

Supplementary Information

Efficient Photocatalytic and Photovoltaic Applications with Nanocomposites between CdTe QDs and NTU-9 MOF

Rajnish Kaur^{1,2}, Aniket Rana³, Rajiv K Singh³, Varun A Chhabra⁴, Ki-Hyun Kim^{5}, Akash Deep^{1,2*}*

¹Central Scientific Instruments Organisation (CSIR-CSIO), Sector 30 C, Chandigarh, 160030, India; ²Academy of Scientific and Innovative Research (AcSIR-CSIO), Sector 30 C, Chandigarh, 160030, India; ³CSIR- National Physical Laboratory, Dr. K.S Krishnan Marg, New Delhi, 110012, India; ⁴Centre for Development of Advanced Computing, Phase VIII, Mohali 160071, India; ⁵Department of Civil and Environmental Engineering, Hanyang University, 222 Wangsimni-Ro, Seoul 04763, Korea

Correspondence: *^{1,2}dr.akashdeep@csio.res.in, Tel: +91-172-2672236; Fax: +91-172-2657287; *³kkim61@hanyang.ac.kr, Tel.: +1-82-2-2220-2325; Fax: +82-2-2220-1945

Table S1. BET surface area properties of various materials used in the study

Material	Surface area (m ² /g)	Pore volume (cm ³ /g)
NTU-9	1205	0.58
CdTe QDs	214	0.18
CdTe/NTU-9	880	0.54

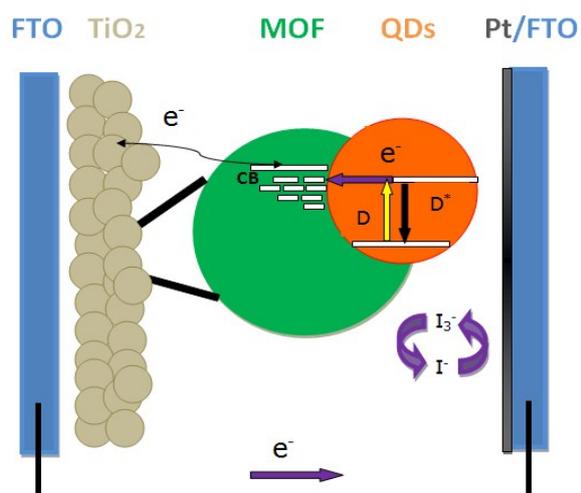


Figure S1. A representative schematic of the proposed CdTe/NTU-9-based solar DSSC.

