Supporting Information

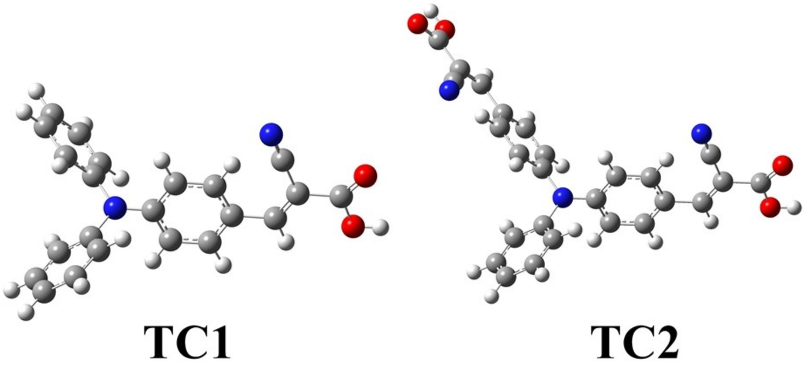
D-π-A type triphenylamine dye covalent functionalized g-C_3N_4 for highly efficient photocatalytic hydrogen evolution

Chao Zhang,†[a] Jiandong Liu,†[a] Xingliang Liu*[a] and Shiai Xu*[a,b]

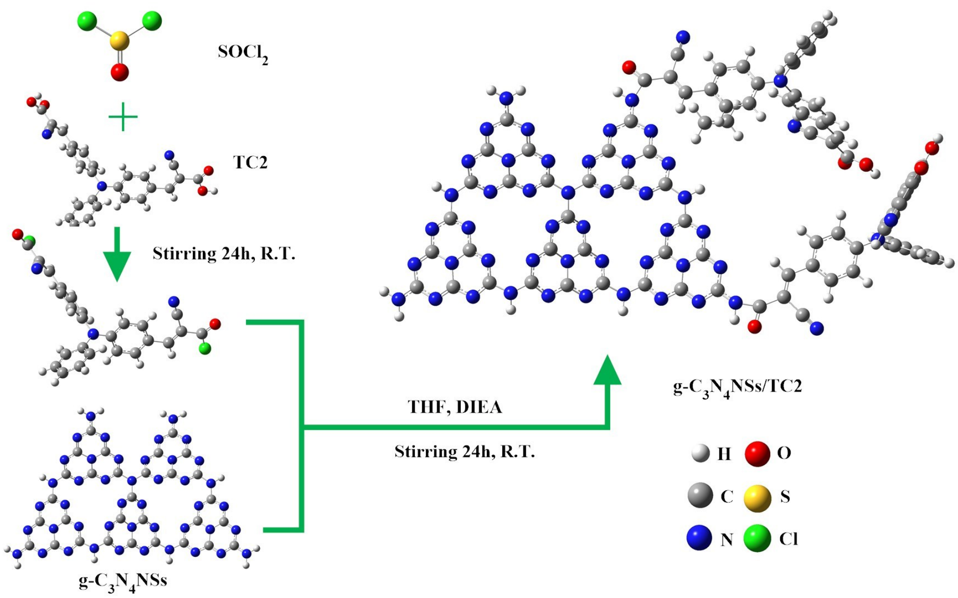
a. School of Chemical Engineering, Qinghai University, Xining 810016, Qinghai, China. E-mail: liuxl1219@163.com

b. Shanghai Key Laboratory of Advanced Polymeric Materials, Key Laboratory for Ultrafine Materials of Ministry of Education, School of Materials Science and Engineering, East China University of Science and Technology, Shanghai 200237, China. E-mail: saxu@ecust.edu.cn

† These authors contributed equally to this work.



Scheme S1 Dyes structure of TC1 and TC2



Scheme S2 Synthesis of g-C_3N_4 NSs/TC2($C_{82}H_{42}N_{50}O_6$)

