Supporting Materials for:

Bi_n(Tu)_xCl_{3n}: a novel sensitizer and its enhancement of BiOCl nanosheets' photocatalytic activity

Liqun Ye,^a Chuqing Gong,^a Jinyan Liu,^a Lihong Tian,^a Tianyou Peng,^a Kejian Deng,^b and

Ling Zan^{* a}

^a College of Chemistry and Molecular Science, Wuhan University, Wuhan 430072, People's Republic of China

^b Key Laboratory of Catalysis and Materials Science of the State Ethnic Affairs Commission and Ministry of Education, South-Central University for Nationalities, Wuhan 430074, People's Republic of China

^{*} Corresponding author. Tel.: 86 27 6875 2919; fax: 86 27 8737 8727; E-mail: irlab@whu.edu.cn



Fig. S1. UV-Vis absorption spectra of NBT in common suspension: (a) BiOCl-3-7; and (b) common BiOCl.



Fig. S2. Reaction of NBT with superoxide ion.



Fig. S3. (a) FT-IR spectra of common BiOCl, BiOCl-3-7-500 and BiOCl-3-7 (1300 cm⁻¹ - 1500 cm⁻¹)



Fig. S4. XPS spectrum of BiOCl-3-7: (a) N1s; (b) S2s.



Fig. S5. TG-DSC curves of BTC-3.



Fig. S6. XRD pattern of BTC-3-500.

The TG-DSC of BTC-3 was showed in Fig. S4. At 500 °C, the rate of weight losses estimated on 47.1% which in accordance with that of BiOCl (47.9%). Furthermore, the XRD pattern displayed that BTC-3-500 (Fig. S5) is BiOCl. Those results indicate that BTC can be transformed to BiOCl at 500°C, and the slight BTC can be removed completely by heat treatment at 500°C. So, BiOCl-3-7-500 can be used as referential sample without BTC.



Fig. S7. CV curves of BTC-3.

The CV curves of the BTC-3 (Fig. S6) was recorded on an u-Autolab III electrochemical analyzer using glassy carbon disks as the working electrode, a Pt-wire auxiliary electrode and Ag/0.01 M $AgNO_3 + 0.1$ M tetrabutylammonium hexafluorophosphate (TBAPF₆) acetonitrile (0.1 M) reference electrode. A drop of the BTC-3 anhydrous acetonitrile solution was placed on the surface of the working electrode and then the solvent was removed to form a BTC-3 film. The scan rate was set at 20 mV/s and the electrolytes were thoroughly deoxygenated by bubbling with high-purity argon for 15 min.

Then the VB/CB band energy was calculated from these E'_{ox} and Er'_{ed} values. $E_{VB}(E_{HOMO}) = E_{onset(ox)} - E_{FOC} + 0.3 \text{ eV}; E_{CB}(E_{LUMO}) = E_{HOMO} - E_g^{opt}$ (eV). Assuming the energy level of ferrocene/ferrocenium (Fc/Fc⁺) to be -0.3 eV below the hydrogen electrode level. The formal potential of Fc/Fc⁺ was measured to be 0.071 eV against an Ag/Ag^+ reference electrode. And $E_g^{opt} = 1240/\lambda_{onset} = 1240/556 = 2.2 \text{ eV}; E_{onset(ox)} =$ 0.363 eV (relative to the Ag/Ag^+ reference electrode). Therefore, $E_{VB}(E_{HOMO}) = 0.363 0.071 + 0.3 = 0.6 \text{ eV}; E_{CB}(E_{LUMO}) = 0.6 - 2.2 = -1.6 \text{ eV}.$



Fig. S8. FT-IR spectra of BiOCl-3-7. (a) before PCD process; (b) after five times PCD processes.



Fig. S9. Cycle runs in the photocatalytic degradation of RhB in the presence of BiOCl-3-7 under visible light irradiation for 1 h.