Electronic Supplementary Information

The Role of Sn in Enhancing the Visible-light Photocatalytic Activity of Bi/BiOBr Heterojunction Hollow Hierarchical Microspheres

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Computational Method. In our theoretical calculations, BiOBr lattice was modeled using a 2×2×4 supercell with a molecular formula of $BiO_{0.969}Br$. Calculations were performed using the Vienna Ab –initio Simulation Package (VASP), [1] which employed a DFT based plane-wave method.[2] Exchange correlation effects were included using the Perdew-Burke-Ernzerhof (PBE).[3] The energy cutoff for the expansion of wave function was set to be 450 eV, which was tested to be enough for both total energies in the systems. The Brillouin zone integration is performed using Monkhorst–Pack grids of 4×4×1 during the iterations; but, to obtain higher quality state densities and to check the stability of the results, this number ofk-points was increased to 8×8×2 after convergence was reached. The atomic position was optimized through PBE calculations with a criterion that required the calculated forces less than 10^{-2}eV/Å.

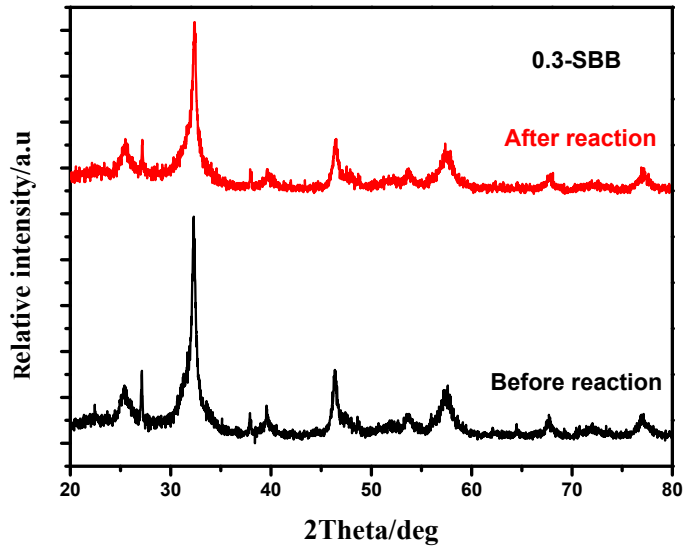
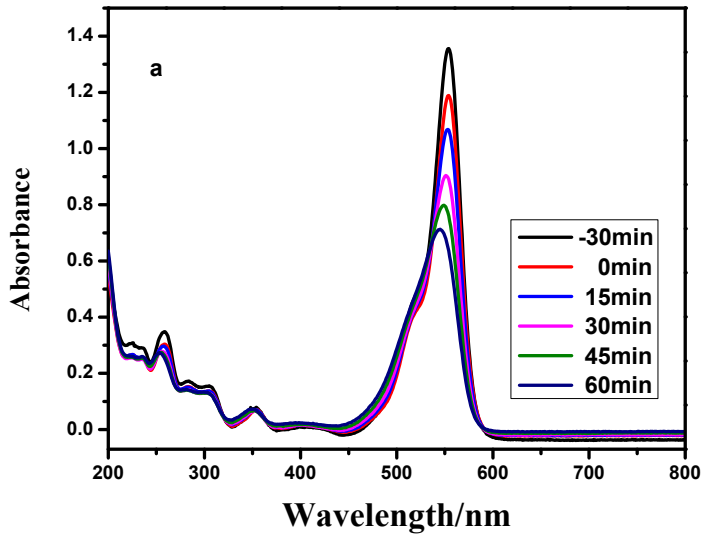


Fig. S1. XRD patterns of 0.3-SBB before and after photocatalytic reaction.



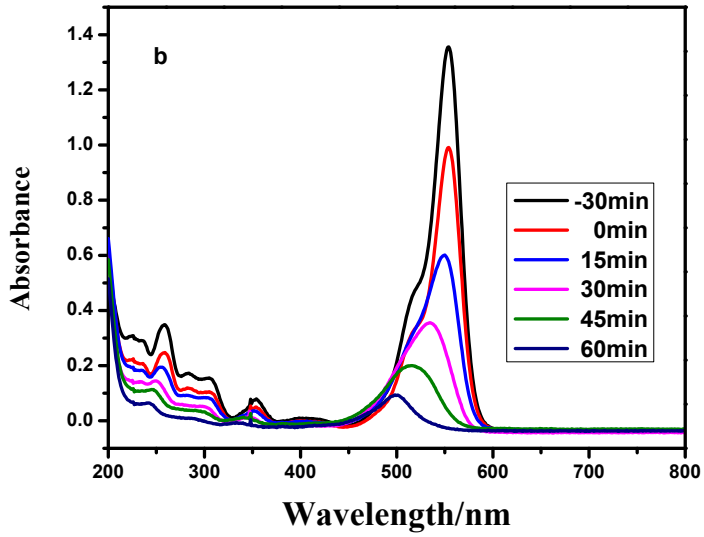


Fig. S2. UV–visible absorption spectral changes observed for the BiOBr/RhB (a) and 0.3-SBB/RhB (b) mixtures as a function of irradiation time under Xe arc lamp ($\lambda > 420$ nm)

References

(1) G. J. Kresse, F. Furthmüller, G. Bechstedt, J. Kresse, Hafner, *Phys. Rev. B,* 1996, **54(15)**, 10304.

(2) W. Kohn and L. J. Sham, *Phys. Rev,* 1965, **140 (4 A)**, 1133-1138.

(3) B. Hammer, L. B. Hansen, and J. K. Nørskov, *Phys. Rev. B*, 1999, **59**, 7413.