

Supplementary Information

BiOBr/carbon nitride heterojunctions: synthesis, enhanced activity and photocatalytic mechanism

Jie Fu, Yanlong Tian, Binbin Chang, Fengna Xi and Xiaoping Dong*

Department of Chemistry, School of Sciences, Zhejiang Sci-Tech University, 5 Second Avenue, Xiasha Higher Education Zone, Hangzhou, 310018, China.

Fax: +86 0571 86843653; Tel: +86 0571 86843228;

E-mail: xpdong@zstu.edu.cn

Details for the preparation of 0.5C₃N₄-0.5TiO₂ and 0.5BiOBr-0.5TiO₂ heterojunctions

The 0.5C₃N₄-0.5TiO₂ sample was synthesized as follows: 0.6 g of TiO₂ particulates (P25, Degussa) were finely ground with 0.6 g of C₃N₄, and then this mixture was heated in a crucible at 400 °C for 2 h. After cooling to room temperature, the 0.5C₃N₄-0.5TiO₂ heterojunction was obtained. For preparing the 0.5BiOBr-0.5TiO₂ photocatalyst, 0.6 g of TiO₂ (P25) powder and 0.24 g of KBr solid were added to 50 mL of water and ultrasonicated for 30 min to get a uniform suspension. Meanwhile, 0.97 g of Bi(NO₃)₃·5H₂O was dissolved in glacial acetic acid to obtain a clear solution. The resulting solution was added rapidly to the suspension and subsequently stirred for 30 min at room temperature. After aging for 3 h, the resulting precipitate was collected by centrifugation, washed thoroughly with water, and finally dried at 70 °C.

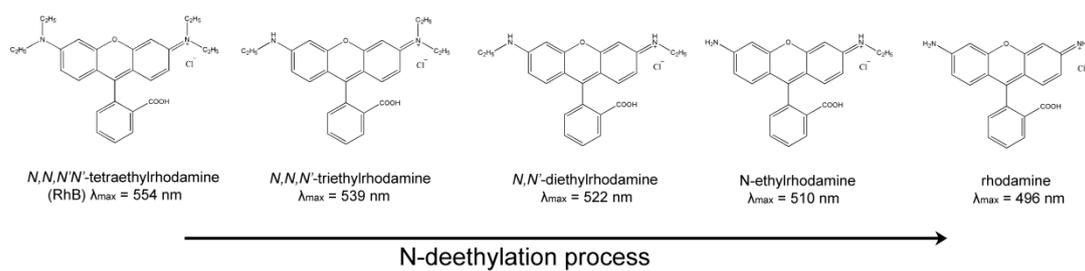


Fig. S1 The stepwise *N*-deethylation of RhB during the photocatalytic process.

Four main de-ethylated intermediates and their corresponding characteristic absorption bands are listed here.

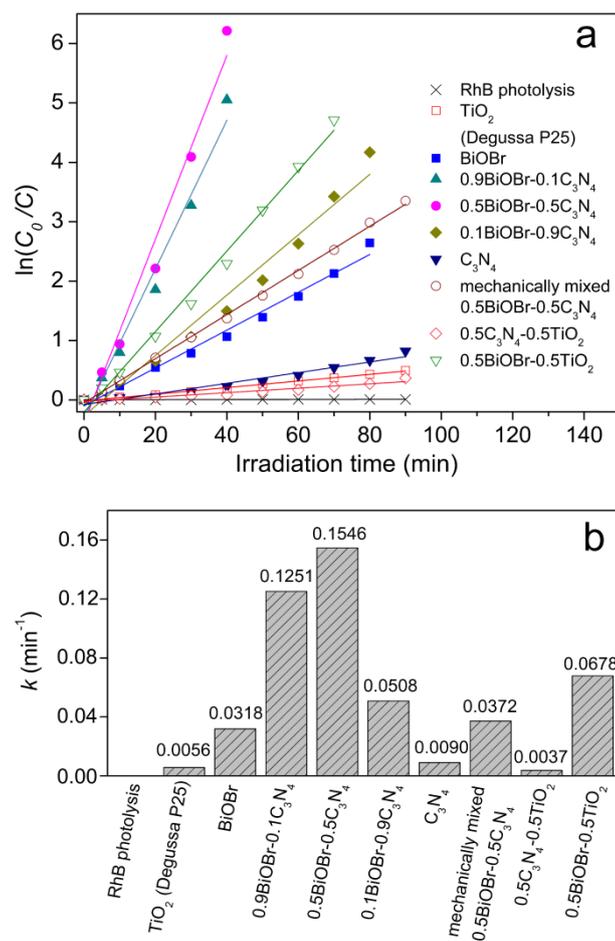


Fig. S2 (a) first-order kinetics plot for the visible light induced photodegradation of RhB over various photocatalysts, and (b) their corresponding rate constants (k).

