Electronic Supplementary Material (ESI) for Materials Chemistry Frontiers.


**Supporting information**

# In-plane Polarization Induced by Hydrogen-bond and π - π Stacking of Functionalized PDIs Supramolecular for Efficient Photocatalytic Degradation toward Organic Pollutants

*Haiyan Li,[a,b] Cong Wang,[a] Xiaojuan Bai,*[a,b] Xuyu Wang,[a] Boxuan Sun,[a] Di Li,[c] Liangchen Zhao,[a] Ruilong Zong[d] and Derek Hao[e]*

[a] Beijing Engineering Research Center of Sustainable Urban Sewage System Construction and Risk Control, Beijing University of Civil Engineering and Architecture, Beijing 100044, China

[b] Beijing Advanced Innovation Center for Future Urban Design, Beijing 100044, China

[c] School of Chemistry and Chemical Engineering, Xi'an University of Architecture and Technology, Xi'an, 710055, China

[d] Department of Chemistry, Tsinghua University, Beijing 100084, China

[e] Centre for Technology in Water and Wastewater (CTWW), School of Civil and Environmental Engineering, University of Technology Sydney (UTS), Ultimo, NSW 2007, Australia

*Corresponding Author E-mail: heixia.1986@163.com, baixiaojuan@bucea.edu.cn

**Supplement of the DFT calculation details**

The DFT calculations process firstly established a molecular model according to the structure of *s*Ami-PDI-HCl, and then optimized the structure by B3LYP-D3BJ/def2-SVP, followed by analysis of NTO, orbital, etc. Specifically, the above model was obtained by drawing molecules and structures in a program interface, generating an input file, and importing them into the Gaussian program for structural optimization. The above steps ensured that the molecular used in DFT calculations was the *s*Ami-PDI-HCl synthesized in this work.

