Supporting Information：

Enhanced photocatalytic activity of the direct Z-scheme black phosphorus/BiOX (X=Cl, Br, I) heterostructures

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Table S1 The calculated lattice parameters of BP and BiOX monolayers

	BP	BiOCl	BiOBr	BiOI
a (Å)	3.298	3.914	3.949	4.020
b (Å)	4.582	3.914	3.949	4.020

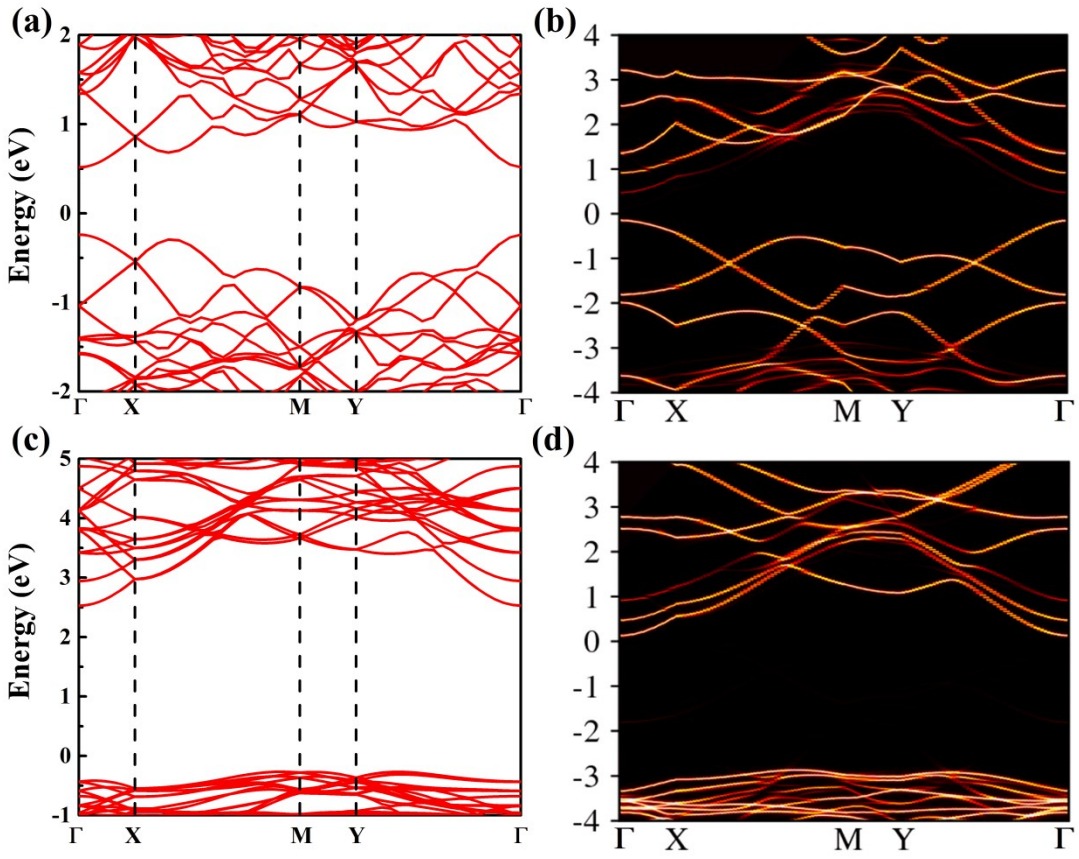

Fig. S1 The band structures (with PBE) for isolated BP (a) and (c) BiOCl monolayers in the BP/BiOCl heterostructure lattice. The unfolded bands derived from the k-projection method are shown in (b) and (d).

