

Electronic supplementary information (ESI) of

Improved photocatalytic activity of TiO₂ nanoparticles through nitrogen and phosphorus co-doped carbon quantum dots: An experimental and theoretical study

H.J. Yashwanth^a, Sachin R. Rondiya^d, Nelson Z. Dzade^{e,f}, Robert L. Z. Hoye^d, Ram J. Choudhary^g, Deodatta M. Phase^g, Sanjay D. Dhole^h, K. Hareesh^{a,b,c,*}

^a*School of Applied Sciences (Physics), REVA University, Bengaluru 560064, India*

^b*Department of Physics, RV College of Engineering, Bengaluru 560059, India*

^c*Center of Excellence on Macro-Electronics, Interdisciplinary Research Center, RV College of Engineering, Bengaluru 560059, India*

^d*Department of Materials, Imperial College London, Exhibition Road, London SW7 2AZ, United Kingdom*

^e*School of Chemistry, Cardiff University, Cardiff, CF10 3AT, Wales, United Kingdom*

^f*Department of Energy and Mineral Engineering, Pennsylvania State University, University Park, PA 16802, United States*

^g*UGC-DAE Consortium for Scientific Research, Indore 452001, India*

^h*Department of Physics, Savitribai Phule Pune University, Pune 411007, India*

*Corresponding author: appi.2907@gmail.com (K. Hareesh)

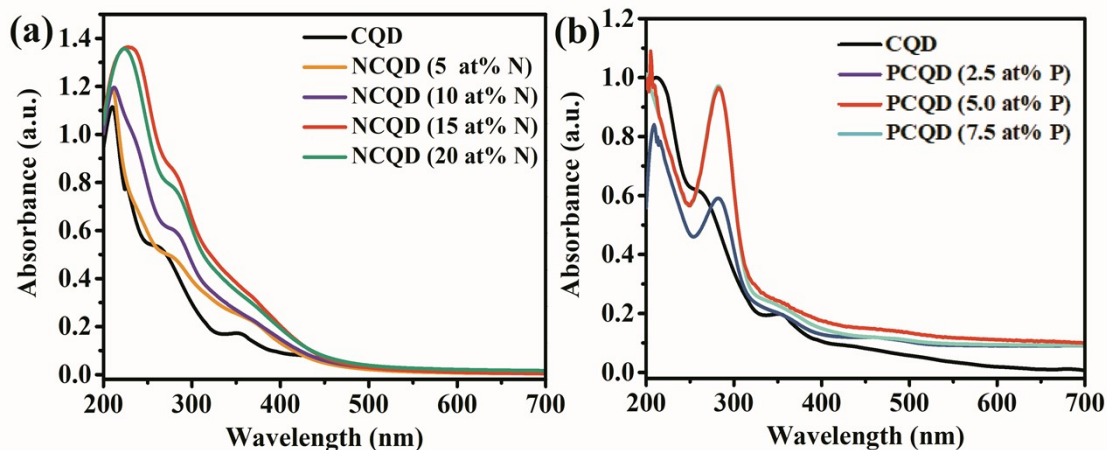


Fig. S1. UV-Visible diffuse reflectance spectra of (a) nitrogen-doped CQDs series and (b) phosphorus doped CQDs series.

