

Supporting Information (SI)

First-Principles Investigation of Nonmetal Doped Single-Layer BiOBr as a Potential Photocatalyst with Low Recombination Rate

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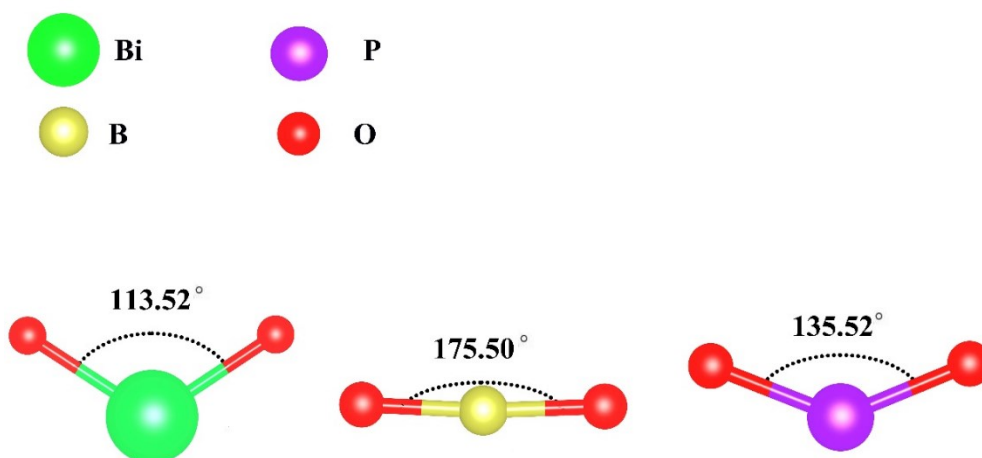


Fig. S1 The optimized bond angle for (a) O-Bi-O, (b) O-B-O, and (c) O-P-O, respectively. The green, golden, purple, and red spheres represent Bi, B, P, and O atoms, respectively.

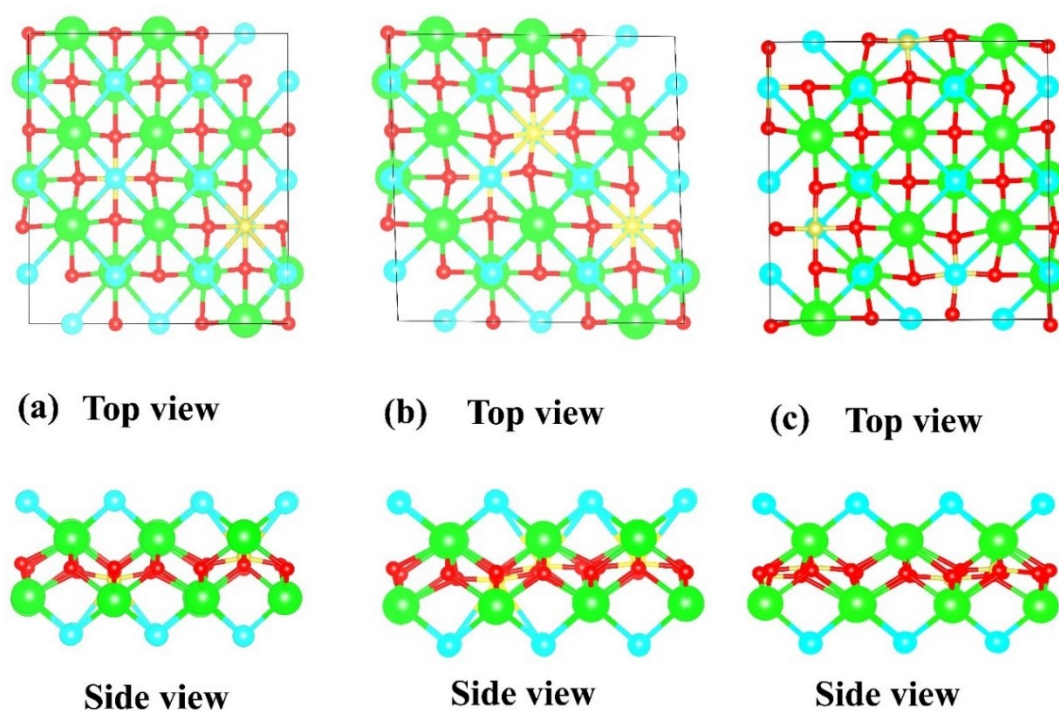


Fig. S2 Optimized atomic structures of B-doped single-layer BiOBr with the B atoms substituting (a) two Bi atoms, (b) three Bi atoms, and (c) four Bi atoms. The green, golden, red, and cyan spheres represent Bi, B, O, and Br atoms, respectively.

