Electronic Supplementary Material (ESI) for New Journal of Chemistry. This journal is © The Royal Society of Chemistry and the Centre National de la Recherche Scientifique 2022

Supplementary information

Donor-acceptor organic nanostructure based on conjugated polymer for improving visible

light driven photocatalytic activity towards degradation of dye in aqueous medium

Ravi Prakash Behere¹, Raj Laxmi¹, Neelam Gupta¹, Uttam Sharma², Santanu Das², Biplab Kumar

Kuila*

¹Department of Chemistry, Institute of Science, Banaras Hindu University, Varanasi Uttar Pradesh

221005, INDIA, Email: <u>bkkuila.chem@bhu.ac.in</u>

²Department of Ceramic Engineering, Indian Institute of Technology (Banaras Hindu University),

Varanasi Uttar Pradesh 221005, INDIA



Figure S1 Zeta potential plot of P3HT NS, PCBA and P3HT-PCBA NS



Figure S2 AFM image of (a) P3HT NS (b) P3HT-PCBA NS



Figure S3 Survey X-ray photoelectron spectroscopy (XPS) spectrum of P3HT-NS (a) and P3HT-PCBA NS (c). C1s spectra P3HT NS (b) and P3HT-PCBA NS (d)



Figure S4 UV-vis absorption spectra of P3HT solution in THF.



Figure S5 PL spectra of PCBA solution, excitation wavelength 320 nm.



Figure S6 Time resolved emission decay curve fitting (a) P3HT NS (b) P3HT-PCBA NS with1:1



weight ratio of P3HT and PCBA.

Figure S7 Cyclic voltammetry of (a) P3HT (b) PCBA (c) P3HT-PCBA hybrid material. The CV curves were recorded by depositing films of the material on glassy carbon electrodes. Platinum was used as the counter electrode, silver-silver chloride as a reference electrode, and 0.1 (M) tetrabutylammonium hexafluorophosphate (Bu_4NPF_6) in acetonitrile as the supporting electrolyte.



Figure S8 optical band gap determination of (a) P3HT NS (b) PCBA (c) P3HT-PCBA NS



Figure S9 UV-vis spectra of MB solution after irradiation with light for different time. No external catalyst was added



Wavelength (nm)

Figure S 10 UV-vis spectra of MB solution after irradiation with light for different time using P3HT NS as photocatalyst.

Table S1. Comparison of Photocatalytic activity of conjugated polymer or conjugated polymer

 composite material for degradation of dye under light irradiation.

Catalyst (amount)	Dye (concentration)	Light used	Efficiency	Time	Rate constant	Whether used as dip photo catalysis or not	Refer ence
Nanostructures (0.062 mg)	blue (0.064 mg)	Xe lamp of a solar simulator)	90.0%	180 min	(min ⁻¹)	NO	51
9,9'- bifluorenylidene- based conjugated microporous/mesopo rous polymers (10 mg)	Rhodamine B (3.75 mg)	Vis [xenon lamp light source (300 W)]	92%	90 min	NA	No	S2
poly(1,3,4- oxadiazole)s	Methylene blue	UV	~100%	180 min	NA	No	S3
P3HT Colloids	Methylene blue	UV	96.6 %	>72 hours	NA	NO	S4
Poly(3- hexylthiophene) Nanostructures	Phenol	UV & Vis	87% (UV light) 16% (Vis light)	240 min	NA	By depositing polymer on quartz glass up to 4 cycles	S5
poly(diphenylbutadi yne) nanostructures	Methyl orange	Vis light	75%	240 min	NA	No	S6
P3HT-TiO ₂	Methyl orange	Vis light	88.5%	10 hours	NA	NO	S7