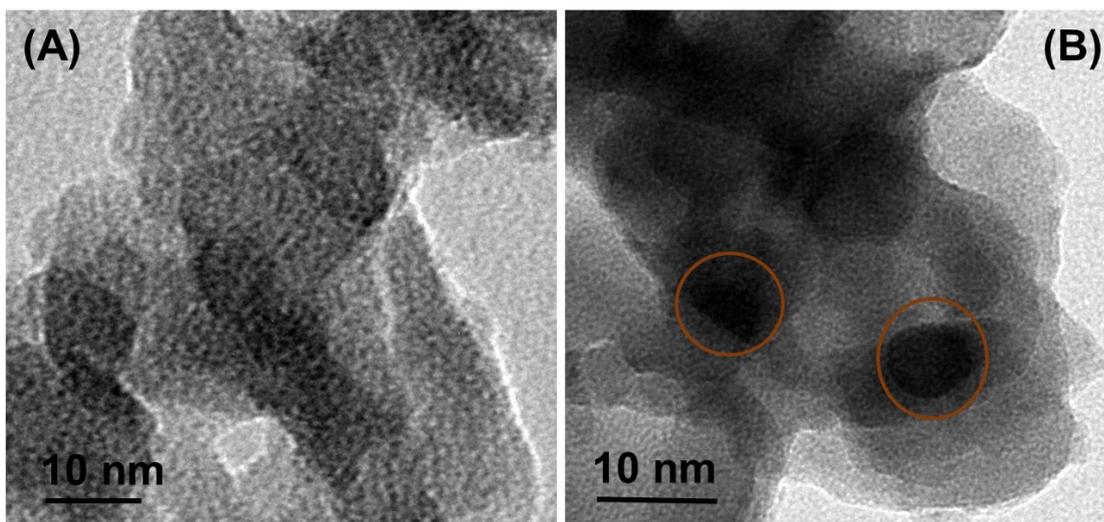


Figure S2. HR-TEM images of (A). NTU-9 MOF and (B). CdTe/NTU-9 composite

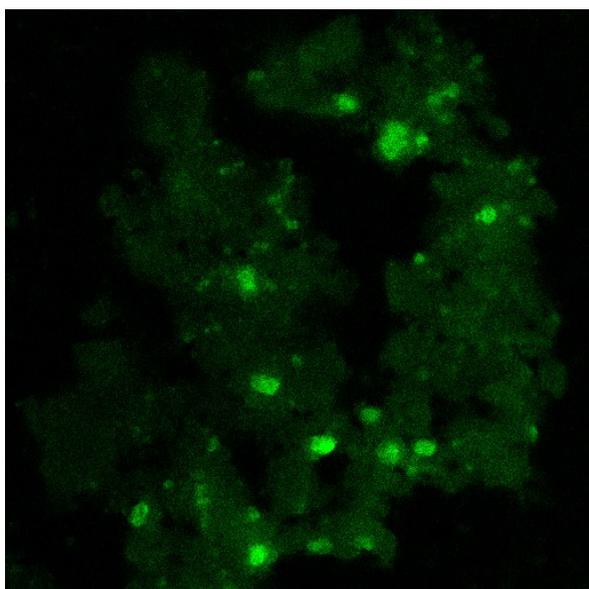


Figure S3: Confocal laser scanning image of CdTe/NTU-9 with distinct fluorescence signals from the embedded QDs.

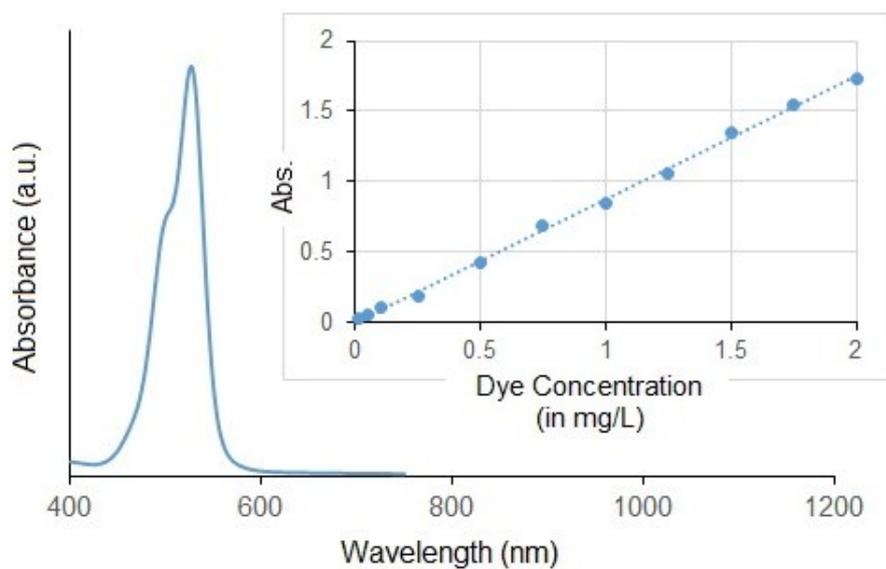


Figure S4. UV-vis spectrum of Rh 6G and its calibration curve.