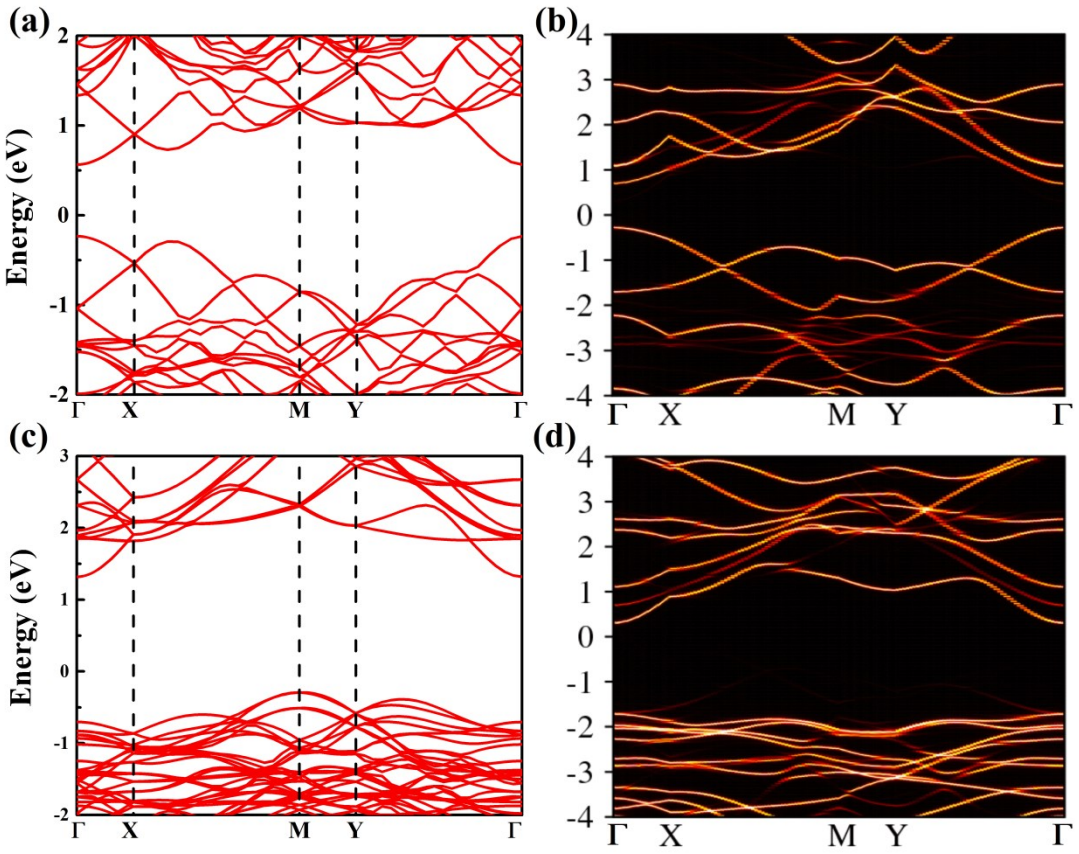

Fig. S2 The band structures (with PBE) for isolated (a) BP and (c) BiOI monolayers in the BP/BiOI heterostructure lattice. The unfolded bands derived from the k-projection method are shown in (b) and (d).

