

Enhancing separation efficiency of photo-induced carriers in Bi₂S₃/BiOCl heterostructure by the cooperative of oxygen vacancies and interfacial electric field

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Mott-Schottky (M-S) analysis:

The 0.2 M Na₂SO₄ solution was used as the electrolyte solution (pH=7). 10 mg of the catalyst was dispersed in 50 μL solution (10:1 by volume of ethanol and Nafion PFSA Polymer), and then uniformly spread on indium-doped tin oxide (ITO) glass (10×20 mm) to dry naturally, and then a working electrode was obtained. Mott-Schottky (M-S) plots were generated under dark with a voltage of 10 mV at a frequency of 1 kHz. In the M-S plot, the flat band potential and the carrier densities of the photoelectrode are measured according to following equation:

$$C^{-2} = (2/\epsilon\epsilon_0qN_q) (E - E_{FB} - kT/q) \quad \text{Equation S1}$$

$$\text{slope} = 2/q\epsilon\epsilon_0A^2N_q \quad \text{Equation S2}$$

Where, C is the space charge capacitance in the semiconductor (obtained from M-S curves), q is the electron charge, ε₀ is the vacuum permittivity (8.85×10⁻¹² F m⁻¹), ε represents the dielectric constant of semiconductor (for BiS/BOC heterojunctions, this value is a fixed value), N_q is the charge donor density (cm⁻³), E is the electrode potential, E_{FB} is fiat band potential, k represents Boltz-mann's constant (1.38×10⁻²³ J K⁻¹), T is the absolute temperature.

The slope (k) of the linear part of the differential capacitance potential curve at a given frequency was used to estimate their charge carrier density. From equations S1 and S2, it can be seen that for BiS/BOC heterojunction, other physical quantities in the equation are fixed values, and the charge donor density (N_q) of BiS/BOC heterojunction is negatively correlated with the obtained k value. That is, the smaller the k value, the larger the N_q, and the greater the photogenerated carrier density of the material; on the contrary, the larger the k value, the smaller the N_q, and the smaller the photogenerated carrier density of the material.

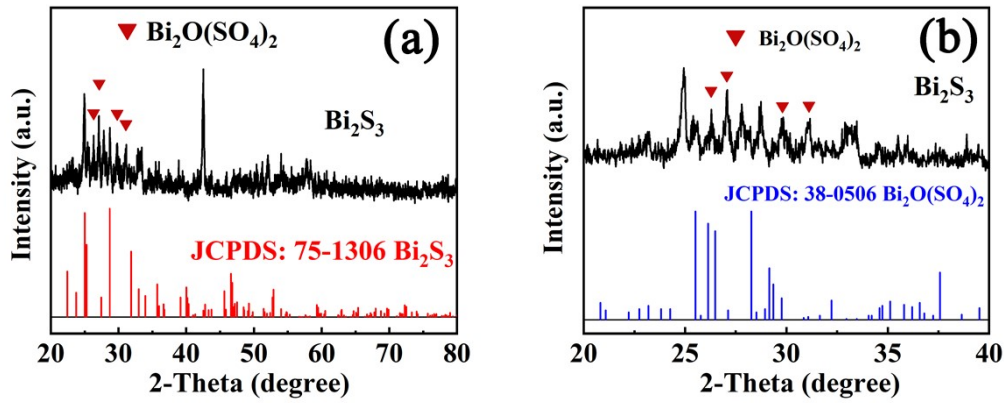


Fig. S1 (a-b) XRD patterns of Bi_2S_3 .