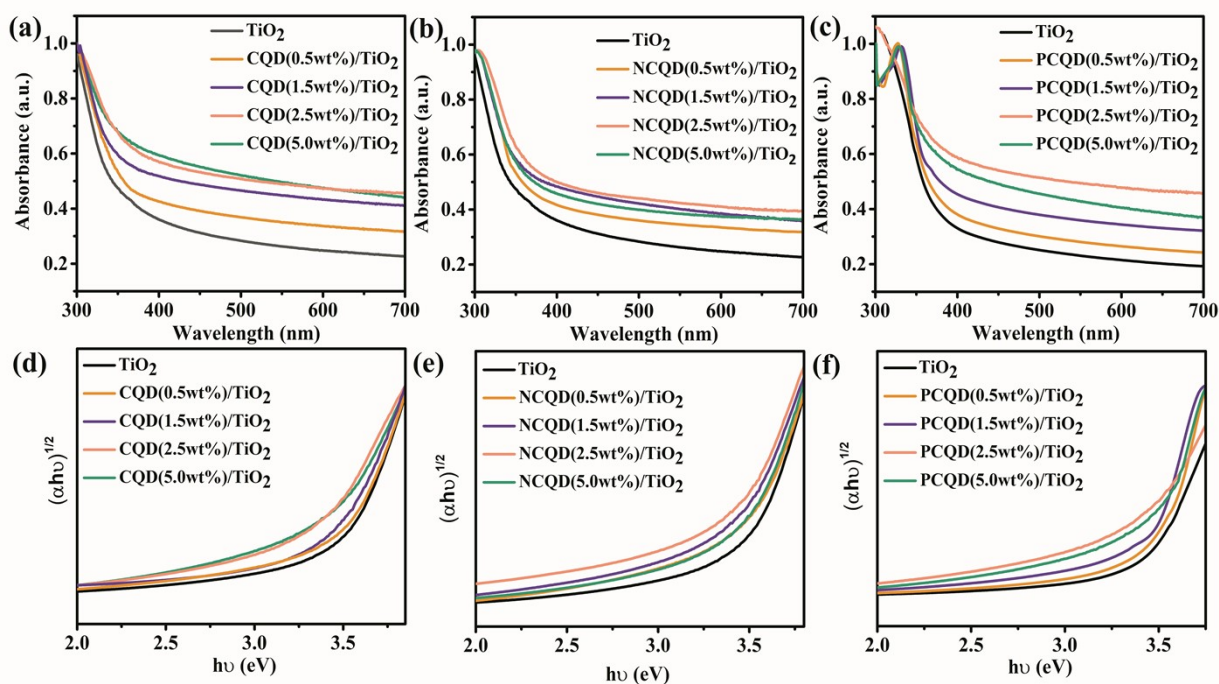


Fig. S2. UV-Visible diffuse reflectance spectra of (a) CT series, (b) NCT series, (c) PCT series, and corresponding Tauc plots of (d) CT series, (e) NCT series, (f) PCT series.

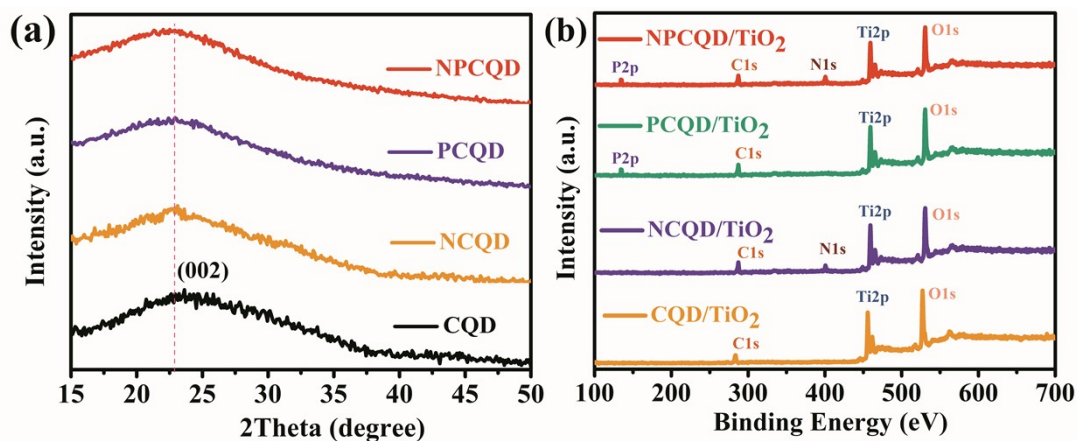


Fig. S3. (a) XRD of CQDs, NCQDs, PCQDs and NPCQDs; (b) XPS survey scan of CT, NCT, PCT and NPCT.