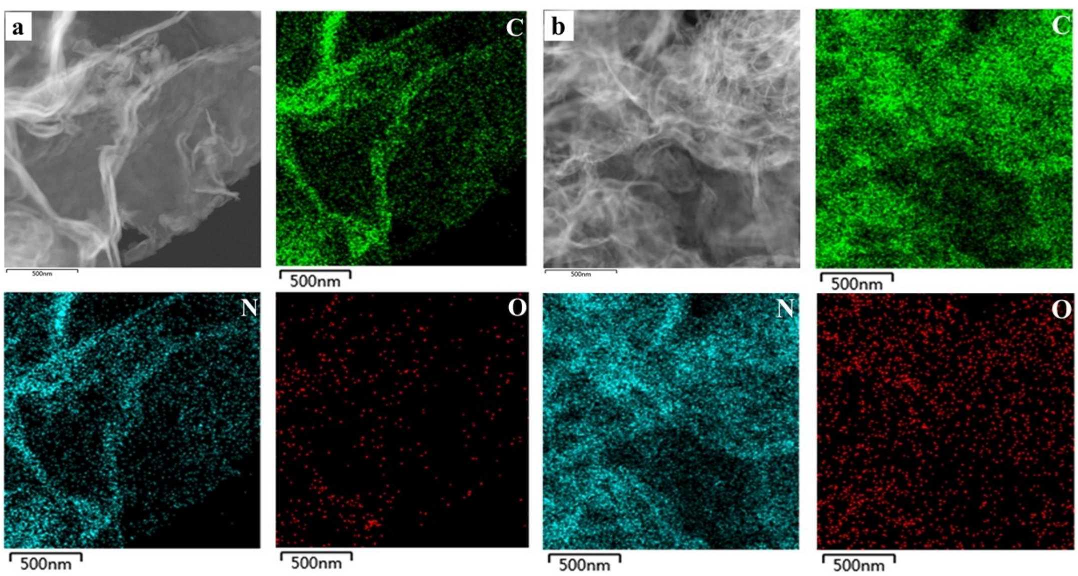


Fig. S1 Typical TEM images of as-prepared sample and elemental mapping (C (green), N (cyan), O (red)) (a) g-

C_3N_4-NSs+TC1, (b) g-C_3N_4 NSs/TC2.

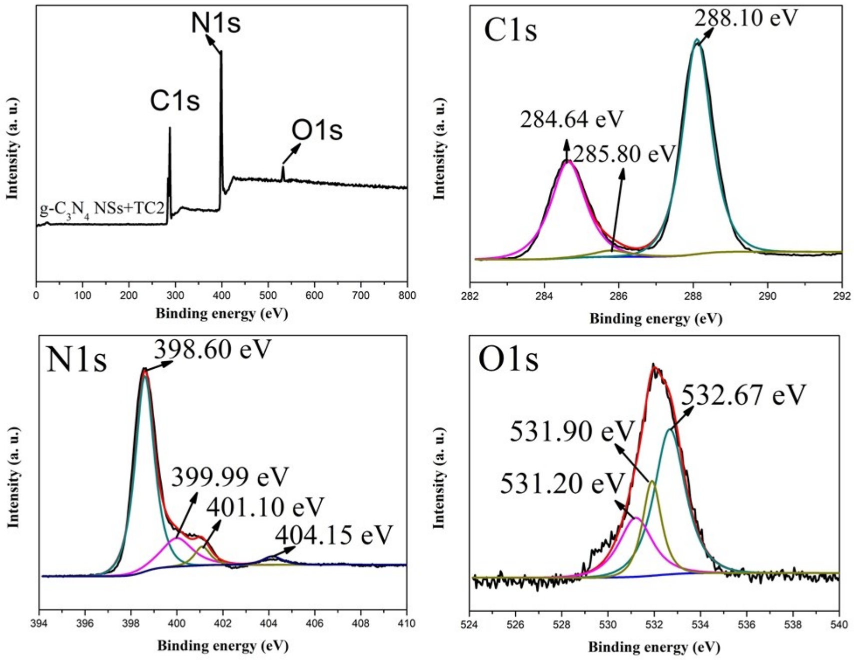


Fig. S2 High-resolution C 1s spectra, N 1s spectra and O 1s spectra of XPS spectra for g-C_3N_4 NSs+TC2.