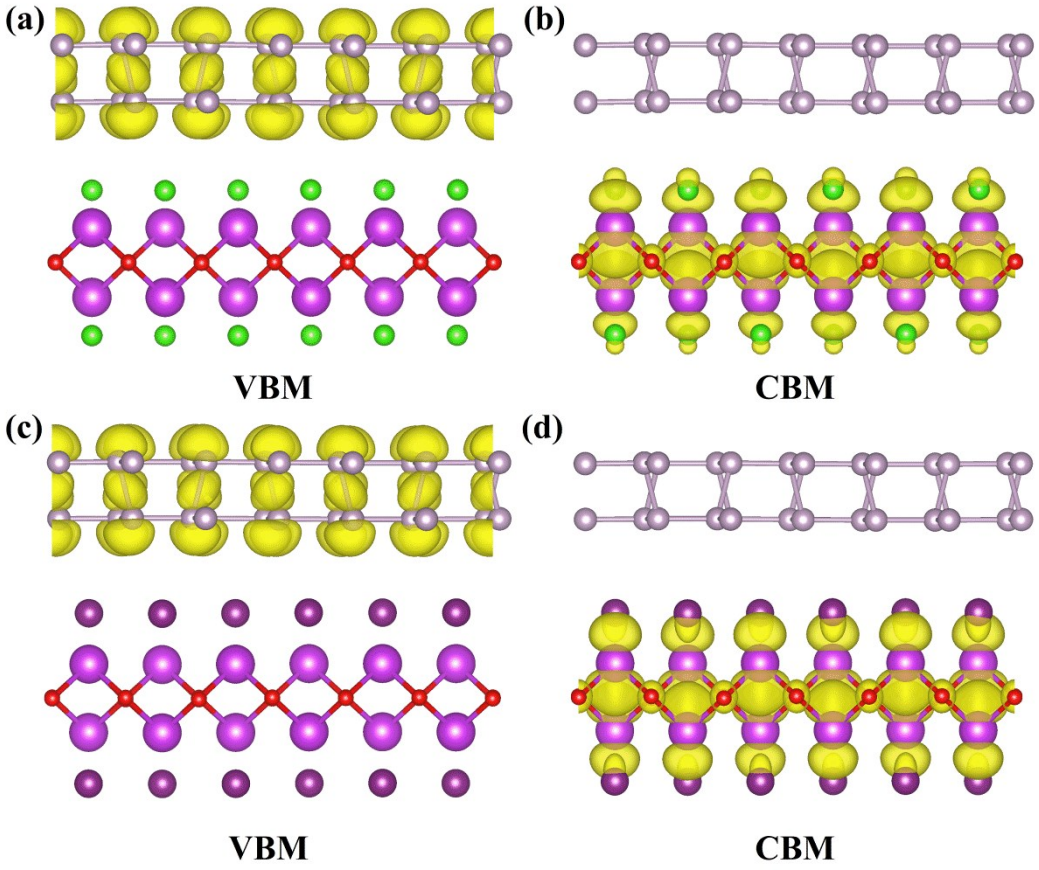

Fig. S3 (a) and (b) show the charge distribution of the VBM and CBM of BP/BiOCl heterostructure, respectively. (c) and (d) show the charge distribution of the VBM and CBM of BP/BiOI heterostructure, respectively.Yellow areas denote electron accumulation.

