

Electronic Supplementary Information

Interfacial Charge Transfer and Enhanced Photocatalytic Performance for the Heterojunction WO₃/BiOCl: First Principles Study[†]

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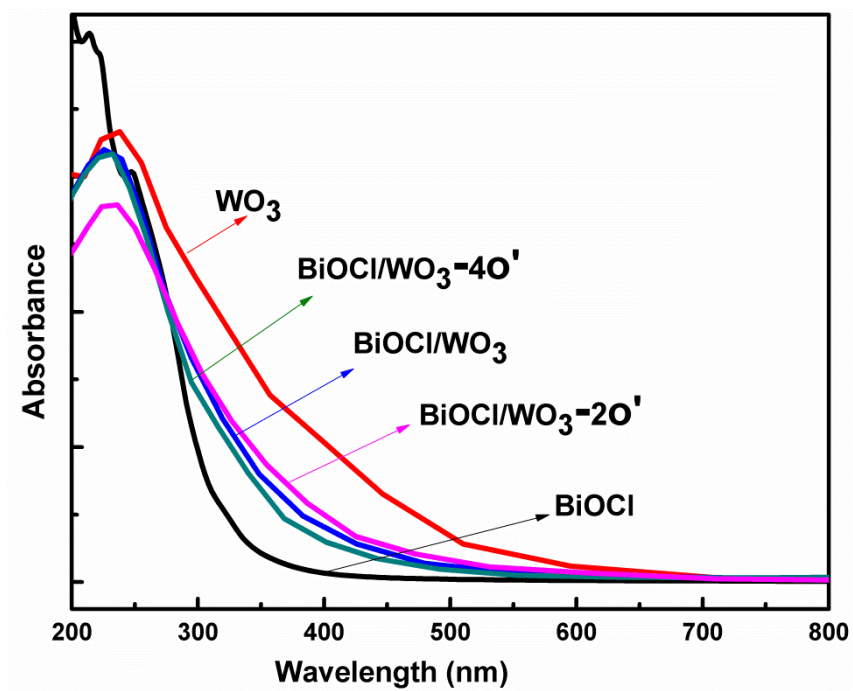


Fig. S1. (color online) Calculated optical absorption spectra of WO_3 , BiOCl and WO_3/BiOCl heterojunction with with stiochemistry, stiochemistry-2, stiochemistry-4 oxygen atoms as a function of wavelength

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The experiment section

The fabrication of BiOCl powder is described details in this paper {W. J. Yang, B. Ma, W. C. Wang, Y. W. Wen, D. W. Zeng and B. Shan, Phys. Chem. Chem. Phys., 2013, 15, 19387.}. The commercial WO₃ (of analytically pure grade) is bought at Tianjin kernel Chemical Reagent Co. Ltd., China. The WO₃/BiOCl composite was synthesized as follows: the specific amounts of BiOCl and WO₃ were dispersed in 10 mL of ethanol separately in beakers and sonificated for 1 hour to obtain a well dispersed homogeneous suspension. The BiOCl solution was then poured into the WO₃ solution and magnetically stirred for 1 hour. The obtained solution was dried at 90 °C for 12 hours and then annealed at 400 °C for 2hours with a rate of 2 °C per minutes.

The PEC performance measurements

The Indium Tin Oxide (ITO) substrates were cleaned by ultrasonication in distilled water, absolute ethanol and isopropanol for 20 min sequentially. The conducting glass substrates were covered and kept area of 1 cm² with high-temperature resistant adhesive tape. Typically, the aqueous slurries of the WO₃ and WO₃/BiOCl samples were spread on an ITO glass substrate by scraper method. The aqueous slurries were fabricated by grinding 500 mg of the WO₃ and WO₃/BiOCl samples, 1g of PEG (Sinopharm Chemical Regent Co. ltd, 400) aqueous solution and 200 μL of water and ethanol. The films were dried in air and then annealed at 120 °C for 10 hour. The photoelectrochemical were measured by an electrochemical analyzer (Correst 310 Instruments) in a standard three-electrode system with the WO₃ and WO₃/BiOCl samples as the working electrodes, a Pt foil as the counter electrode and a saturated Ag/AgCl as a reference electrode under simulated sunlight illumination. A 1.0 M Na₂SO₄ aqueous solution was used as the electrolyte.

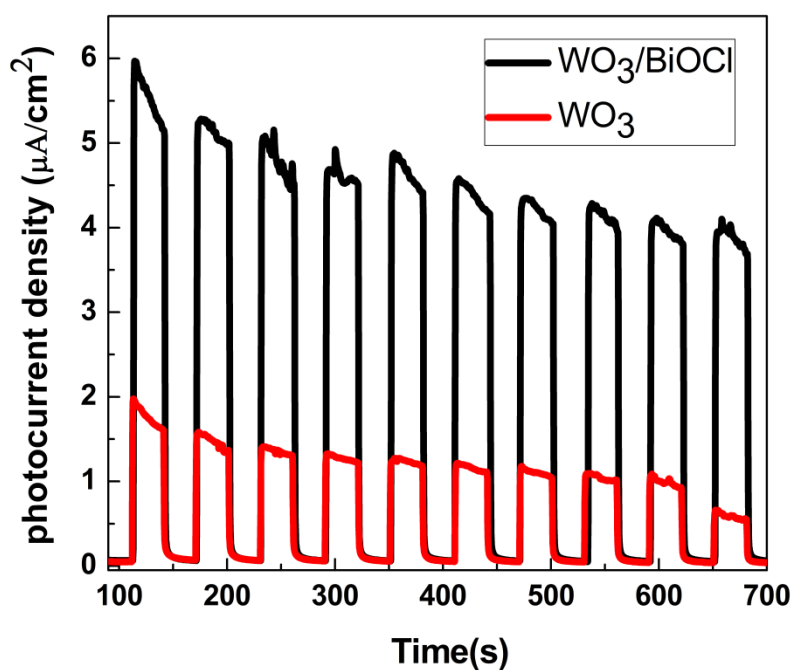


Fig.S2. (color online) Transient photocurrent density *vs.* time plotted for the WO_3 and heterojunction WO_3/BiOCl samples in 1 M Na_2SO_4 aqueous solutions under UV-*vis* irradiation at 0.2 V *vs.* Ag/AgCl.