Supplementary Information

Self-Assembly and Boosted Photodegradation Properties of Perylene Diimide via Different Solvent

Ruizhe Yang[a], Jinyuan Liu[a], Bin Wang[a], Rong Wang[a], Yanhua Song[b], Yingjie Hua[c], Chongtai Wang[c], Yuanbin She[d], Junjie Yuan[a], Hui Xu[a,*], Huaming Li [a,*]

[a] *School of Chemistry and Chemical Engineering, Institute for Energy Research, Jiangsu University, Zhenjiang 212013, Jiangsu, China*

[b]*School of Environmental and Chemical Engineering, Jiangsu University of Science and Technology, Zhenjiang, Jiangsu, 212003, PR China*

[c]*School of Chemistry and Chemical Engineering, Key Laboratory of Electrochemical Energy Storage and Energy Conversion of Hainan Province, HainanNormal University, Haikou 571158, Hainan, China*

[d]*State Key Laboratory Breeding Base of Green Chemistry-Synthesis Technology, College of Chemical Engineering, Zhejiang University of Technology, Hangzhou 310014, Zhejiang, China*

1. Characterization of as-prepared samples

The crystalline structures of the self-assembled PDI were analyzed via X-ray diffraction (XRD) on a Shimadzu XRD-6000 with Cu Ka radiation in the range of 2θ from 10 ° to 80 °. The morphology of the products was observed by a scanning electron microscope (SEM, Hitachi S-3500 N). The chemical environment of as-prepared photocatalysts was analyzed by X-ray photoelectron spectroscopy (XPS) using VG MultiLab 2000 system with a monochromatic Mg-Kα source operated at 20 kV. The Diffuse reflection spectra (DRS) of the samples were acquired on Shimadzu UV-2450 spectrophotometer in the range of 200-800 nm, and BaSO4. was used as a reference. Fourier transform infrared (FT-IR) spectra were recorded on a Nicolet Nexus 470 spectroscopy. The Brunauer-Emmett-Teller (BET) specific surface area of the samples was evaluated in the relative pressure range of 0.1-0.9. by N_2 adsorption/desorption using TriStar II 3020. The photoluminescence (PL) spectra of the samples were obtained via on QuantaMaster&TimeMaster Spectrofluorometer at room temperature. The photocurrents and electrochemical impedance spectroscopy (EIS) were measured on a CHI660B electrochemical system. Electron spin resonance (ESR) spectra were conducted on a Bruker model ESR JES-FA200 spectrometer.

2. Photocatalytic activity measurements

The photocatalytic activities of a series of self-assembled PDI were investigated by the photodegradation of 10 mg/L bisphenol A (BPA) and 10 mg/L Rhodamine B (RhB) as target pollutants. Typically, 10 mg and 50 mg self-assembled PDI photocatalysts were respectively added to the Pyrex photocatalytic reactors for the photodegradation of 50 mL RhB and 50 mL BPA. A visible light source was obtained by a 250 W Xe arc lamp with an appropriate UV cutoff filter (λ> 400 nm). The temperature was maintained at 30 °C using a flow cooling water system to avoid thermal catalysis. Before the light irradiation, the suspension of target pollutants and photocatalysts was magnetically stirred for 30 min in the dark to reach adsorption-desorption equilibrium. At certain time intervals, 3 mL solution was sampled and centrifuged to remove the particulates for the following analysis. The concentrations of the probe pollutants were measured by a UV–vis spectrophotometer at maximum

absorption wavelength (553 nm for RhB) and high-performance liquid chromatography (HPLC, Agilent, 1260 Infinity) with a C18 column (250 mm×4.6 mm, 5 μm particle sizes). Millennim 32 software was employed to acquire and process chromatographic data. The mobile phase was a mixture of methanol/water (75:25, volume ratio), and the flow rate was 1.0 mL/min.

3. Results and figures

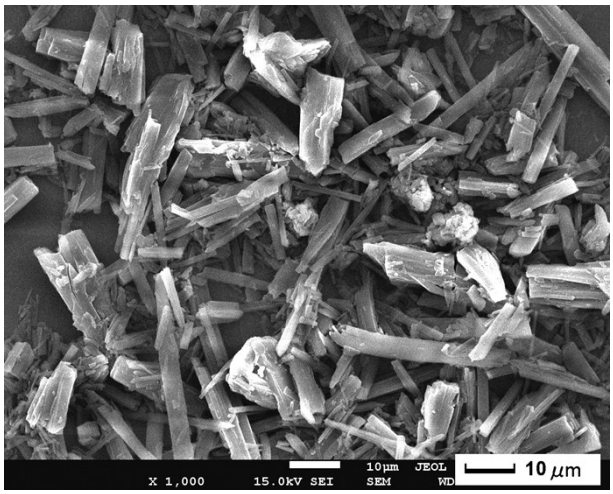

Fig. S1. SEM images of PDI (deionized water).

