

Supporting Information

Engineering chemically bonded S-scheme heterojunction between 5,10,15,20-Tetrakis(4-sulfophenyl)porphyrin and Bi₄O₅Br₂ for efficient photocatalytic water purification

Shijie Li^{a,b,c,*}, Yanbo Wang^a, Kexin Dong^a, Fang Yang^d, Yang Guo^e, Xiaobing Wang^f, Yanping Hou^{g,*}, Bin Zhang^{a,*}

^a Zhejiang Key Laboratory of Pollution Control for Port-Petrochemical Industry, School of Petrochemical Engineering & Environment, College of Food Science and Pharmacy, National Engineering Research Center for Marine Aquaculture, Zhejiang Ocean University, Zhoushan, Zhejiang Province, 316022, China.

^b Pingyang Institute of Science and Technology Innovation, Wenzhou 325400, China

^c School of Environmental and Chemical Engineering, Zhaoqing University, Zhaoqing, 526061, China

^d School of Mechanical and Automotive Engineering, Shanghai University of Engineering Science, Shanghai, 201620, China

^e Key Laboratory of Soil Environmental Management and Pollution Control, Nanjing Institute of Environmental Sciences, Ministry of Ecology and Environment, Nanjing 210042, China

^f School of Chemistry and Civil Engineering, Shaoguan University, Shaoguan, 512005, China;

^g School of Resources, Environment and Materials, Guangxi University, Nanning 530004, China

* Corresponding authors

* E-mail: lishijie@zjou.edu.cn (S.J. Li); houyp@gxu.edu.cn (Y.P. Hou); zhangbin@zjou.edu.cn (B. Zhang)

Experiment

1.1. Characterizations

The crystallographic phase composition of the TPPS/BiBr samples was determined by X-ray diffraction (XRD, Rigaku MiniFlex 600) with Cu K α radiation ($\lambda = 1.5406 \text{ \AA}$), scanning over a 2θ range of $10\text{--}80^\circ$. Surface chemical states, along with elemental composition, were analyzed by XPS (Escalab 250Xi) with a monochromatic Al K α source. High-resolution TEM (JEOL JEM-2100) was harnessed to reveal the microstructure, while SEM-EDX (Thermo Fisher Scientific) was utilized for morphological and elemental analysis. Electrochemical measurements were carried out on a CHI 660E workstation employing a standard three-electrode configuration. The bandgap energies were determined from UV-Vis diffuse reflectance spectra (Shimadzu UV-2600). Water contact angle (WCA) measurements, conducted with an SDC-100 contact angle analyzer (Shengding Precision Instrument Co., Dongguan, China), were used to probe the surface wettability of the synthesized catalysts. Photoluminescence spectra of the catalysts were recorded on a Bio-Rad F-7000 fluorescence spectrophotometer.

1.2. Density functional theory (DFT) simulations

DFT simulations of the catalysts were performed using the VASP 5.4.4 package.

1.3. Intermediates and toxicity analyses

HPLC-HRMS analysis was first executed to unravel the degradation pathway of TC on TPPS/BiBr, providing accurate structural assignments for the intermediates, whose potential toxicities were then estimated using the T.E.S.T. software.

Figures

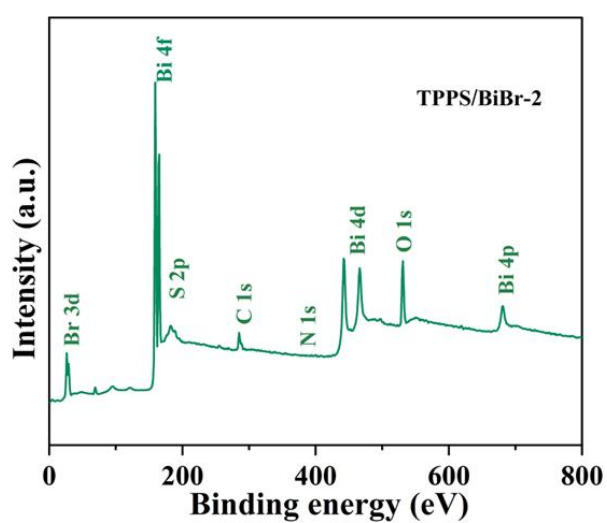


Fig. S1. Survey XPS spectrum of TPPS/BiBr-2.

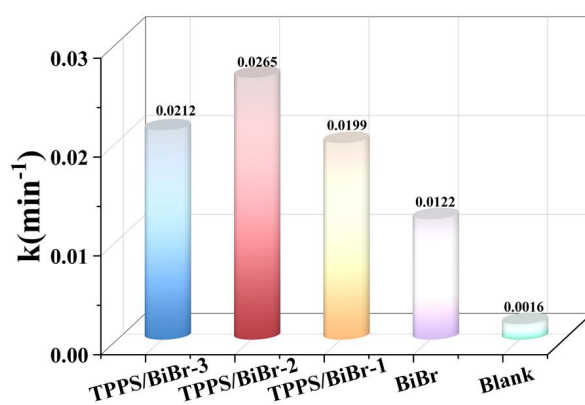


Fig. S2. The k values of BiBr, and TPPS/BiBr heterojunctions.