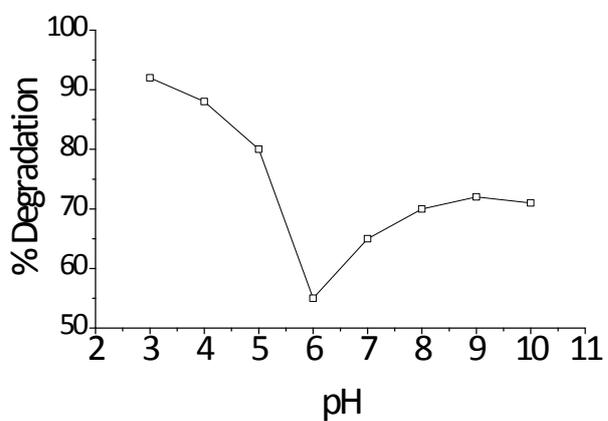


Figure S5. Photodegradation of 5 mg/L Rh 6G under varying conditions of pH; concentration of photocatalyst = 5 mg/L, reaction time = 30 min, and excitation wavelength = 500 nm.

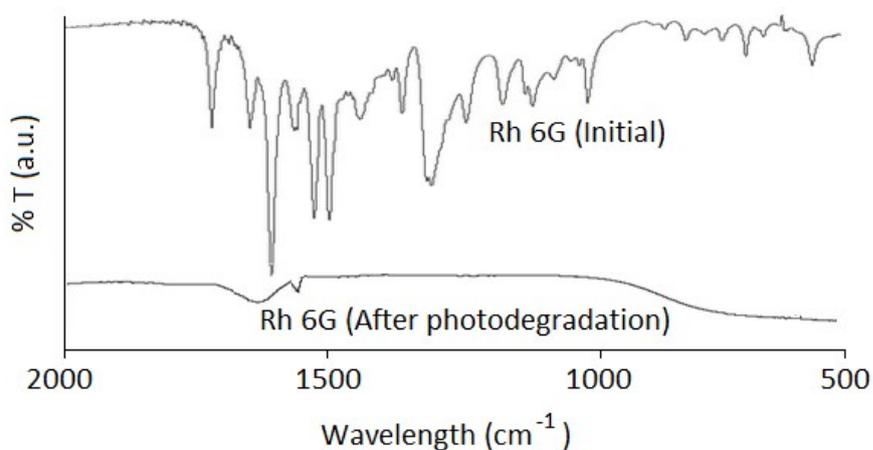


Figure S6. FTIR spectra of Rh 6G dye: comparison between before and after photodegradation.