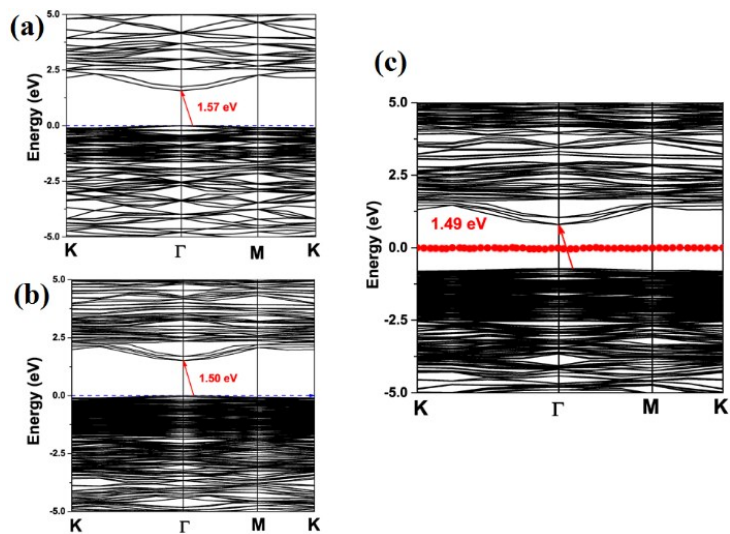


Fig. S3 Electronic band structure of pristine BiOBr layer (a), SubB (b), and SubP (c) systems using PBE-SOC. The horizontal dashed blue line signifies the Fermi level which is set to zero.

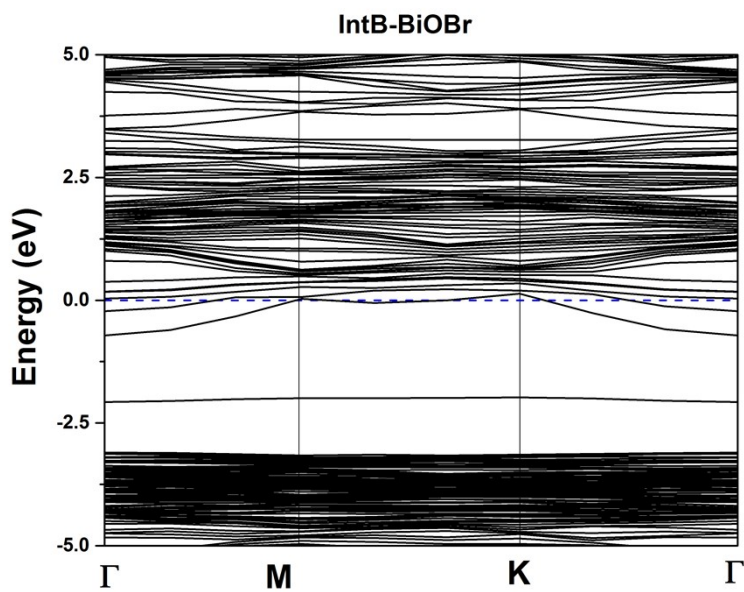


Fig. S4 Electronic band structure of interstitial B doped BiOBr layer. The horizontal dashed blue line signifies the Fermi level which is set to zero.

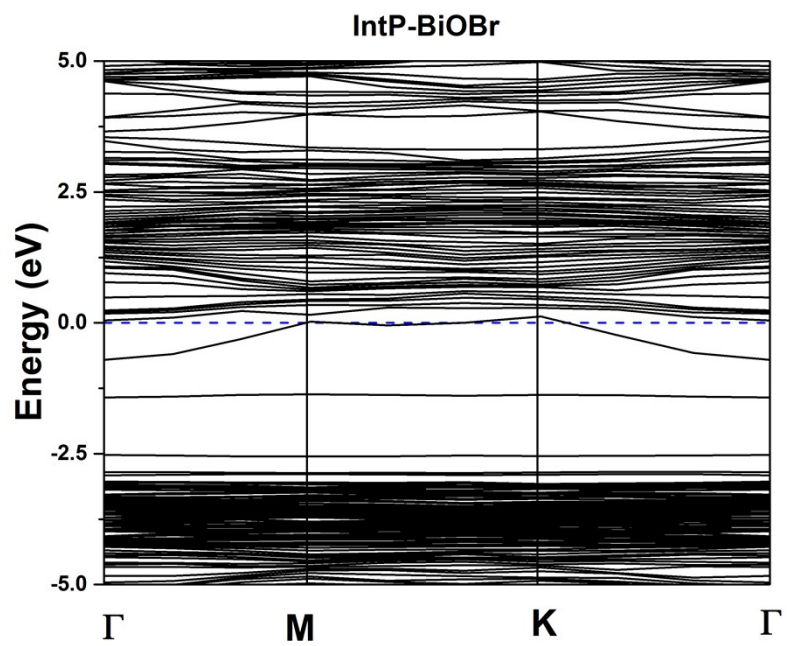


Fig. S5: Electronic band structure of interstitial P doped BiOBr layer. The horizontal dashed blue line signifies the Fermi level which is set to zero.