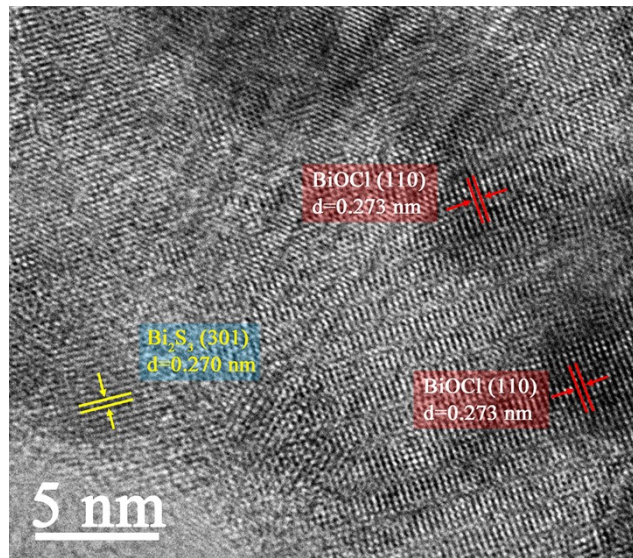
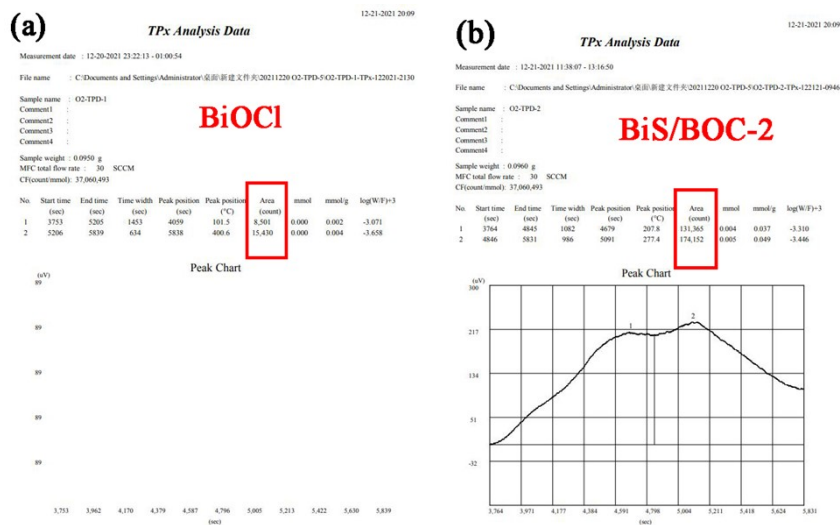


Fig. S2 The HRTEM image of BiS/BOC-4.



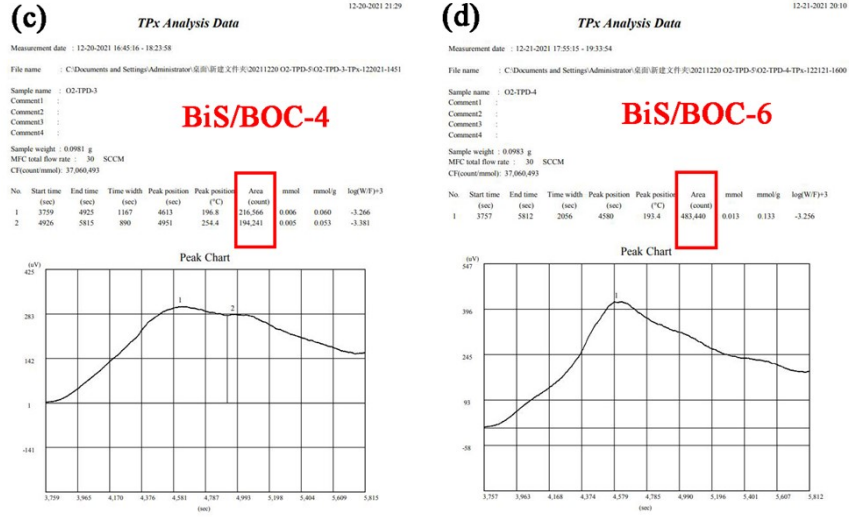


Fig. S3 The O₂-TPD profile of (a) BiOCl, (b) BiS/BOC-2, (c) BiS/BOC-4 and (d) BiS/BOC-6.