PEDOT nanostructures	Phenol Methyl orange	Vis	100% (phenol) 100 %(MO)	240 min 180 min	NA	No	S8
P3HT-ZnO composite	Rhodamine B (RhB)	Vis	100%	80 min	0.03127 min ⁻¹	No	S9
P3HT-PCBM (5 mg)	Rhodamine B (RhB) (2ppm)	Vis [186 w/m ² or Mercury xenon lamp (200W)]	95.1%	120 min	0.0219	Yes (by depositing thin film on glass slide), up to 3 cycles	S10
Perylene diimide based porous conjugated polymer	Methylene blue	UV light(150 W Xe light-source)	≈75 %	200 min	N A	NO	S11
triazine-based covalent organic polymer (20 mg)	Methyl orange, Methylene blue & RhB	Visible light(LED (10 W) or natural light irradiation)	67% MO, 78% RhB and 57% MB degradatio n under visible light in presence of f 30% H ₂ O ₂	MO (12 hours) RhB(150 min) MB (100 min)	MO(0.00151 min ⁻¹) RhB(0.00871 min ⁻¹) MB(0.00610 min ⁻¹) at 30 °C	NO	S12
P3HT-phenyl C-61 butyric Acid hybrid nanostructure (0.5 mg)	Methylene blue (0.256 mg)	20 Watt white LED bulb	87.5%	270 min	7.82 X10 ⁻³ min ⁻¹	Yes, flexible dip catalytic membrane up to 4 th cycle	This work

Photocatalyst	Scavenger	Trapped species	Degradation
			(%)
	No scavenger	/	82.5%
P3HT-PCBA NS	benzoquinone (BQ)	$\cdot O_2^-$	80%
	isopropanol (IPA)	·OH	81%
	Triethanolamine (TEOA)	h^+	75%
	AgNO ₃	e	37%

 Table S2 Effects of different scavengers on the photocatalytic efficiency of phenol degradation.

References

- S1 B. Jana, S. Bhattacharyya and A. Patra, *Phys. Chem. Chem. Phys.*, 2015, 17, 15392–15399.
- S2 B. Wang, Z. Xie, Y. Li, Z. Yang and L. Chen, *Macromolecules*, 2018, **51**, 3443–3449.
- S3 X. Ran, L. Duan, X. Chen and X. Yang, J. Mater. Sci., 2018, 53, 7048–7059.

- S4 E. González-Juárez, E. García-Hernández, C. D. Arrieta-González, R. Salgado-Delgado,
 M. Güizado-Rodríguez, V. Barba and A. Espinosa-Roa, *Polym. Bull.*, 2021, 78, 6455–6472.
- D. Floresyona, F. Goubard, P.-H. Aubert, I. Lampre, J. Mathurin, A. Dazzi, S. Ghosh, P. Beaunier, F. Brisset, S. Remita, L. Ramos and H. Remita, *Appl. Catal. B Environ.*, 2017, 209, 23–32.
- S. Ghosh, N. A. Kouamé, L. Ramos, S. Remita, A. Dazzi, A. Deniset-Besseau, P.
 Beaunier, F. Goubard, P.-H. Aubert and H. Remita, *Nat. Mater.*, 2015, 14, 505–511.
- S7 D. Wang, J. Zhang, Q. Luo, X. Li, Y. Duan and J. An, *J. Hazard. Mater.*, 2009, 169, 546–550.
- S. Ghosh, N. A. Kouame, S. Remita, L. Ramos, F. Goubard, P.-H. Aubert, A. Dazzi, A. Deniset-Besseau and H. Remita, *Sci. Rep.*, 2015, 5, 18002.
- S9 H. Liu, M. Li, J. Yang, C. Hu, J. Shang and H. Zhai, *Mater. Res. Bull.*, 2018, 106, 19–27.
- S10 P. Ramar, B. V Aishwarya and D. Samanta, Chem. Commun., 2021, 57, 12964–12967.
- S11 L. Li and Z. Cai, *Polym. Chem.*, 2016, 7, 4937–4943.
- S12 N. Xu, R.-L. Wang, D.-P. Li, X. Meng, J.-L. Mu, Z.-Y. Zhou and Z.-M. Su, *Dalt. Trans.*, 2018, 47, 4191–4197.