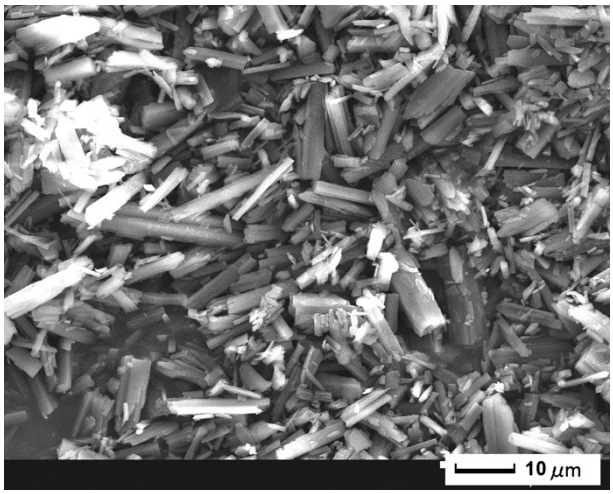

Fig. S2. SEM images of PDI (ethanol).

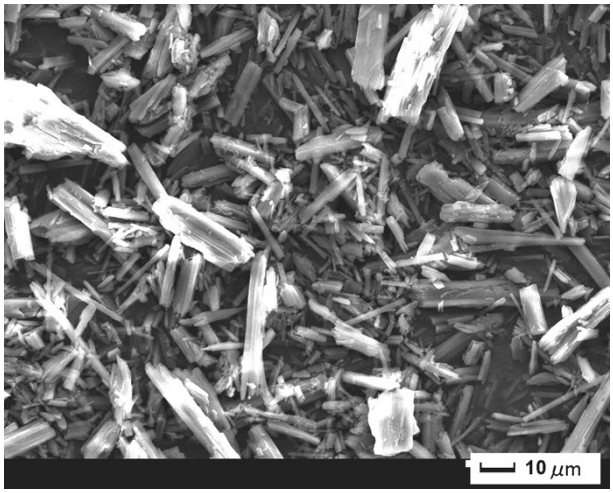

Fig. S3. SEM images of PDI (methanol).

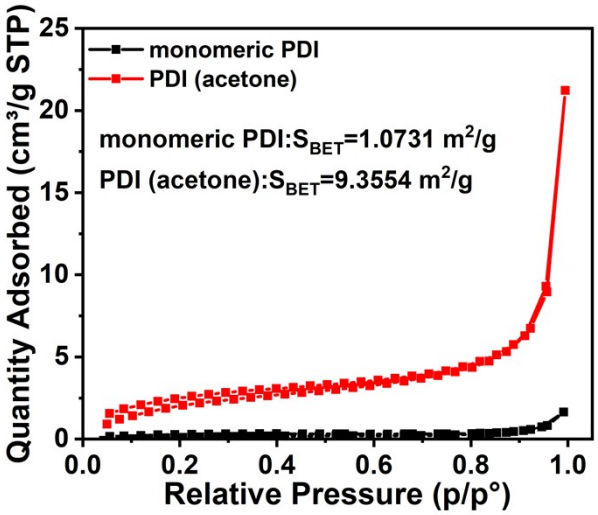

Fig. S4. N_2 adsorption and desorption isotherms of monomeric PDI and PDI (acetone).

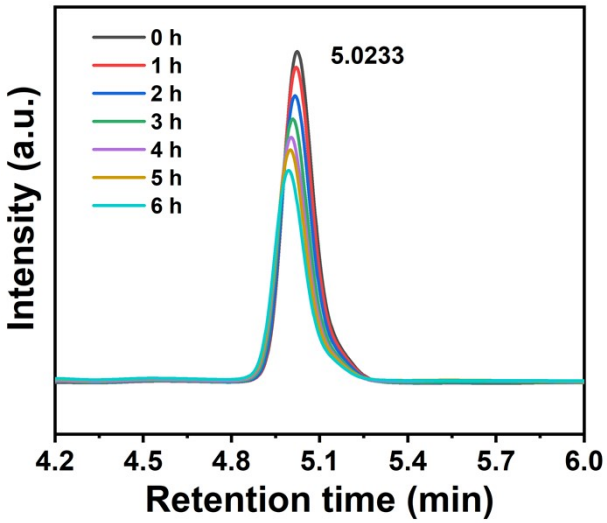

Fig. S5. HPLC spectrums of BPA solution degraded by monomeric PDI.