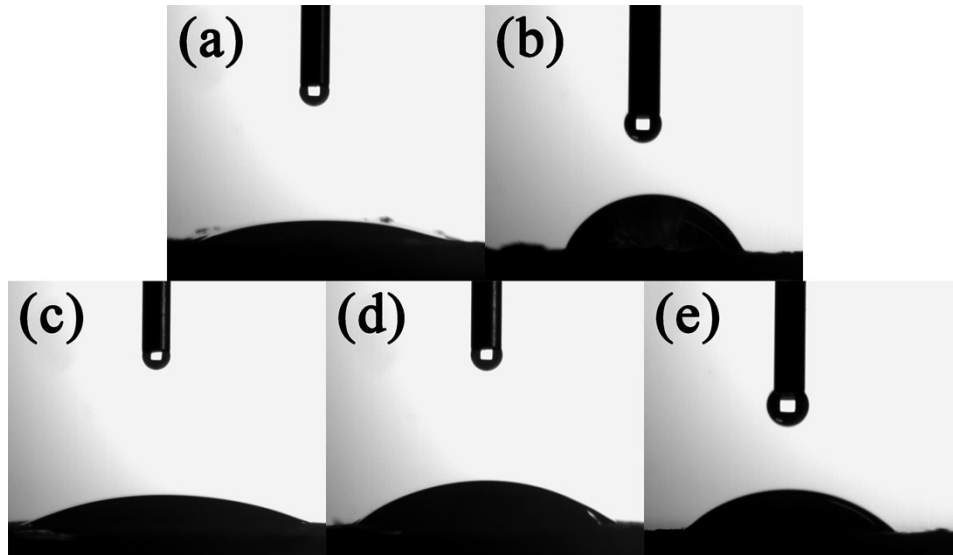


Fig. S4 Water contact angle of the as-prepared samples: (a) BiOCl, (b) Bi₂S₃, (c) BiS/BOC-2, (d) BiS/BOC-4, (e) BiS/BOC-6.

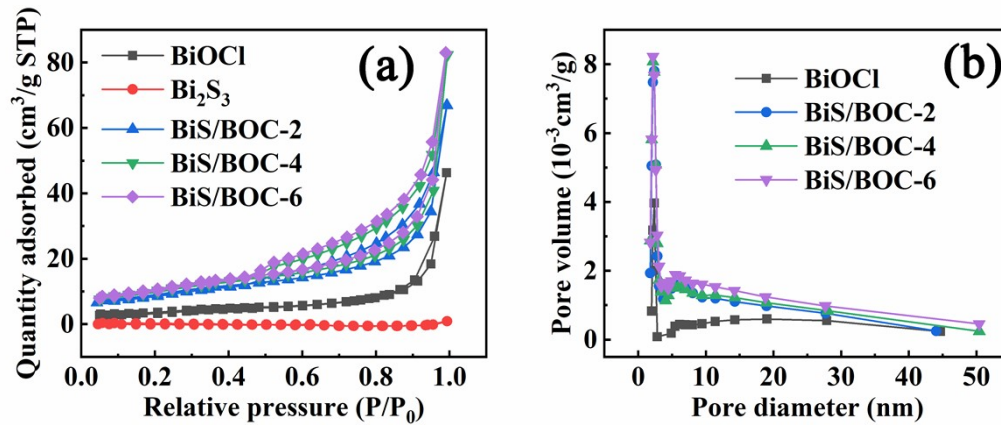


Fig. S5 (a) Nitrogen sorption isotherms curves and (b) pore volume distribution plots of the as-prepared samples.

