Electronic Supplementary Information

Nanosheet-Constructed Porous BiOCl with Dominant {001} Facets for Superior Photosensitized Degradation

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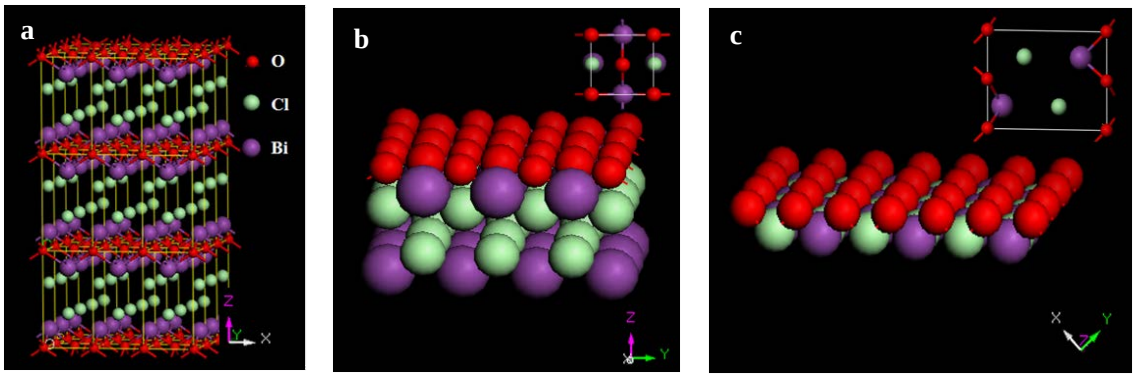


Fig. S1 The structure model illustration of BiOCl crystals (3×3 lattices): (a) three-dimensional projection; (b) (001) and (c) (110) surface. Inset in b and c is the corresponding top view (1×1 lattice).

The atomic structure of (001) facets and (110) facets were characterized by the high density of oxygen atoms (Fig. S1b, c), the oxygen density (OD) for the (001) facets and (110) facets were calculated as follows:

For 1×1 lattice and the top face

$$OD_{(001)} = (1+4\times¼)/a^2 = 2a^{-2} \quad (1)$$

For BiOCl crystal, it has a tetragonal structure with lattice constants of a =b = 3.883 Å and c = 7.347 Å, as estimated from the XRD data, therefore,

$$c = 7.347/3.883a = 1.892a \quad (2)$$

$$OD_{(110)} = (2\times½+4\times¼)/(2^{1/2}\times a\times c) = 2/(2.676a^2) = 0.7474a^{-2} \quad (3)$$

$$OD_{(001)}/OD_{(110)} = 2.68 \quad (4)$$

The aforementioned structural characteristics reveal that the (001) surface atomic structure contains terminal oxygen atoms, and the oxygen density on the (001) facets is much higher than that on the (110) facets, which is responsible for the high adsorption ability of RhB.

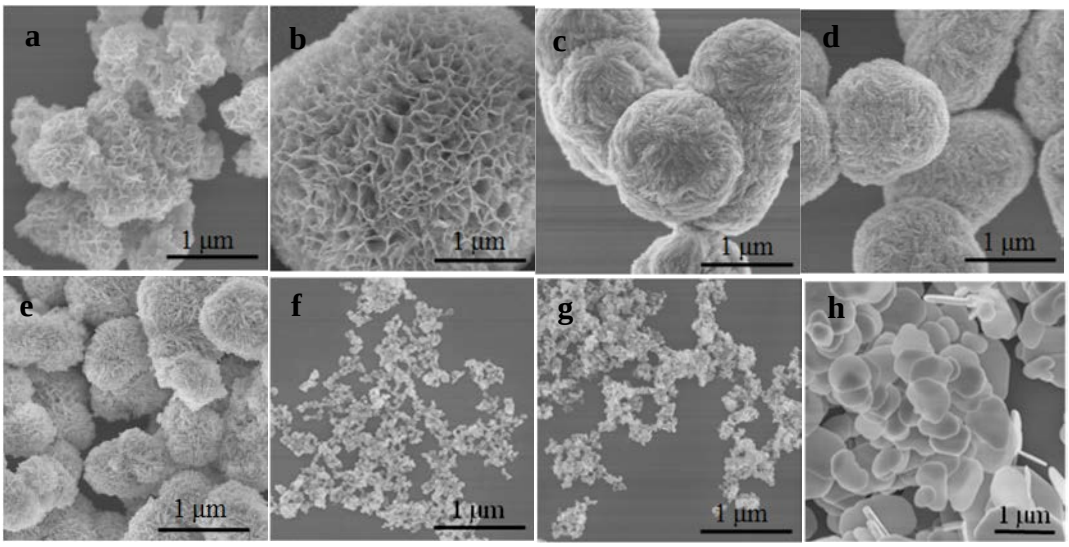


Fig. S2 SEM images of the as-made BiOCl nanostructures preprared in the presence of different water content by hydrothermal treatment at 110 ^{o}C for 6 h: (a) 1 ml, (b) 5 ml, (c) 10 ml, (d) 15 ml, (e) 20 ml, (f) 25 ml, (g) 35 ml and (h) 40 ml