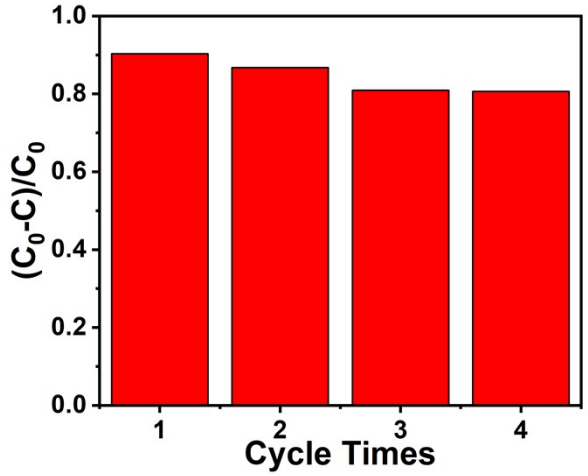

Fig. S6. The cycle experiment for the photodegradation of BPA under visible light of PDI (acetone).

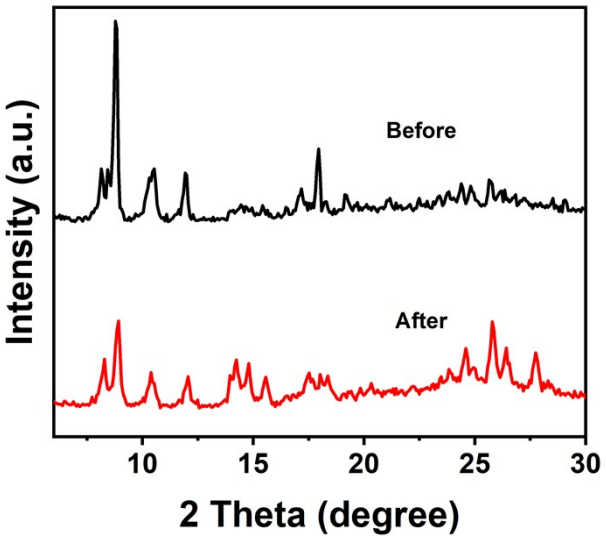

Fig. S7. XRD patterns of PDI (acetone) material before and after the recycle experiment.

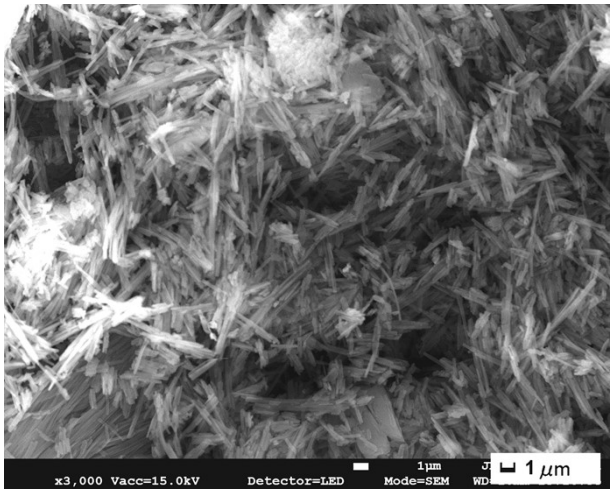

Fig. S8. The SEM image of the PDI (acetone) sample after cycling.