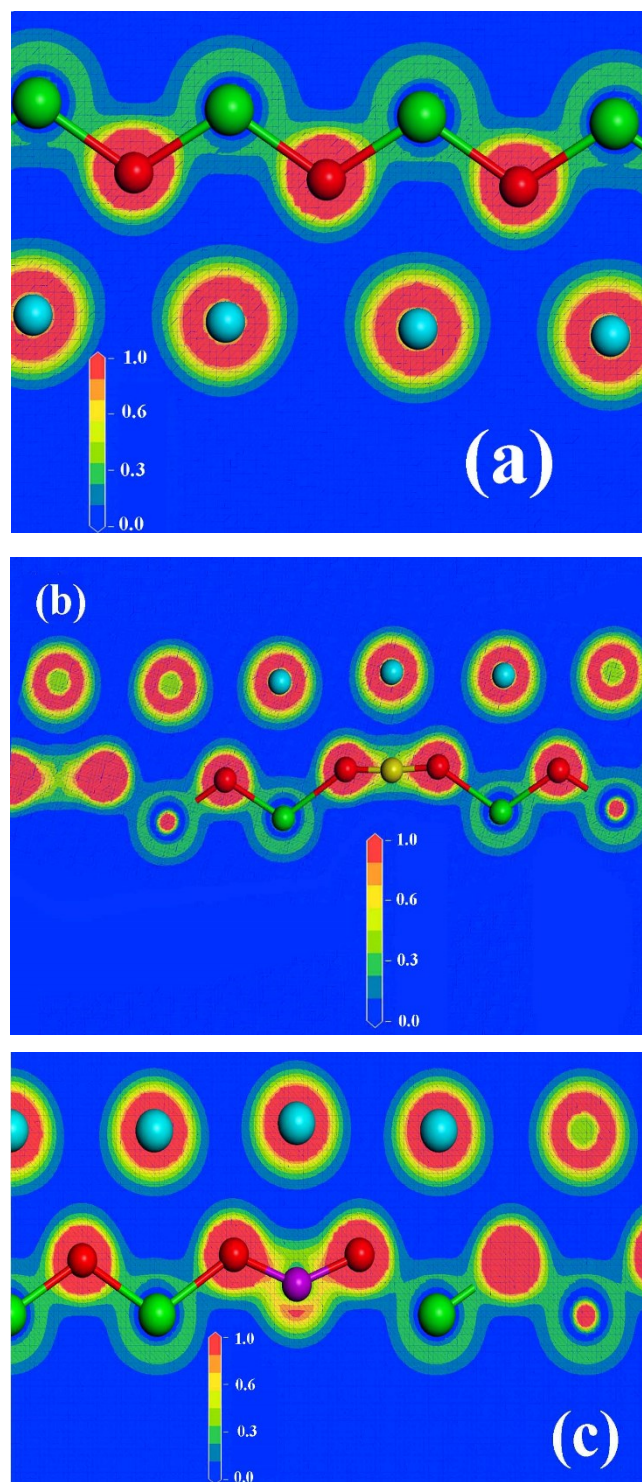


Fig. S6 The electron density distribution of pristine BiOBr (a), and boron (b) and phosphorus (c) substituted single-layer BiOBr. The green, golden, purple, red, and cyan spheres represent Bi, B, P, O, and Br atoms, respectively.

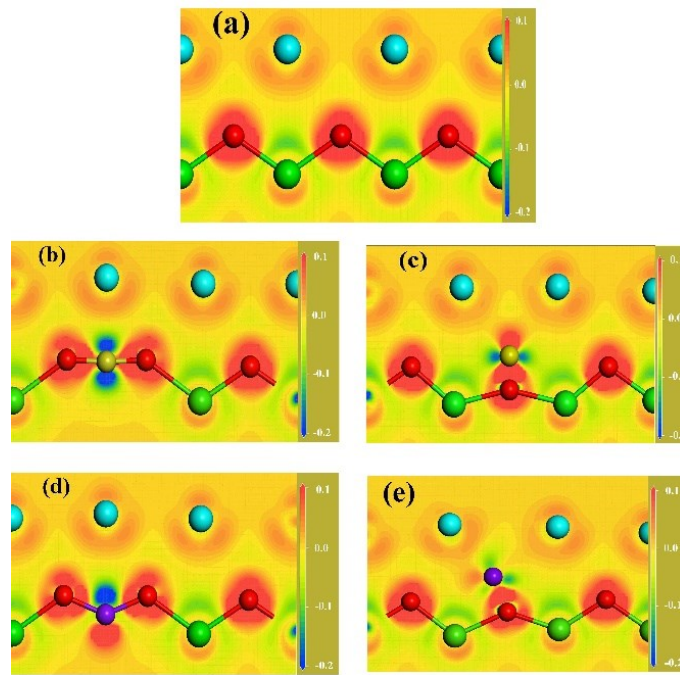


Fig. S7 The corresponding charge density difference of (a) pristine, (a) B_{Sub} , (b) B_{Inter} , (c) P_{Sub} , and (d) P_{Inter} doped single-layer BiOBr. The color scale runs from -0.2 at bottom (blue) to +0.1 electrons/ \AA^3 at the top (red). The green, golden, purple, red, and cyan spheres represent Bi, B, P, O, and Br atoms, respectively.