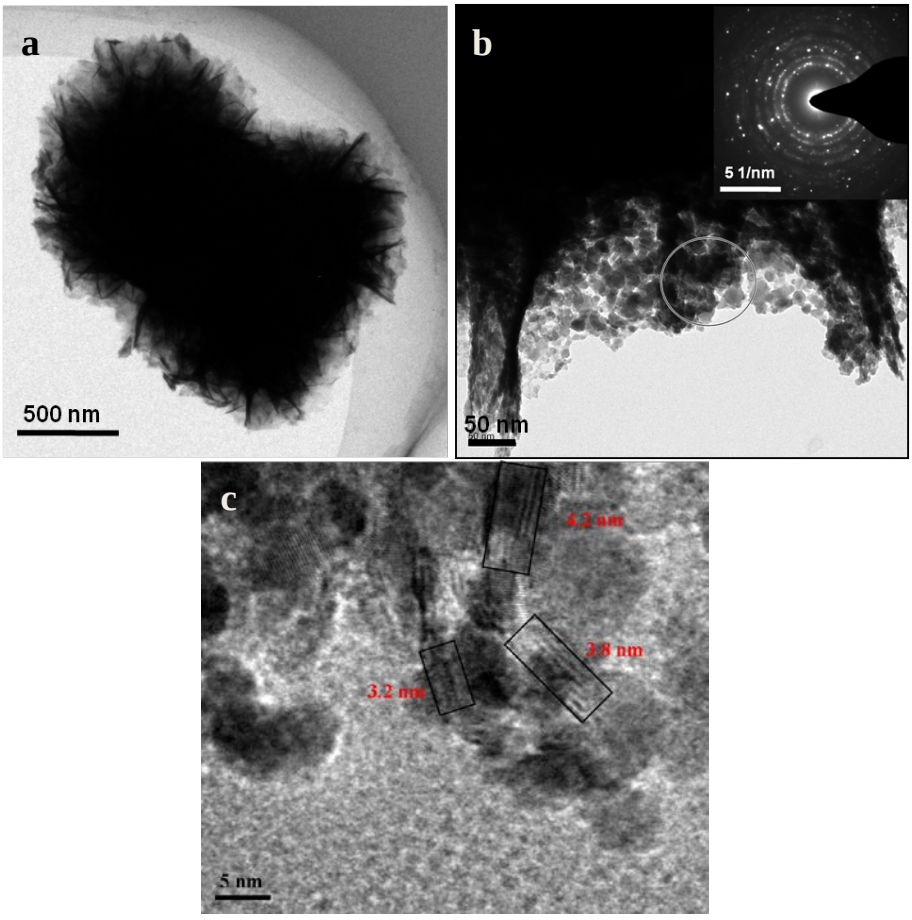
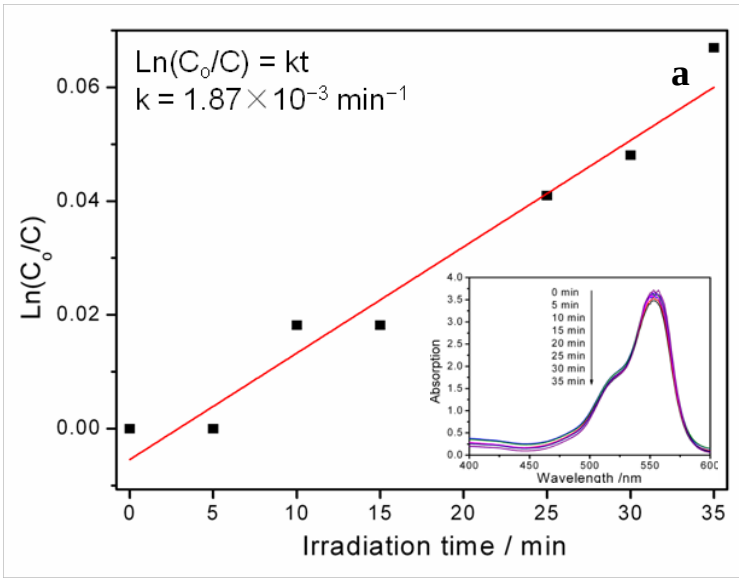


Fig. S3 TEM images of a typical flowerlike hierarchical structure of BiOCl (a and b). The inset in b) is the corresponding SAED pattern and c) HRTEM image of the BiOCl flower.