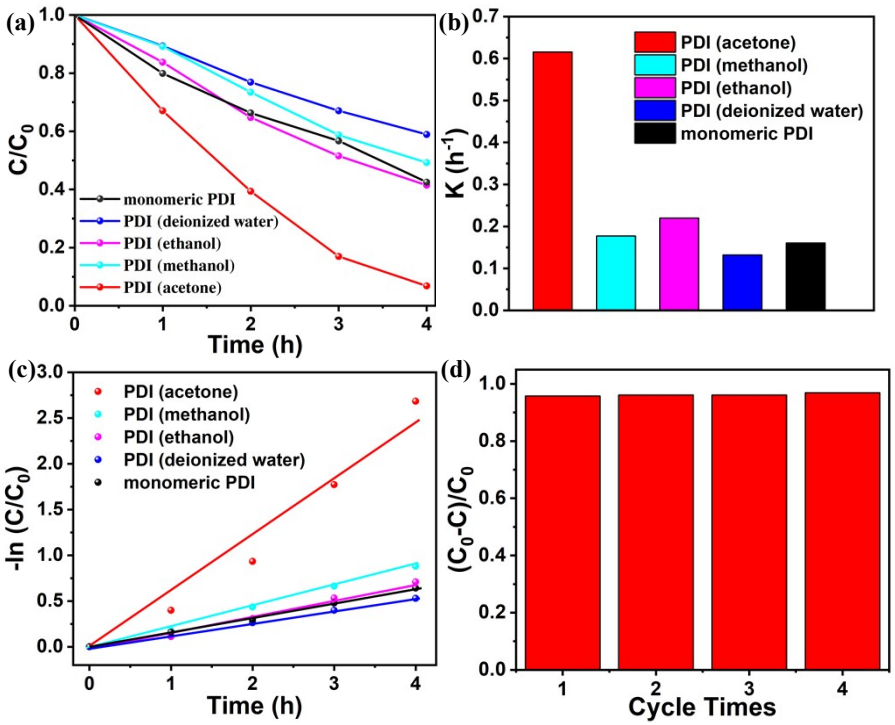

Fig. S9. (a) Photocatalytic degradation of RhB over different samples, (b) apparent rate constants of the prepared samples for RhB degradation, (c) the kinetic fit for degradation of RhB, (d) The cycle experiment for the photodegradation of RhB under visible light of PDI (acetone).

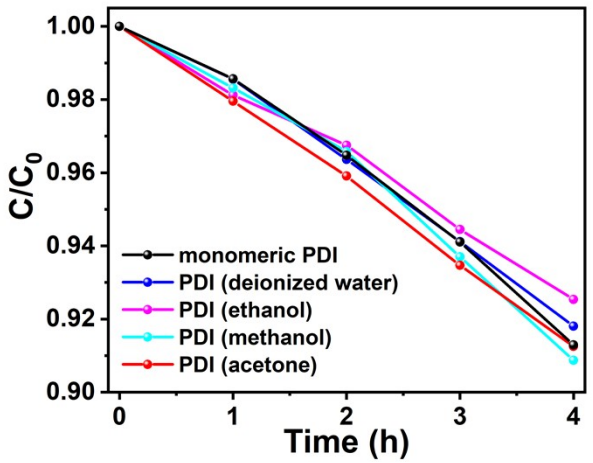

Fig. S10. The adsorption efficiencies of as-prepared samples for degradation RhB.

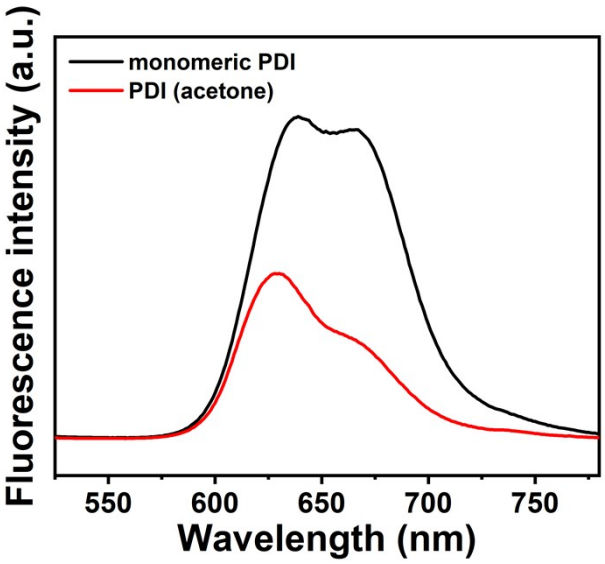

Fig. S11. PL emission spectra of monomeric PDI and PDI (acetone) under photoexcitation at 500 nm.

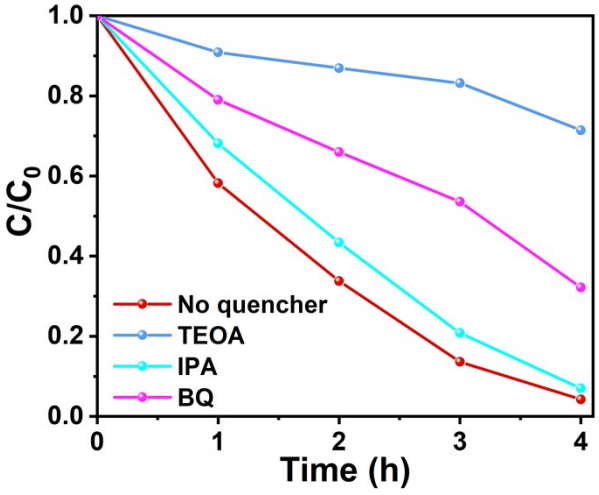

Fig. S12. Trapping experiment of active species during the photocatalytic degradation of RhB over PDI (acetone) material under visible light irradiation.