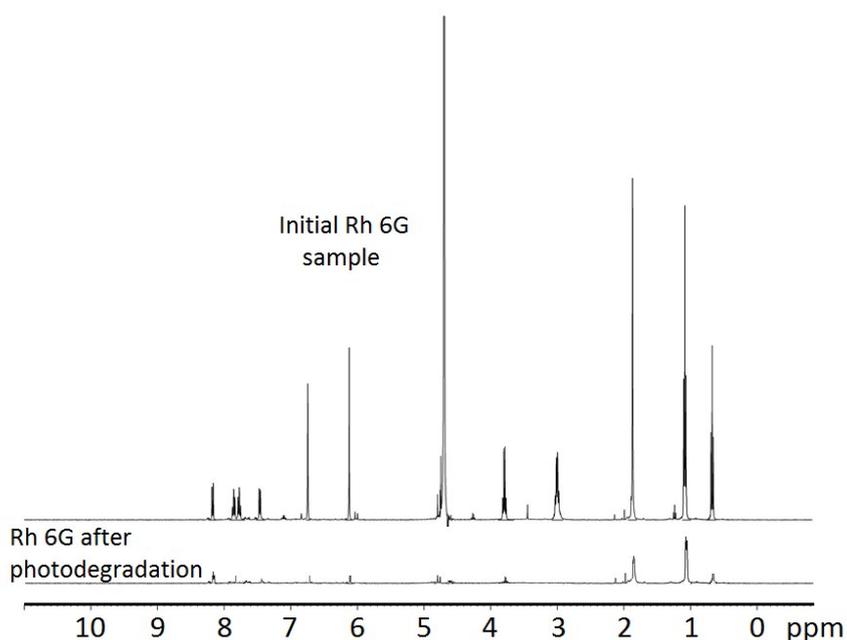


Figure S7. NMR of Rh 6G dye: comparison between before and after photodegradation. (Procedure: A 1 L solution of 1 mg/L Rh 6G mixed with 5 mg/mL of CdTe/NTU-9 was irradiated under solar light for 30 minutes. The contents were then centrifuged at 10,000 rpm. The remaining solvent was further evacuated using a rotary evaporator. The remaining residue was dissolved in 1 mL of D₂O for analysis.)

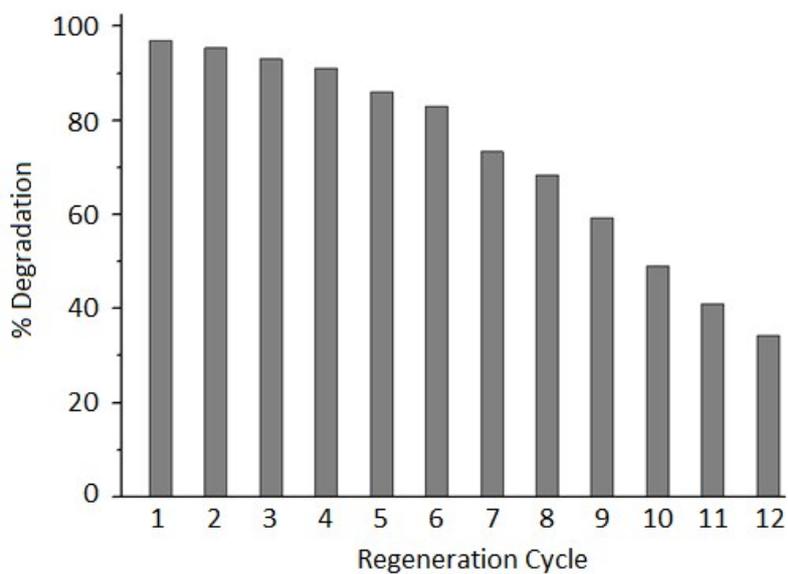


Figure S8. Photodegradation of 1 mg/L Rh 6G with 5 mg/mL CdTe/NTU-9 photocatalyst during successive regeneration cycles (reaction time = 30 min and excitation wavelength = 500 nm).

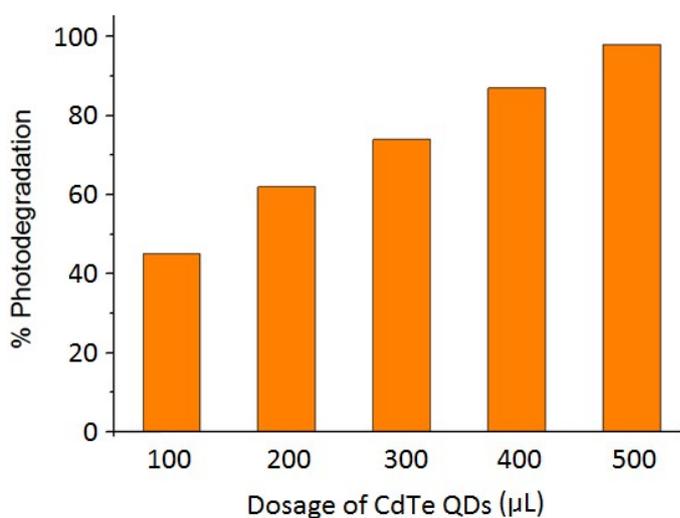


Figure S9. Photodegradation of 1 mg/L Rh 6G with varying contents of CdTe in CdTe/NTU-9 composites (duration of the photodegradation experiment = 30 min and excitation wavelength = 500 nm).