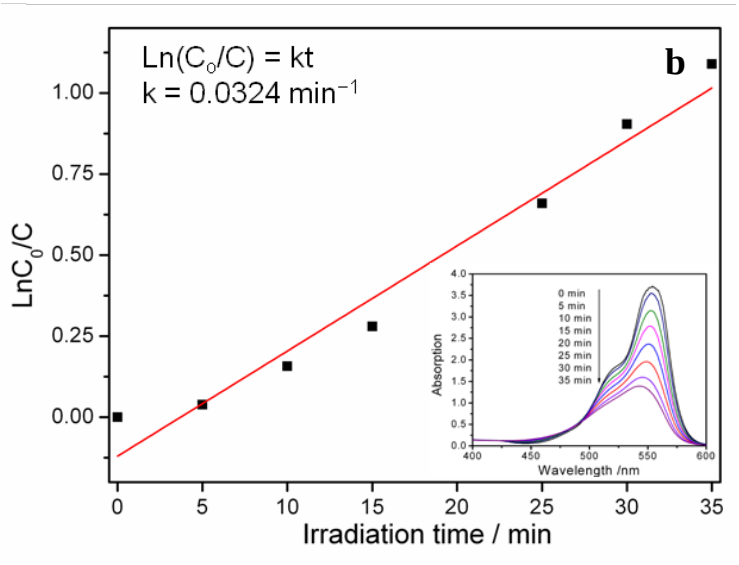


Fig. S4 Degradation rate of RhB over P25 (a) and BiOCl nanoplates (B) under visible light irradiation, with the insets are the corresponding absorption profiles of RhB against irradiation time.

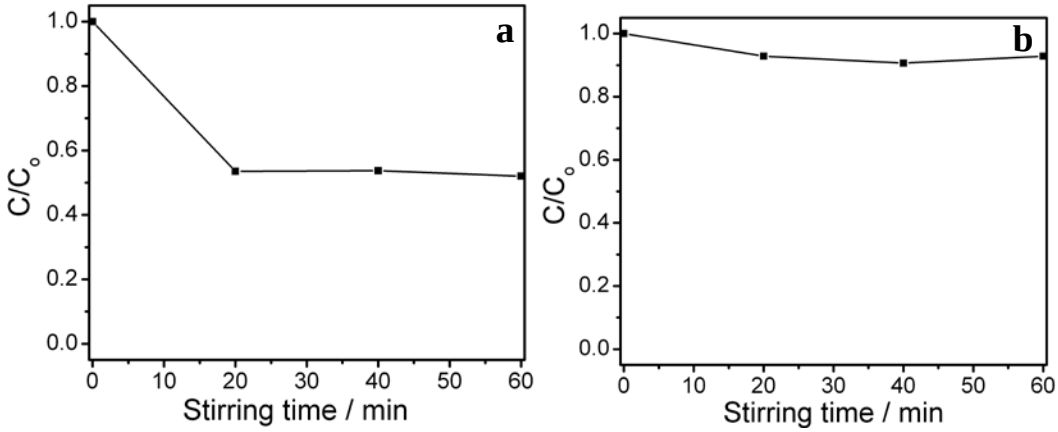


Fig. S5 Remaining concentration of MB (a) and MO (b) against stirring time in the dark in the presence of BiOCl micro-flowers. The original concentration of MB and MO was 20 mg L^{-1}, respectively.

Mean thickness calculations:

As shown in Fig. S6, the mean thickness of the nanosheets is 3.7 nm. Besides, we used the XRD data to estimate the average thickness of the nanosheets using Scherrer's equation. The average thickness, D, were determined using eqn (5):

$$D = K\lambda/(B\cos\theta) \quad (5)$$

Where λ is the wavelength of X-ray radiation (0.15406 nm), K is the Scherrer's constant (K = 0.9), θ is the diffraction angle, B is the full-width-at-half-maximum of the (001) plane (in radian) and D is the mean particle size.

The mean thickness calculated for the BiOCl nanosheets is around 3.82 nm, which was consistent with the result measured in the HRTEM image and TEM image. Therefore, we used 4 nm as the thickness of the nanosheets.

Band gap calculations:

For an inorganic semiconductor, the conduction band (CB) position at the point of zero charge can be calculated by the following empirical formula:[1]

$$E_{CB} = X - E^e - 0.5E_g \quad (6)$$

where E_{CB} is the potential of the conduction band, X is the absolute electronegativity of the semiconductor, which is defined as the geometric mean of the absolute electronegativity of the constituent atoms, E^e is the energy of free electrons on the hydrogen scale (ca. 4.5 eV), and E_g is the band gap of the semiconductor.

Then, the potential of the valence band can be calculated by the following empirical formula:

$$E_{VB} = E_g + E_{CB} \quad (7)$$

References:

1. H. F. Cheng, B. B. Huang, X. Y. Qin, X. Y. Zhang and Y. Dai, *Chem. Commun.*, 2012, **48**, 97; S. S. Liu, D. P. Yang, D. K. Ma, S. Wang, T. D. Tang and S. M. Huang, *Chem. Commun.*, 2011, **47**, 8013.

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