Electronic Supplementary Material (ESI) for RSC Advances.

Electronic Supplementary Information

A nine-fold enhancement of visible-light photocatalytic hydrogen production of g-C_3N_4 with TCNQ by forming conjugated structure

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Characterization of g-C_3N_4 and TCNQ-C_3N_4 photocatalysts

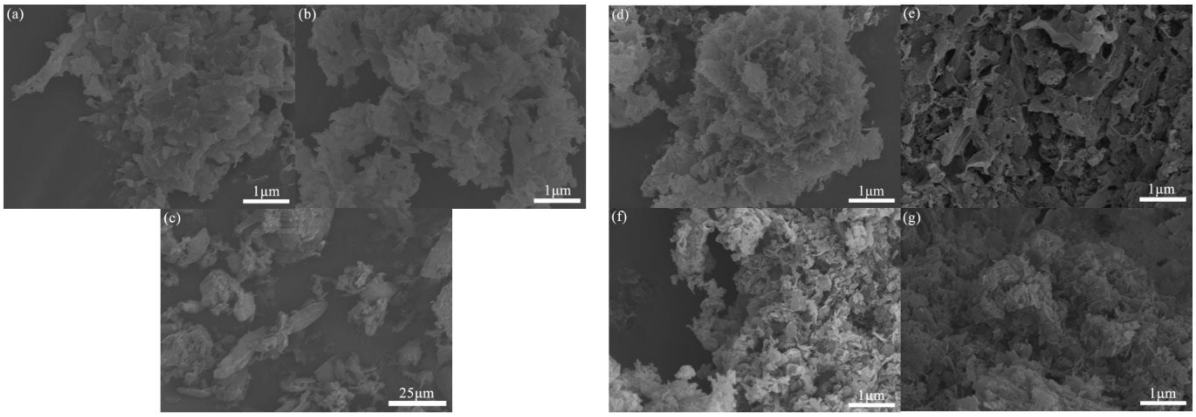

Fig. S1 (a) SEM images of: (a) g-C_3N_4 (bulk); (b) g-C_3N_4 (APTES); (c) TCNQ; (d) 2%TCNQ-C_3N_4; (e) 5%TCNQ-C_3N_4; (f) 10%TCNQ-C_3N_4; (g) 15%TCNQ-C_3N_4.

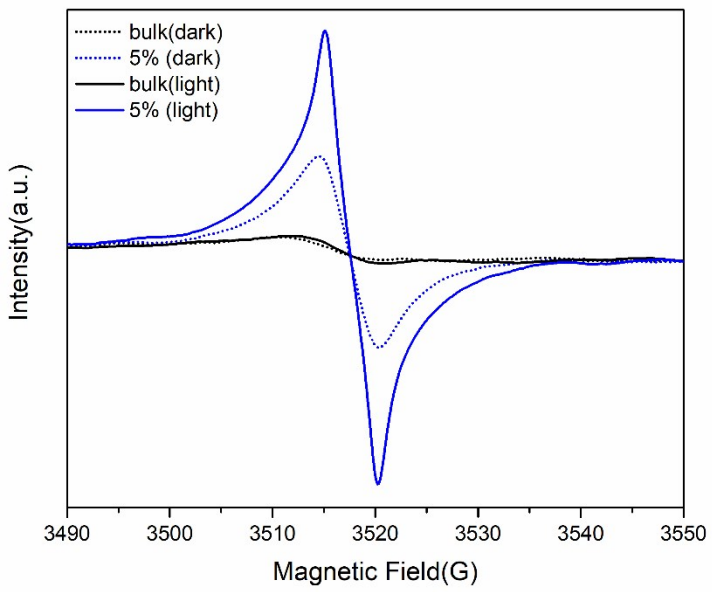

Fig. S2 EPR spectra of bulk g-C_3N_4 and 5%TCNQ-C_3N_4.