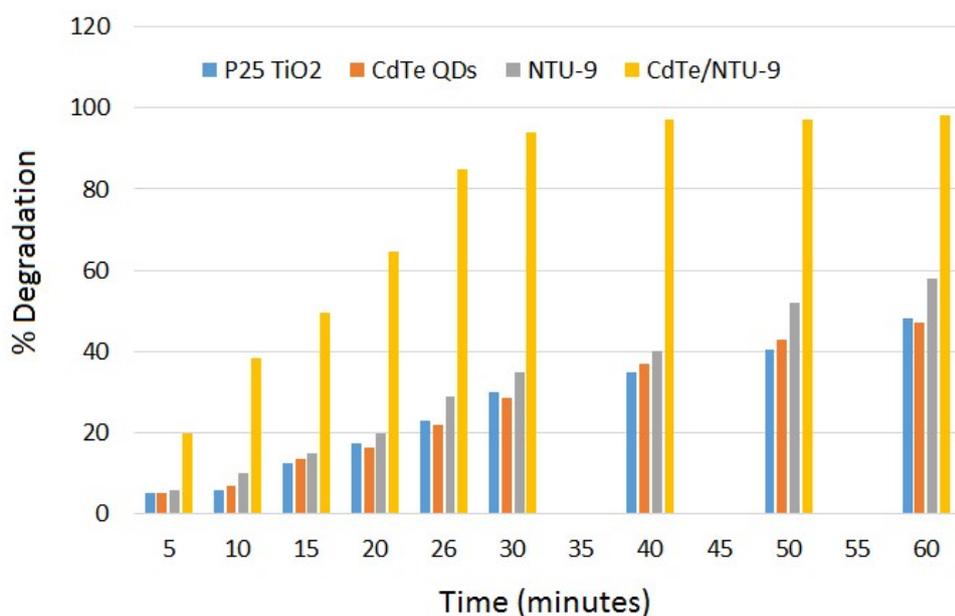


Figure S10. Photodegradation of 1 mg/L Rh 6G with CdTe/NTU-9, CdTe QDs, NTU-9, and P-25 TiO₂ (concentration of photocatalyst = 5 mg/L and excitation wavelength = 500 nm).

Table S2. Comparison of different photocatalyst systems for Rhodamine 6G

S. No.	Photocatalyst composition	Degradation time	Reference
1.	Cu-FeZSM-5 zeolite catalyst	45 minutes	1
2.	Iron(III)-based metal-organic frameworks	60 minutes	2
3.	Graphene-metal oxide composite	200 minutes	4
4.	Molybdophosphate-based Fe-MOF	120 minutes	3
5.	ZnO@Graphene composite	120 minutes	5
6.	p-BiOI@n-ZnTiO ₃ heterojunction	150 minutes	6
7.	CdTe@Eu-MOF	60 minutes	7

References:

1. W. Zhu, X.-Y. Yang, Y.-H. Li, J.-P. Li, D. Wu., Y. Gao and F.-Y. Yi, *Inorg. Chem. Commun.*, 2015, **49**, 159-162.
2. B. Li and H. Cao, *J. Mater. Chem.*, 2011, **21**, 3346-3349.
3. J. Zhang, Z. Xiong and X.S. Zhao, *J. Mater. Chem.*, 2011, **21**, 3634-3640.
4. K.G.M. Laurier, F. Vermoortele, R. Ameloot, D.E. De Vos, J. Hofkens and M.B.J. Roefsaers, *J. Am. Chem. Soc.*, 2013, **135**, 14488-14491.
5. R.V. Prihod'ko and N.M. Soboleva, *J. Chem.*, 2013, **2013**, 8.
6. K.H. Reddy, S. Martha and K.M. Parida, *Inorg. Chem.*, 2013, **52**, 6390-6401
7. R. Kaur, K. Vellingiri, K.-H. Kim, A.K. Paul and A. Deep, *Chemosphere*, 2016, **154**, 620-627.