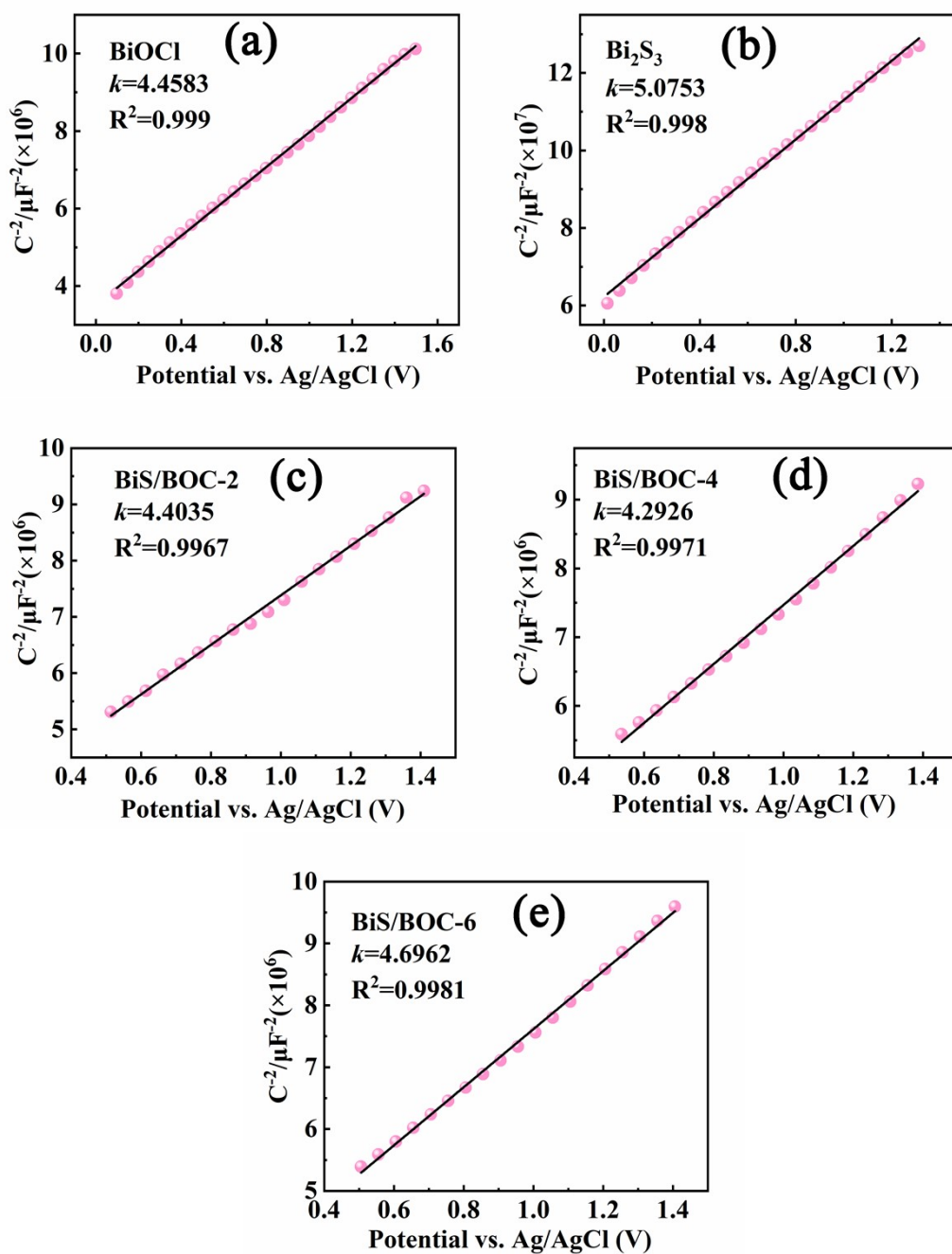


Fig. S6 (a-e) The slope (k) of the linear part of the differential capacitance potential curve at a given frequency (1000 KHz) for the prepared sample.



Fig. S7. Photocatalytic reaction conditions (a) dark reaction, (b) light reaction.

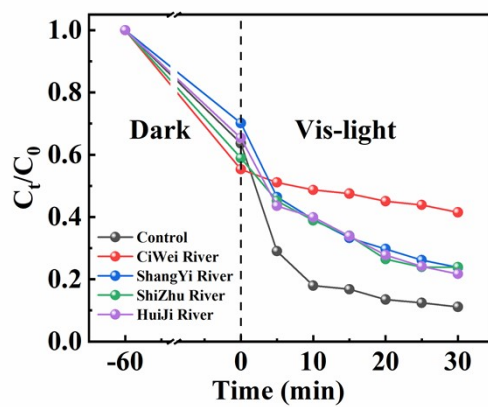


Fig. S8 Photocatalytic activity of BiS/BOC-4 for purify TC-HCl (20 mg/L) in different natural water matrices.