Calculated apparent quantum yield (AQY) at different wavelength

AQY (%)=

$$\frac{2 \times number\ of\ evolved\ H_2\ molecules}{number\ of\ inciednt\ photons} \times 100\% = \frac{2 \times M \times N_A}{S \times P \times t \times \frac{\lambda}{\hbar \times c}} \times 100\%$$

In the formula, M is the amount of H_2 molecules per hour (μmol h^{-1}); N_A is the Avogadro constant (6.02×10^{23} mol^{-1}); S is the irradiation area ($1.5 \times 1.5 \times \pi$ cm^2); P is the intensity of monochromatic light (W cm^{-2}), detected by optical power meter; t is the light irradiation time (1h); λ is the wavelength of the monochromatic light (nm); $\hbar$ is the Plank constant (6.626×10^{-34} J s); c is the speed of light (3×10^8 m s^{-1}).

Table S1. Calculated AQY at different wavelengths

Wavelength (nm)	Light intensity (10^{-3} W cm^{-2})	Amount of H_2 (μmol h^{-1})	AQY (%)
365	32.00	4.2053	0.34
420	20.00	4.4398	0.50
450	15.51	3.5703	0.48
485	15.40	2.3199	0.30
535	2.76	0.7838	0.50
595	0.79	0.8947	1.79
630	5.62	0.5840	0.16

λ=365 nm:

$$AQY\ (\%) = \frac{2 \times 4.2053 \times 10^{-6} \times 6.022 \times 10^{23}}{\pi \times 1.5^2 \times 32.00 \times 10^{-3} \times 3600 \times \frac{365 \times 10^{-9}}{6.626 \times 10^{-34} \times 3 \times 10^{8}}} = 0.34\%$$

λ=420 nm:

$$AQY\ (\%) = \frac{2 \times 4.4398 \times 10^{-6} \times 6.022 \times 10^{23}}{\pi \times 1.5^2 \times 20.00 \times 10^{-3} \times 3600 \times \frac{420 \times 10^{-9}}{6.626 \times 10^{-34} \times 3 \times 10^{8}}} = 0.50\%$$

λ=450 nm:

$$AQY\ (\%) = \frac{2 \times 3.5703 \times 10^{-6} \times 6.022 \times 10^{23}}{\pi \times 1.5^2 \times 15.51 \times 10^{-3} \times 3600 \times \frac{450 \times 10^{-9}}{6.626 \times 10^{-34} \times 3 \times 10^{8}}} = 0.48\%$$

λ=485 nm:

$$AQY\ (\%) = \frac{2 \times 2.3199 \times 10^{-6} \times 6.022 \times 10^{23}}{\pi \times 1.5^2 \times 15.40 \times 10^{-3} \times 3600 \times \frac{485 \times 10^{-9}}{6.626 \times 10^{-34} \times 3 \times 10^{8}}} = 0.30\%$$

λ=535 nm:

$$AQY\ (\%) = \frac{2 \times 0.7838 \times 10^{-6} \times 6.022 \times 10^{23}}{\pi \times 1.5^2 \times 2.76 \times 10^{-3} \times 3600 \times \frac{535 \times 10^{-9}}{6.626 \times 10^{-34} \times 3 \times 10^{8}}} = 0.50\%$$

λ=595 nm:

$$AQY\ (\%) = \frac{2 \times 0.8947 \times 10^{-6} \times 6.022 \times 10^{23}}{\pi \times 1.5^2 \times 0.79 \times 10^{-3} \times 3600 \times \frac{595 \times 10^{-9}}{6.626 \times 10^{-34} \times 3 \times 10^{8}}} = 1.79\%$$

λ=630 nm:

$$AQY\ (\%) = \frac{2 \times 0.5840 \times 10^{-6} \times 6.022 \times 10^{23}}{\pi \times 1.5^2 \times 5.62 \times 10^{-3} \times 3600 \times \frac{630 \times 10^{-9}}{6.626 \times 10^{-34} \times 3 \times 10^{8}}} = 0.16\%$$