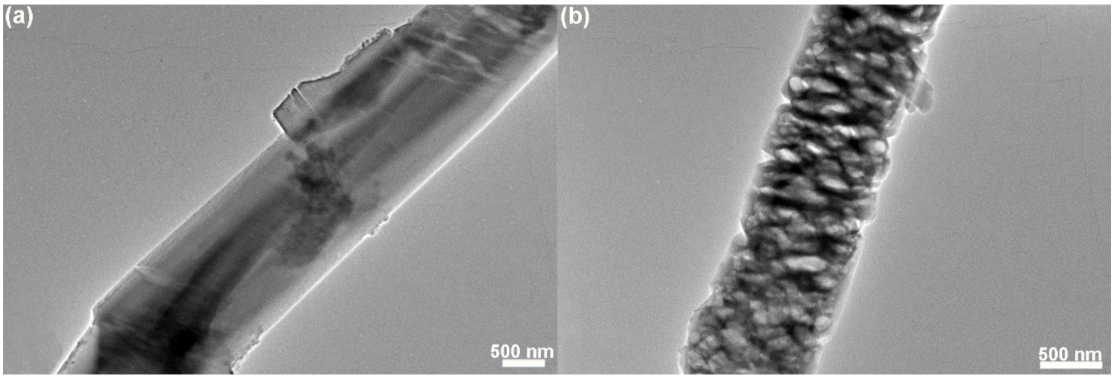

Fig. S1 TEM images of an individual nanorod (a) before and (b) after electron beam irradiation.