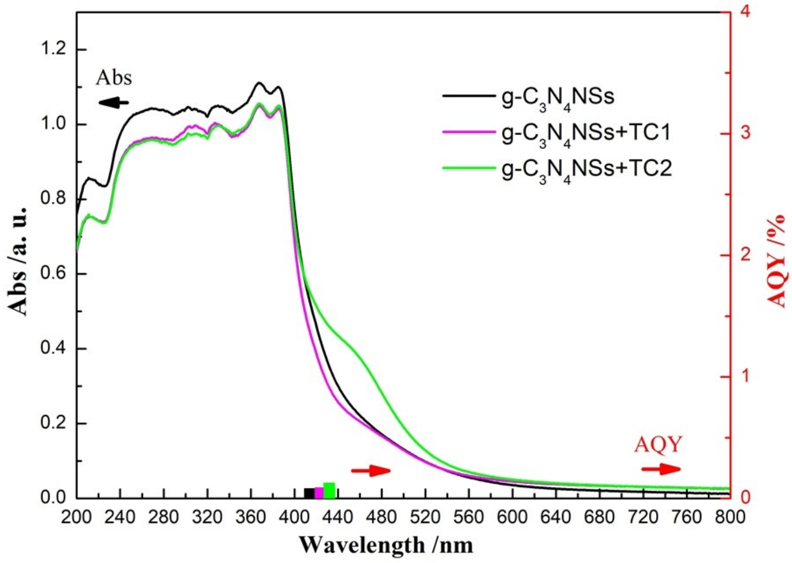


Fig. S3 Wavelength-dependent AQY and DRS spectrum of g-C_3N_4 NSs, g-C_3N_4 NSs+TC1s and g-C_3N_4 NSs+TC2 in AA under λ=420nm.

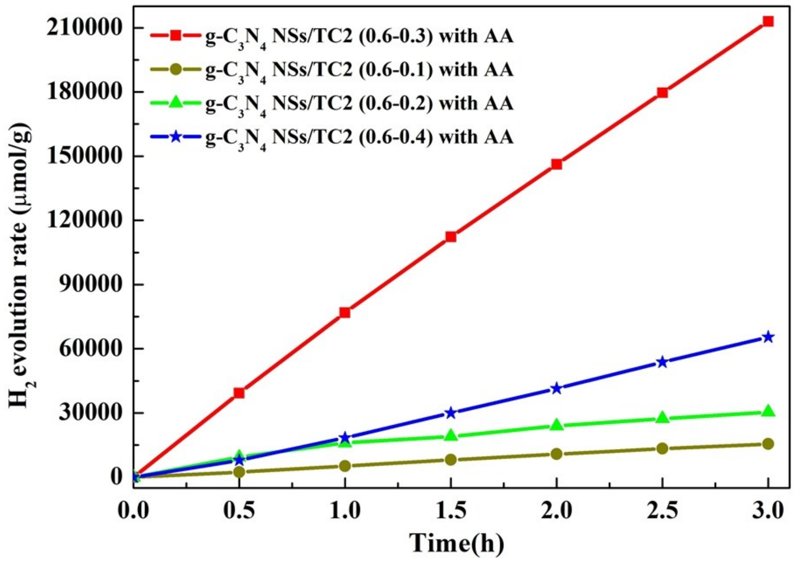


Fig. S4 Photocatalytic H_2 evolution as a function of reaction time with different mass ratio of dye TC2 and g-C_3N_4 composed g-C_3N_4 NSs/TC2 samples in AA under λ ≥400 nm.

Table S1. The corresponding hydrogen production, light intensity for the calculation of AQY and the obtained AQY value of g-C_3N_4/TC1.

Band-pass filters	Photon flux (μmol m^{-2} s^{-1})	The irradiation area S(cm^2)	The calculated photon moles (mol/s)	The H_2 volume of g-C_3N_4/TC1 for1hour(ml/h)	The calculated H_2 moles of g-C_3N_4/TC1(mol/s)	The obtained AQY value of g-C_3N_4/TC1
420 nm	108.9	23.75	2.586×10^{-7}	4.00	4.547×10^{-8}	35.16%
500 nm	153.1	23.75	3.636×10^{-7}	4.33	4.922×10^{-8}	27.07%
520 nm	198.0	23.75	4.702×10^{-7}	3.50	3.979×10^{-8}	16.92%
600 nm	239.9	23.75	5.697×10^{-7}	1.35	1.535×10^{-8}	5.39%

Table S2. The corresponding hydrogen production, light intensity for the calculation of AQY and the obtained AQY value of g-C_3N_4/TC2.