The first-order model, $\ln(C_0/C) = kt$, was applied to fit the experimental data, where C_0 and C are the concentrations of RhB solution at times 0 (after stirring in the dark for 60 min) and t , respectively, and k is the first-order rate constant.

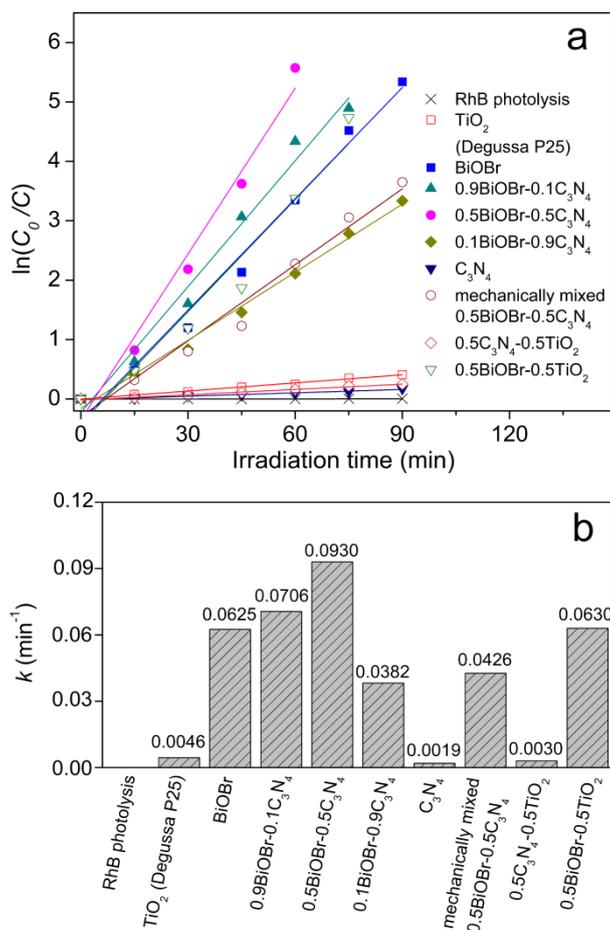


Fig. S3 (a) first-order kinetics plot for the degradation of RhB over various photocatalysts under indoor light irradiation, and (b) their corresponding rate constants (k).

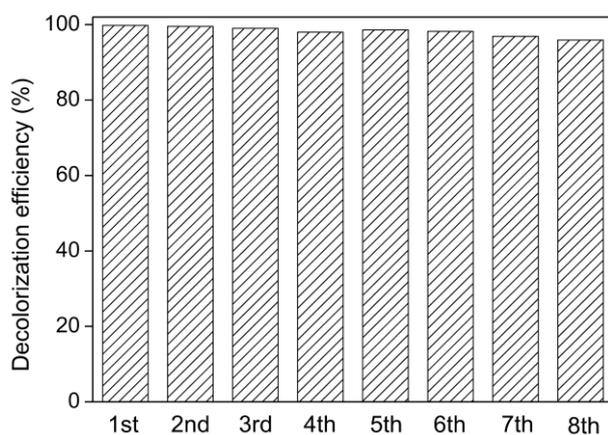


Fig. S4 The decolorization efficiency of RhB using 0.5BiOBr-0.5C₃N₄ heterojunction after 150 min of indoor light irradiation in each cycle.

The decolorization efficiency was estimated as: $\eta (\%) = (A_0 - A)/A_0 \times 100\%$

Where A_0 is the equilibrium absorbance of RhB solution at 554 nm (after stirring in the dark for 60 min), and A is the absorbance of final solution at 496 nm (after indoor light irradiation for 150 min).