**Figures**

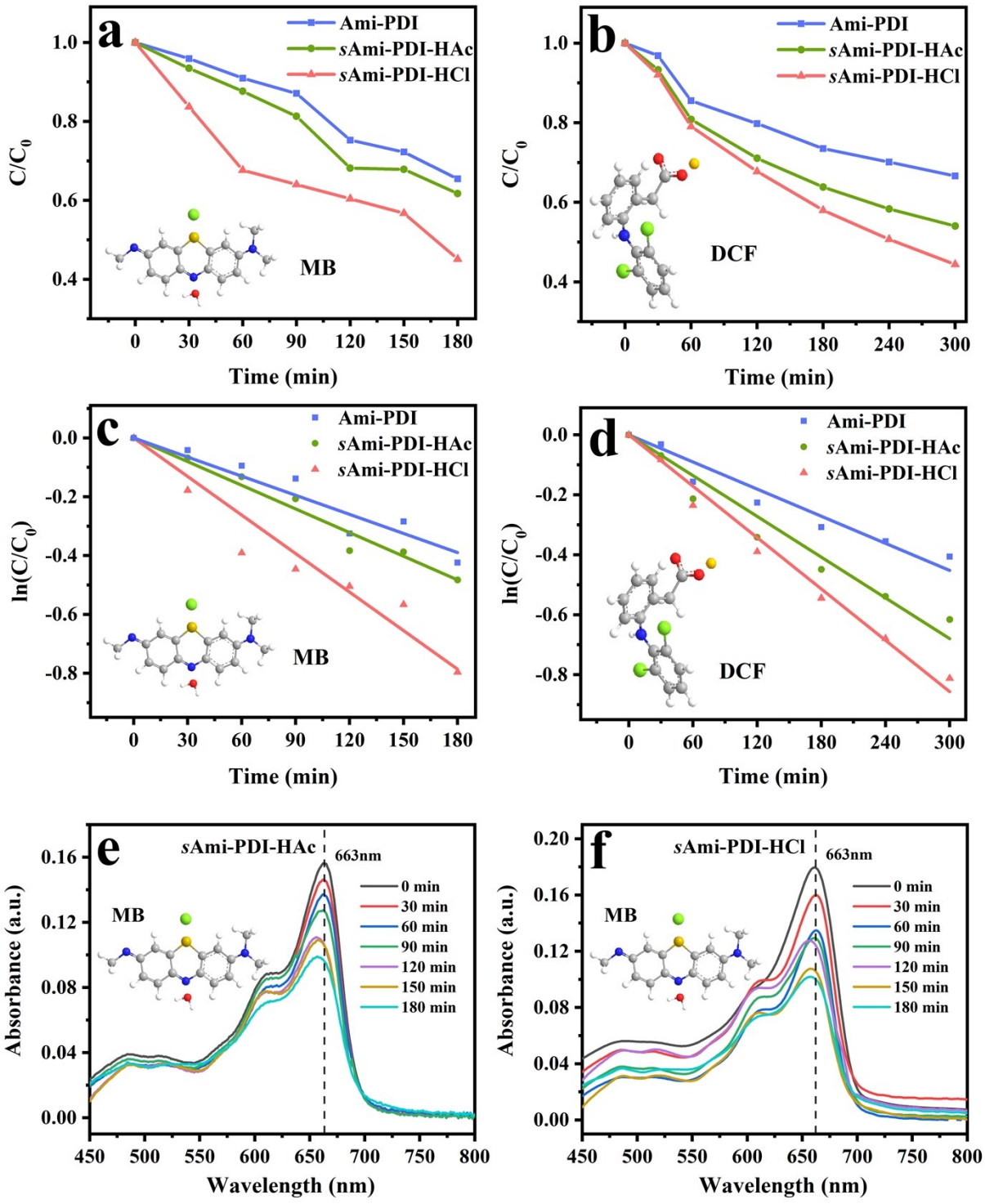


**Fig. S1** Photodegradation performance on MB (a) and DCF (b) by using Ami-PDI, *s*Ami-PDI-HAc and *s*Ami-PDI-HCl under visible light irradiation (λ ≥ 420 nm). The pseudo-first-order kinetic

fitting curve of Ami-PDI, *s*Ami-PDI-HAc and *s*Ami-PDI-HCl for MB (c) and DCF (d). The UV absorption spectrum of MB degraded by *s*Ami-PDI-HAc (e) and *s*Ami-PDI-HCl (f).

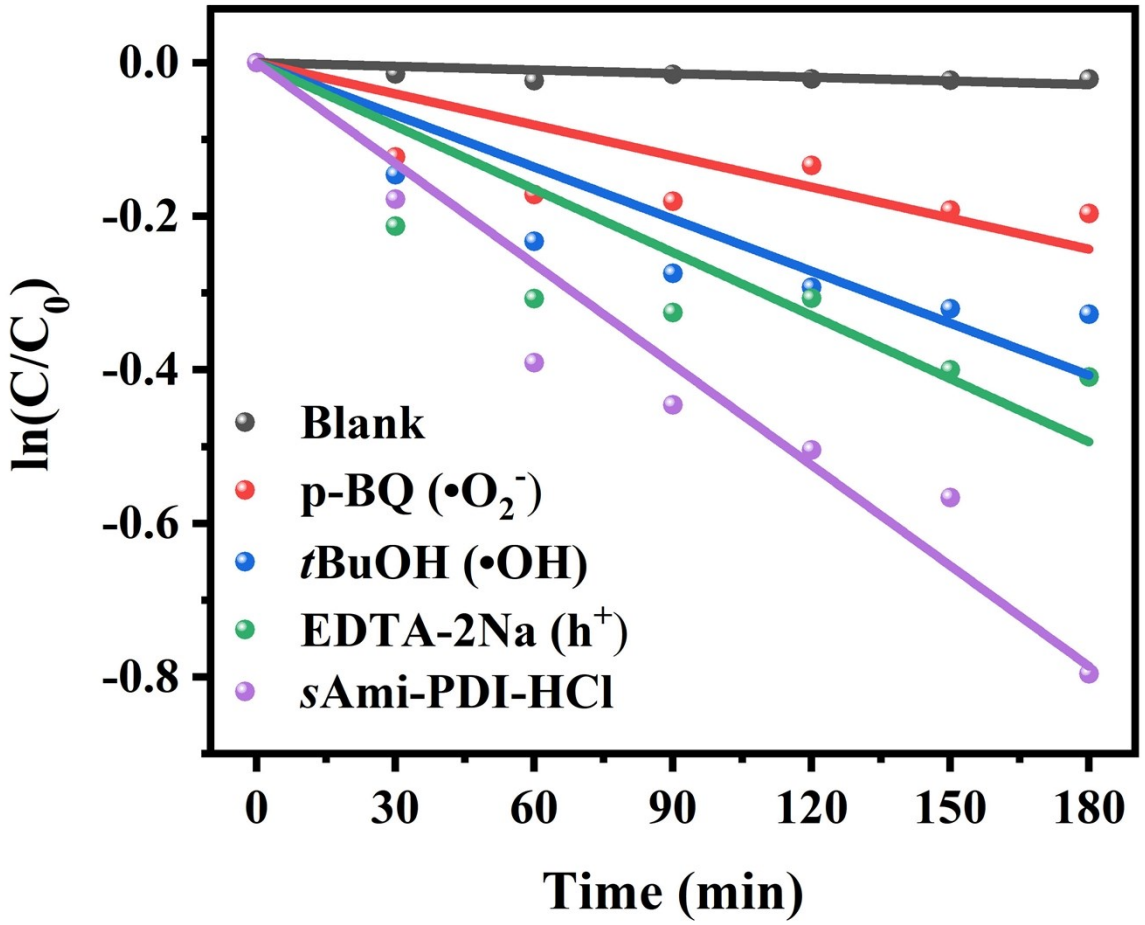


**Fig. S2** The pseudo-first-order kinetic fitting curve of different scavengers on MB degradation by *s*Ami-PDI-HCl.