Band-pass filters	Photon flux (μmol m^{-2} s^{-1})	The irradiation area S(cm^2)	The calculated photon moles (mol/s)	The H_2 volume of g-C_3N_4/TC2 for 1 hour(ml/h)	The calculated H_2 moles of g-C_3N_4/TC2(mol/s)	The obtained AQY value of g-C_3N_4/TC2
420 nm	108.9	23.75	2.586×10^{-7}	3.12	3.547×10^{-8}	27.43%
500 nm	153.1	23.75	3.636××10^{-7}	2.10	2.387×10^{-8}	13.14%
520 nm	198.0	23.75	4.702×10^{-7}	2.00	2.274×10^{-8}	9.67%
600 nm	239.9	23.75	5.697×10^{-7}	0.26	2.956×10^{-9}	1.04%

The specific calculation process example: Apparent quantum yields (AQY) calculation for g-C_3N_4/TC1 sample

1. The calculated H_2 moles produced from g-C_3N_4/TC1: for band-pass filter λ= 420 nm

Volume of gas liberated in reaction = 4.0 ml/h = 0.0040L/h

Form std. gas equation **PV= nRT**

$n = 0.004L \times 1\ atm / 0.082\ L.atm\ mol-1\ K^{-1} \times 298\ K$

The corresponding amount of H_2 in moles = 0.000164 moles/h = 4.547×10^{-8} moles/s

2. The calculated photon moles (mol/s):for band-pass filter λ= 420 nm

Photon flux (μmol m^{-2} s^{-1})=108.9 μmol m^{-2} s^{-1}

The irradiation area S(cm^2)=23.75cm^2

The calculated photon moles (mol/s)=108.9×23.75/10000×0.000001=2.586×10^{-7} mol/s

3. The calculated AQE %:for band-pass filter λ= 420 nm

$$AQY(\%)=\frac{2\times \text{number of evolved } H_2 \text{ molecules}}{\text{number of incident photons}}\times 100$$

$$AQY(\%)=\frac{2\times 4.547\times 10^{-8}}{2.586\times 10^{-7}}\times 100$$

$$AQY(\%)=35.16\%$$

The calculation process is similar with the above calculation example and the relevant data shoud be made adaptive adjustments for other samples.

Table S3. The comparison of other dye-sensitized g-C_3N_4 for photocatalytic H_2 production.

Photocatalyst	Reaction conditions	Wavelength of incident light (λ)	H_2 production activity	AQY/%	Ref.
MgPc-mpg-C_3N_4/Pt	10vol% TEOA	λ≥640 nm	4.5μmol h^{-1} (λ≥640 nm)	0.07% (λ= 660 nm)	S1
Zn-tri-PcNc-1-g-C_3N_4/Pt co-adsorbed CDCA	5μmol g^{-1} dye, 50 mM AA	λ≥500 nm,	125.2μmol h^{-1}	1.85% at (λ= 700 nm)	S2
ZnPcNcs-Pt/g-C_3N_4	5μmol g^{-1} dye, 50 mM AA	λ≥500 nm,	263μmol h^{-1}	0.97%	S3
Zn-tri-PcNc-2-g-C_3N_4/Pt	5μmol g^{-1} dye, 50 mM AA	λ≥500 nm,	132μmol h^{-1}	1.13% (λ= 685 nm)	S4
EY-mpg-C_3N_4/Pt	15% TEOA, H2PtCl6	λ≥420 nm	115.5μmol h^{-1}	20.5%(λ=490 nm), 14.4%(λ= 520 nm), 19.4% (λ= 550 nm)	S5
ErB-Pt/g-C_3N_4 nanosheets	5% TEOA, 0.2g ErB	λ≥550 nm	162.5μmol h^{-1}	33.4% (λ= 460 nm)	S6
P3HT-g-C_3N_4	3wt% P3HT, Na_2S-Na_2SO_3	λ≥400 nm	162.5μmol h^{-1}	2.9% (λ= 420 nm)	S7
BF-g-C_3N_4/Pt	10% TEOA	λ≥420 nm	1619.0μmol g^{-1} h^{-1}	none	S8
g-C_3N_4/TC1/Pt	saturated AA solution	λ≥400 nm	73555.8 μmol·h^{-1}·g^{-1}	35.2%(λ=420 nm), 27.1%(λ= 500nm), 16.9%(λ=520 nm), 5.4%(λ= 600 nm)	This work
g-C_3N_4/TC2/Pt	saturated AA solution	λ≥400 nm	70986.8μmol·h^{-1}·g^{-1}	27.4%(λ=420 nm), 13.1%(λ= 500nm), 9.6%(λ=520 nm), 1.04%(λ= 600 nm)	This work

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