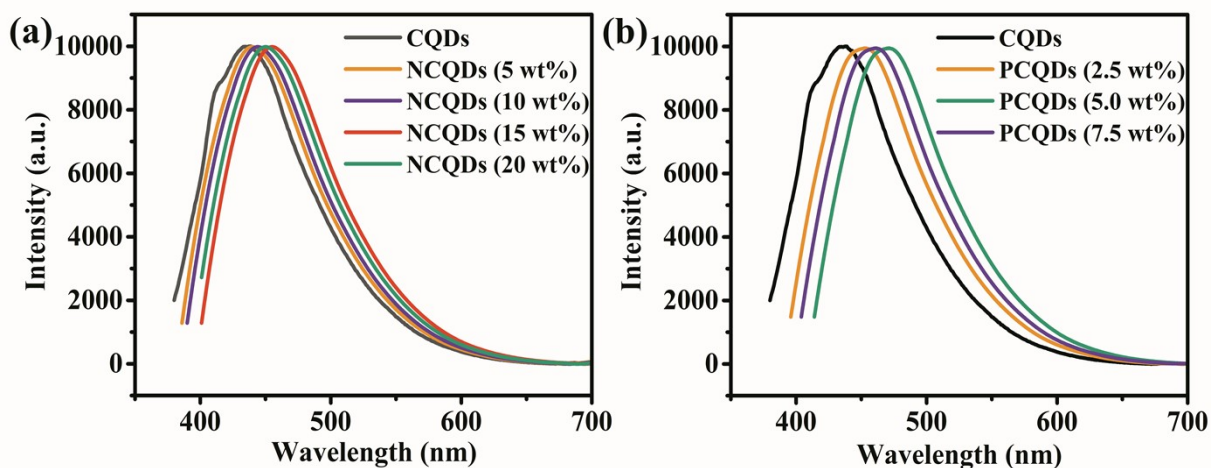


Fig. S4. Photoluminescence emission spectra of (a) nitrogen doped CQDs (b) phosphour doped CQDs at excitation wavelength of 360 nm.