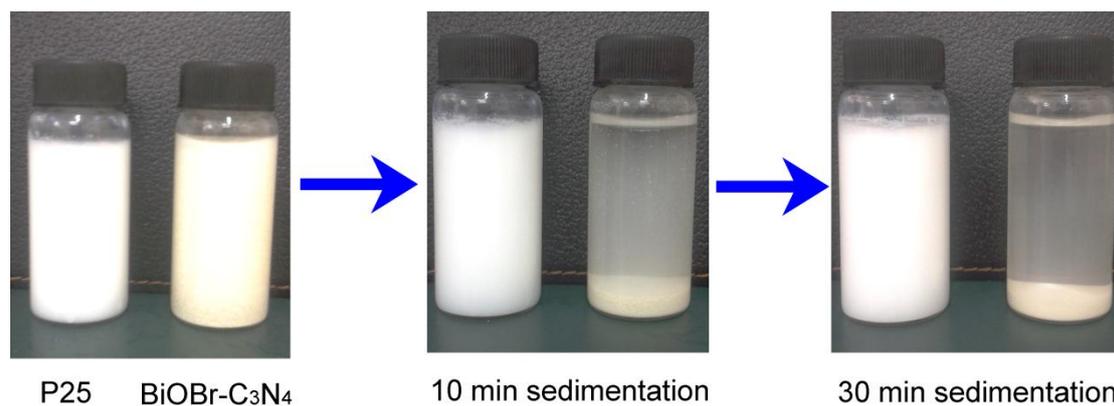


Fig. S5 Sedimentation of TiO₂ nanocatalyst (P25) and 0.5BiOBr-0.5C₃N₄ heterojunction in water.

It is clear that most of 0.5BiOBr-0.5C₃N₄ particles have settled within 10 min and a nearly complete separation can be realized after 30 min by a simple sedimentation. On the contrary, in the case of P25, almost no changes can be observed.

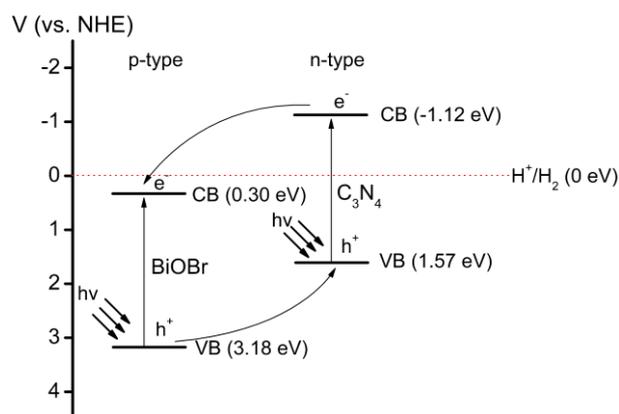


Fig. S6 Proposed energy levels of BiOBr and C₃N₄ and the scheme for the separation and transport of photogenerated charges at the interface of BiOBr-C₃N₄ heterojunctions.

Due to the well-aligned straddling band-structures of BiOBr-C₃N₄, the excited electrons would be concentrated in the CB of BiOBr, and the holes would be collected by the VB of C₃N₄. This effectively inhibits the recombination of photogenerated electrons-holes pairs.

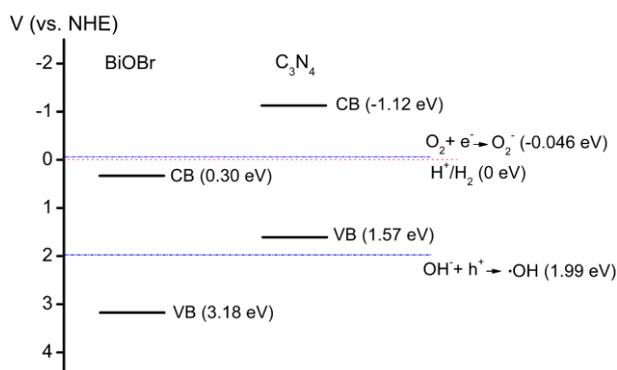


Fig. S7 Proposed energy levels of BiOBr and C₃N₄ compare with the standard redox potentials of ·OH/OH and O₂/O₂⁻.

Obviously, the excited electrons in the CB potential of BiOBr are not negative enough to reduce the O₂ molecule, and holes in the VB of C₃N₄ are not positive to oxidize OH. Thus, both the photogenerated electrons in BiOBr and holes in C₃N₄ cannot bring any hydroxyl radicals to the photocatalytic system.