Table S1. Comparison of the photocatalytic degradation activity for BPA of some reported system using traditional catalyst.

Catalysts	Light Source	Reaction Condition	Removal Efficiency	Reference
PDI (acetone)	250 W Xe lamp, $\lambda > 400$ nm	50 mg catalysts; 50 mL10 mg/L BPA	Remove 95 % in 6 h	This work
N-doped TiO_2	LED Flood Light; 30 W)	0.5 g catalysts; 6 ppm 500 mL BPA	Remove 91.3 % in 6 h	S1
Vc-C_3N_4	350 W Xe lamp, $\lambda > 420$ nm	30 mg catalysts; 100 mL 10 mg/L BPA	Remove 90.0% in 7 h	S2
In_2O_3/ OGCN	57 mW/cm^2 Xe, $\lambda > 420$ nm	50 mg catalysts; 50 mL BPA	Remove 91.0% in 3 h	S3
TiO_2@MIL-101(Cr)	125-W mercury lamp	40 mg catalysts; 80 mL 50mg/L BPA	Remove 92.4% in 4 h	S4
GO@B–TiO_2	300 W Xe lamp	40 mg catalysts; 40 mL 10mg/L BPA	Remove 47.8% in 6 h	S5
CeO_2/BP	300 W Xe lamp	50 mg catalysts; 100 mL 50mg/L BPA	Remove 82.3% in 3 h	S6
Bi microspheres	500 W I lamp 380-830 nm	10 mg catalysts; 100 mL 10mg/L BPA	Remove 47.4% in 3 h	S7
α-Fe_2O_3	300 W Xe lamp	50 mg catalysts; 50 mL 30mg/L BPA	Remove 91% in 6 h	S8
$BiVO_4$/GR/ Bi_2O_3	150 W metal halide lamp	100 mg catalysts; 100 mL 10mg/L BPA	Remove nearly 100% in 8 h	S9
g-C_3N_4 nanotubes	300 W Xe lamp, $\lambda > 400$ nm	20 mg catalysts; 100 mL 10mg/L BPA	Remove 90% in 5 h	S10

Reference:

1. R. Kamaludin, M. H. D. Othman, S. H. S. A. Kadir, A. F. Ismail, M. A. Rahman and J. Jaafar, *Water, Air, Soil Pollut.*, 2018, **229**, 363.

2. X. Liang, G. Wang, X. Dong, G. Wang, H. Ma and X. Zhang, *ACS Appl. Nano Mater.*, 2019, **2**, 517-524.

3. A. Uddin, A. Rauf, T. Wu, R. Khan, Y. Yu, L. Tan, F. Jiang and H. Chen, *J. Colloid Interface Sci.*, 2021, **602**, 261-273.

4. Y. Tang, X. Yin, M. Mu, Y. Jiang, X. Li, H. Zhang and T. Ouyang, *Colloids Surf., A*, 2020, **596**, 124745.

5. I. Altin, X. Ma, V. Boffa, E. Bacaksız and G. Magnacca, *Mater. Sci. Semicond. Process.*, 2021, **123**, 105591.

6. C. He, H. Qian, X. Li, X. Yan, S. Zuo, J. Qian, Q. Chen and C. Yao, *J. Mater. Sci.: Mater. Electron.*, 2019**, 30**, 593-599.

7. F. Zhang, Y. Zhao, Y. Li, G. Wu and J. Zhao, *J. Colloid Interface Sci.*, 2017, **505**, 519-527.

8. C. Ye, K. Hu, Z. Niu, Y. Lu, L. Zhang and K. Yan, *J. Water Process Eng.*, 2019, **27**, 205-210.

9. P. Qiu, B. Park, J. Choi, M. Cui, J. Kim and J. Khim, *J. Alloys Compd.*, 2017, **706**, 7-15.

10. F. Xu, Z. Mo, J. Yan, J. Fu, Y. Song, W. El-Alami, X. Wu, H. Li and H. Xu, *J. Colloid Interface Sci.*, 2020, **560**, 555-564.