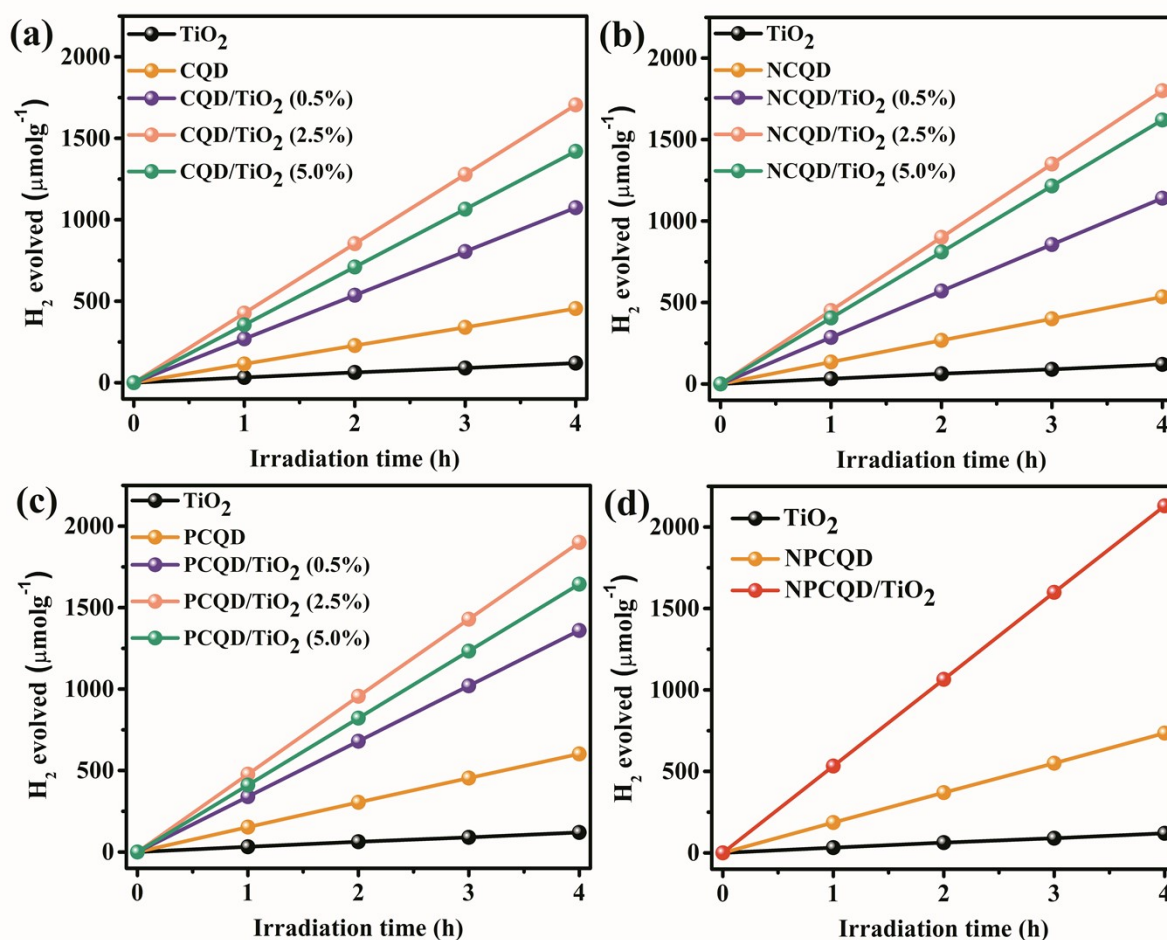


Fig. S5. Photocatalytic hydrogen production of (a) CT photocatalysts, (b) NCT photocatalysts, (c) PCT photocatalysts and (d) NPCT photocatalyst.

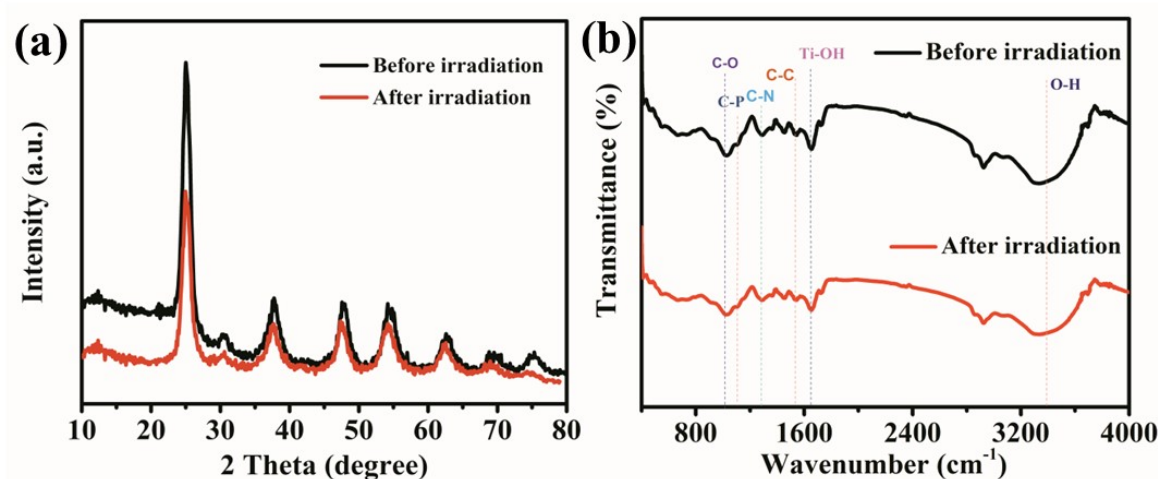


Fig. S6. (a) XRD and (b) FTIR spectra of NPCT photocatalyst before and after photocatalytic activity.

