Nitrogen defected polymeric carbon nitride for efficient photocatalytic H_2 evolution and RhB degradation under visible light irradiation

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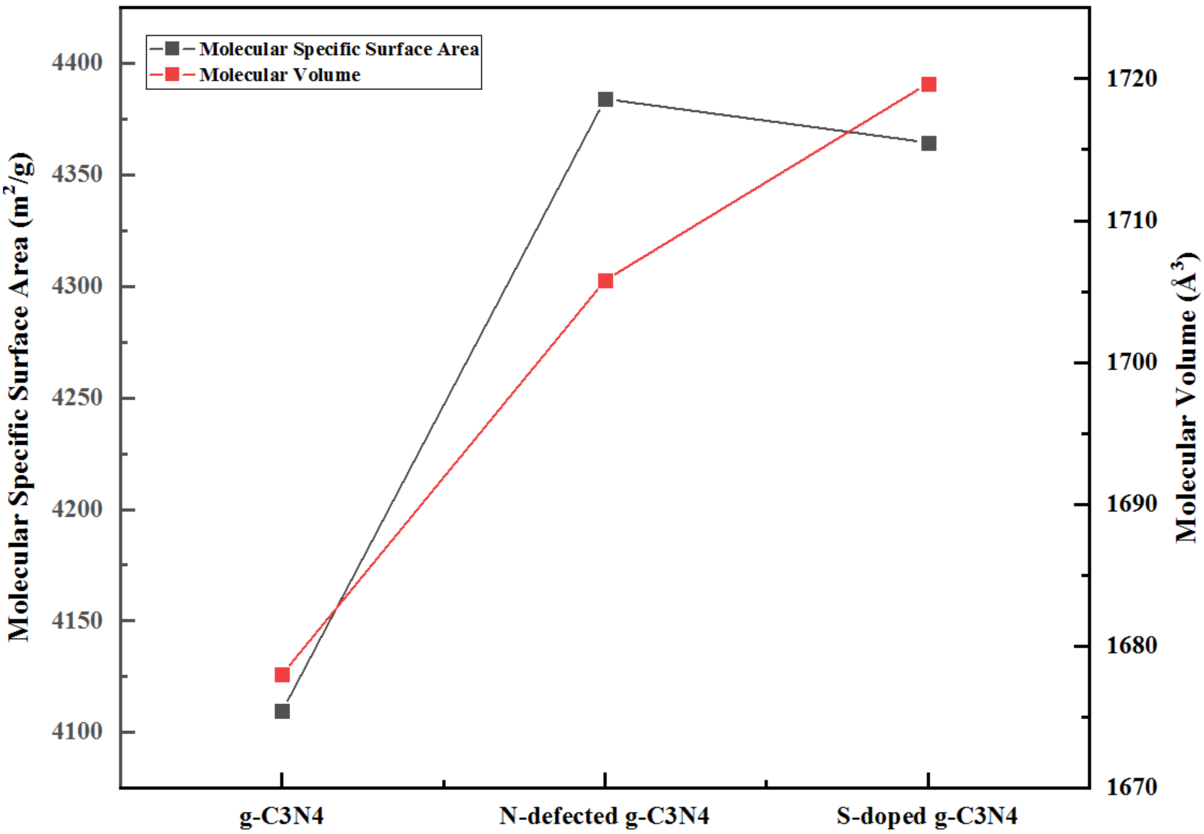

Figure S1. Calculated specific surface areas and molecular volumes of the three molecules.

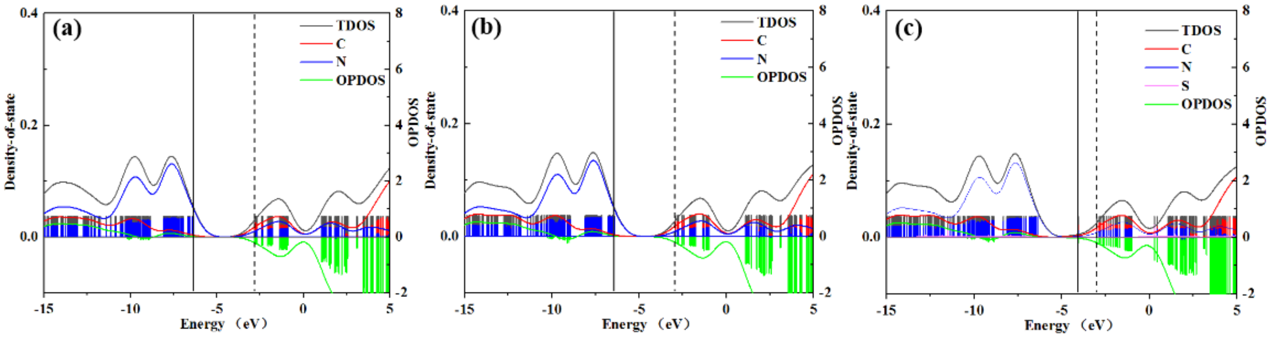

Figure S2. Calculated total, partial, and overlapped population density of states of (a) pure, (b) N-defected, and (c) S-doped g-C_3N_4 with N defection at the B3LYP/6-31G* theory level. Solid line: HOMO energy; dashed line: LUMO energy.

Table.S1 Comparison of the reported hydrogen evolution rate (HER) of g-C_3N_4 photocatalysts from different literatures.

Photocatalyst (precursors)	HER rate [μmol/(h▪g)]	Light source	Reaction conditions	Reference
2SCN (melamine and trithiocyanuric acid)	4140	500 W Xe lamp, λ > 420 nm	3 wt% Pt 17 vol% TEOA	This work
g-C_3N_4 microwire (melamine)	1688	500 W Xe lamp, λ > 380 nm	1 wt% Pt 17 vol% TEOA	[5]
g-C_3N_4 (urea)	3327	300 W Xe lamp, λ >420 nm	3 wt% Pt TEOA	[4]
g-C_3N_4 (melamine and urea)	3100	300 W Xe lamp, λ ≥ 400 nm	3 wt% of Pt 20 vol% TEOA	[2]
g-C_3N_4 (dicyandiamide)	310	300 W Xe lamp, λ > 440 nm	3 wt% Pt 10 vol% TEOA	[1]
g-C_3N_{4-x} (melamine)	3068	500 W Xe lamp, λ > 420 nm	2 wt% Pt 10 vol% TEOA	[7]
g-C_3N_4 (melamine)	1288	300 W Xe lamp, λ > 420 nm	3 wt% Pt 15 vol% TEOA	[6]
P/g-C_3N_4 (melamine)	1596	300 W Xe lamp, λ ≥ 400 nm	2 wt% Pt 20 vol% TEOA	[3]

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nitride for greatly extended visible light photocatalytic hydrogen evolution. Nano Energy **2018**, 44, 73-81.
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