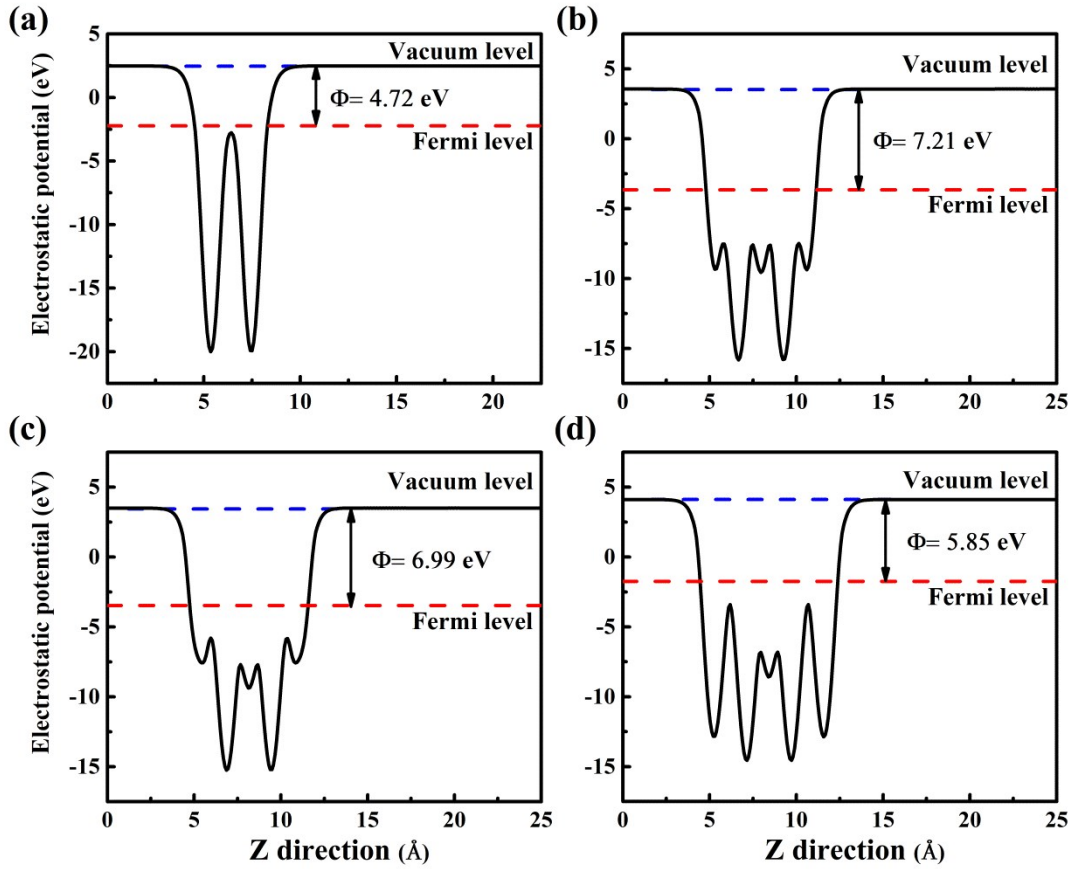

Fig. S4 The electrostatic potentials along Z direction of the isolated (a) BP, (b) BiOCl, (c) BiOBr and (d) BiOI.

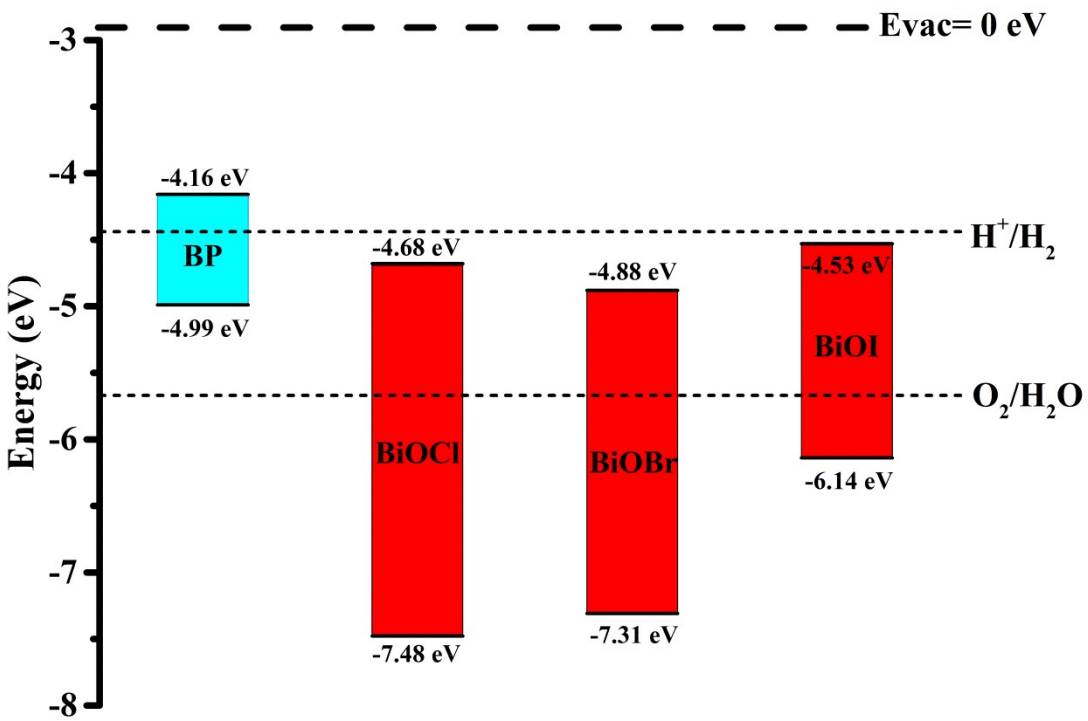

Fig. S5 Diagrams of the band edge positions of isolated BP, BiOCl, BiOBr and BiOI.