Table

Table TS1. Comparison of photocatalytic hydrogen produced by carbon quantum dots and TiO₂ based photocatalysts.

SI No	Method	catalysts	Hydrogen produced	reference
1	Hydrothermal method	CQD/TiO ₂ nanosheets	7.9 μmol/h	R1
2	Hydrothermal method	CQD/TiO ₂	472 μmol g ⁻¹ h ⁻¹	R2
3	Hydrothermal method	NCQD/TiO ₂ nanotube	30.12 μmol cm ⁻² h ⁻¹	R3
4	Hydrothermal method	CQD/P25	8.3 μmol/h	R4
5	Thermolysis	CQDs/Pt@TiO ₂	3323 μmol g ⁻¹ h ⁻¹	R5
6	Hydrothermal method	NCQD/P25	58.6 nmol h ⁻¹	R6
7	Hydrothermal method	CQD/P25	2.43 mmol g ⁻¹ h ⁻¹	R7
8	Hydrothermal method	NPCQD/TiO ₂ nanoparticles	533 μmolh ⁻¹ g ⁻¹	This work
9	Hydrothermal method	PCQD/TiO ₂ nanoparticles	478 μmolh ⁻¹ g ⁻¹	This work
10	Hydrothermal method	NCQD/TiO ₂ nanoparticles	451 μmolh ⁻¹ g ⁻¹	This work
11	Hydrothermal method	CQD/TiO ₂ nanoparticles	427 μmolh ⁻¹ g ⁻¹	This work

References:

[R] Y. Sui, L. Wu, S. Zhong, Q. Liu, Carbon quantum dots/TiO₂ nanosheets with dominant (001) facets for enhanced photocatalytic hydrogen evolution. *Appl. Surf. Sci.* 480 (2019) 810-816.

- [R2] I. Sargin, G. Yanalak, G. Arslan, I.H. Patir, Green synthesized carbon quantum dots as TiO₂ sensitizers for photocatalytic hydrogen evolution. *Inter. J. Hydro. Ener.* 44 (2019) 21781-21789.
- [R3] Q. Wang, J. Cai, G.V. Biesold-McGee, J. Huang, N.Y. Hau, S. Hongtao, J. Wang, Y. Lai, Z. Lin, Silk fibroin-derived nitrogen-doped carbon quantum dots anchored on TiO₂ nanotube arrays for heterogeneous photocatalytic degradation and water splitting, *Nano Energy*, 78 (2020) 105313.
- [R4] H. Yu, Y.F. Zhao, C. Zhou, L. Shang, Y. Peng, Y.H. Cao, L.Z. Wu, C.H. Tunga, T. Zhang, Carbon quantum dots/TiO₂ composites for efficient photocatalytic hydrogen evolution, *J. Mater. Chem. A* 2 (2014) 3344.
- [R5] Y. Zhou, S. Yang, D. Fan, J. Reilly, H. Zhang, W. Yao, J. Huang, Carbon quantum dot/TiO₂ nano hybrids: Efficient photocatalysts for hydrogen generation via intimate contact and efficient charge separation, *ACS Appl. Nano Mater.* 2 (2019) 1027-1032.
- [R6] R. Shi, Z. Li, H. Yu, L. Shang, C. Zhou, G.I.N. Waterhouse, T. Zhang, Effect of nitrogen doping level on the performance of N-doped carbon quantum dot/TiO₂ composites for photocatalytic hydrogen evolution, *ChemSusChem*, 10 (2017), 4650-4656.
- [R7] H. Zhao, X. Yu, C.F. Li, W. Yu, A. Wang, Z.Y. Hu, S. Larter, Y.L.M.G. Kibria, H. Jinguang, Carbon quantum dots modified TiO₂ composites for hydrogen production and selective glucose photo reforming, *J. Ener. Chem.* 64 (2022) 201-208.