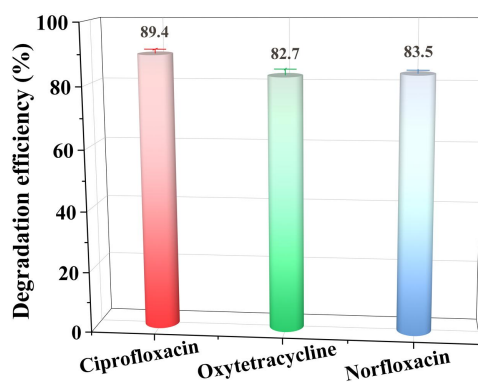


Fig. S3. The catalytic performance of TPPS/BiBr-2 in degrading other antibiotics.

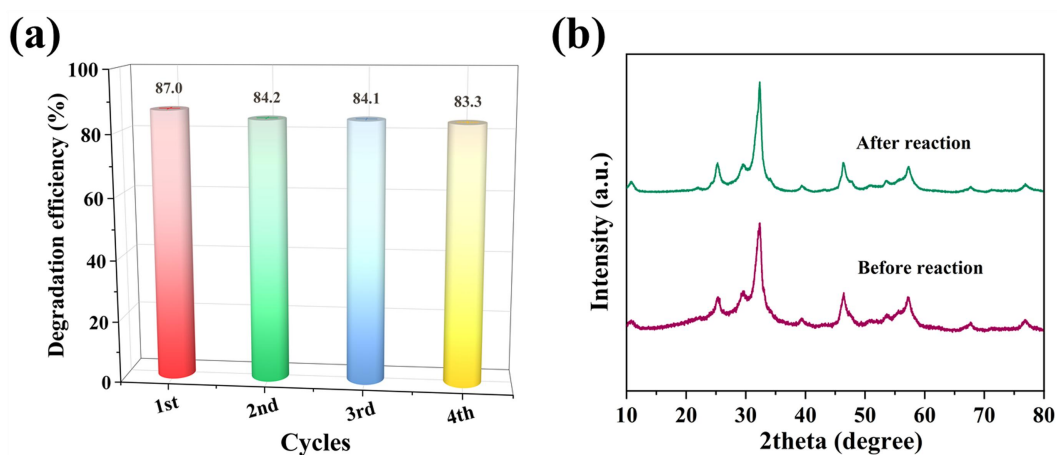


Fig. S4. (a) Cycling test of TPPS/BiBr-2. (b) The XRD results of the fresh and recycled TPPS/BiBr-2.

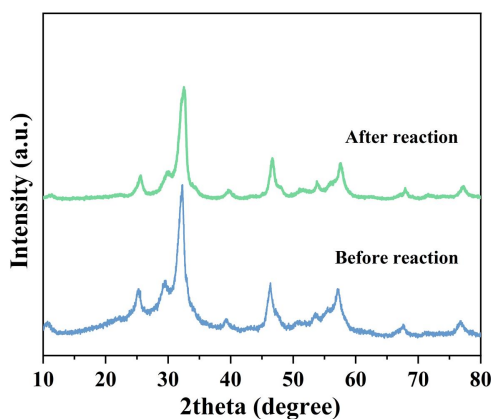


Fig. S5. The XRD results of the fresh and the used TPPS/BiBr-2 after continuous photocatalysis.

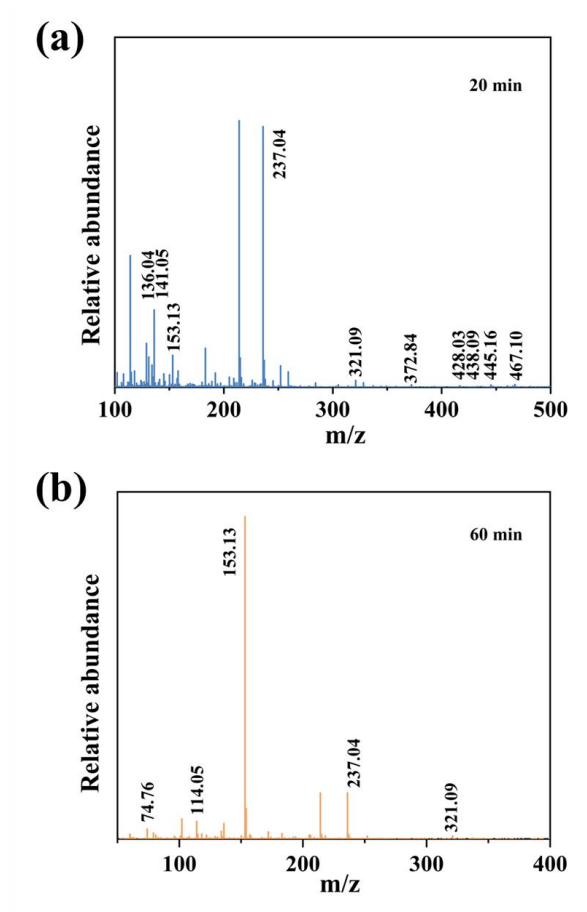


Fig. S6. HPLC-MS of the TC degradation intermediates over TPPS/BiBr-2.