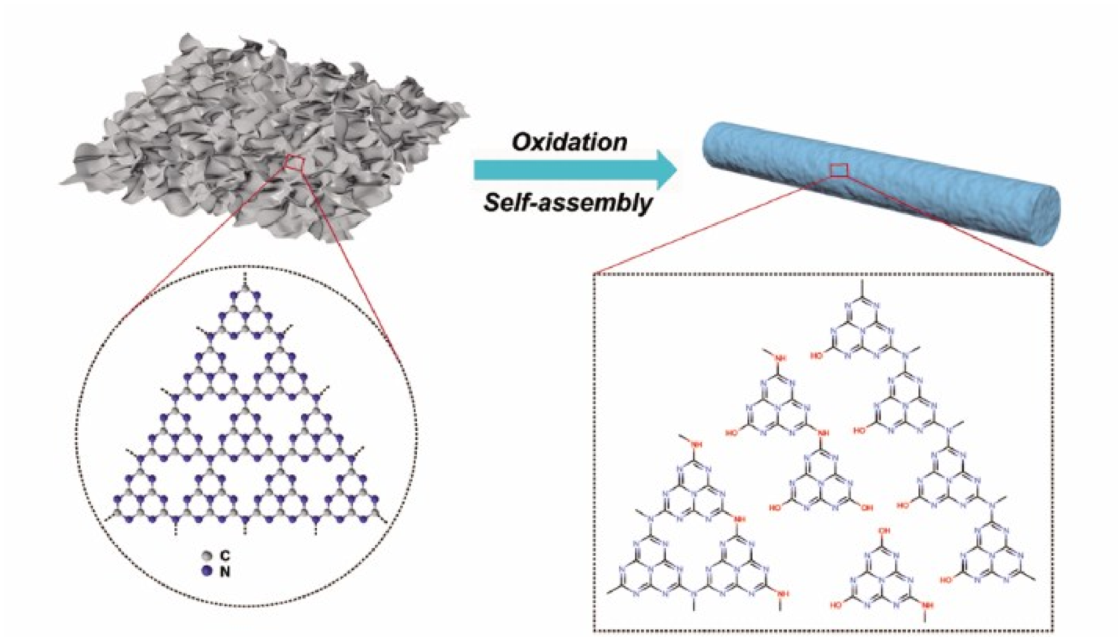

Fig. S2 Schematic illustration for self-assembly process of the OCN

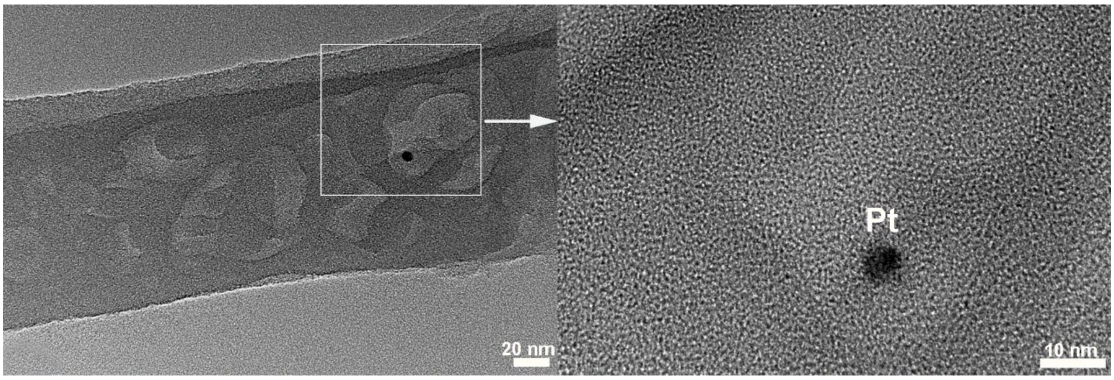

Fig. S3 Typical TEM images of the OCN for photocatalytic H_2 evolution after long-term cycles.

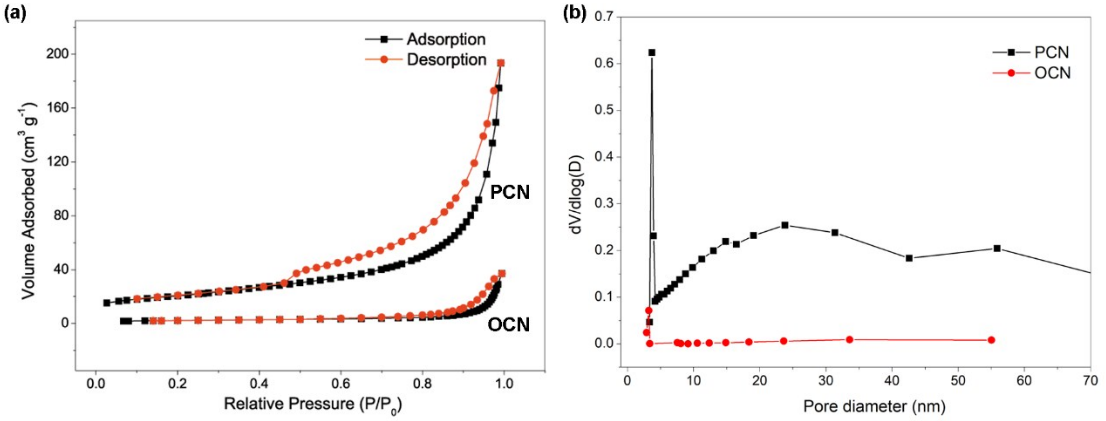

Fig. S4 (a) N_2 adsorption-desorption isotherms and (b) corresponding pore size distributions of the PCN and OCN.

Table S1 Quantification analysis of the C/N ratio and atomic percentage of the C-N=C, N-$(C)_3$ and C-NH configurations by XPS analysis.

Sample	C/N	C-N=C	N-$(C)_3$	C-NH
PCN	0.69	0.448	0.325	0.227
OCN	0.71	0.291	0.511	0.198

Table S2 Hydrogen evolution rates over a series of CN-based photocatalysts.

Catalyst	Pt (wt %)	Sacrificial Agents	λ (nm)	HER Rate (mmol h^{-1} $g_{catalyst}^{-1}$)	Ref.
C_3N_4 aerogel	3	TEOA, 10 vol %	> 420	0.33	1
g-C_3N_4/Ni	0	TEOA, 10 vol %	> 420	0.11	2
C_3N_4 microspheres	3	TEOA, 15 vol %	> 420	0.18	3
g-C_3N_4/CoO	3	TEOA, 10 vol %	> 400	0.65	4
C_3N_4 nanotubes	3	TEOA, vol %	> 420	5.24	5
g-C_3N_4 nanosheets	3	TEOA, 10 vol %	> 420	9.0	6
C_3N_4	3	TEOA, 20 vol %	> 420	0.61	7
(C_{ring})-C_3N_4	3	/	> 420	0.37	8
a-CN	1	TEOA, 10 vol %	> 420	2.04	9
g-C_3N_4/CdS	1	0.05 M Na_2S-Na_2SO_3	> 420	5.69	10
g-C_3N_4/CQDs	3	Methanol, 25 vol %	> 420	3.54	11
g-C_3N_4/PtCo	/	TEOA, 10 vol %	> 400	0.96	12
Au/SnO_2/g-C_3N_4	/	Methanol, 20 vol %	> 400	0.77	13
g-C_3N_4/C	1	TEOA, 10 vol %	> 420	2.59	14
1D OCN	1	TEOA, 10 vol %	> 400	1.48	**this work**

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