Supplementary Materials: Electronic Structure and Optical Properties of BiOI as a Photocatalyst Driven by Visible Light

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**Figure S1.** The comparison of total and partial density of states of BiOI by different density functional theory (DFT) methods.
**Figure S2.** The imaginary part and the real part of the dielectric functions of BiOI along two polarization direction and polycrystalline model by generalized-gradient approximation (GGA) method.

**Figure S3.** The imaginary part and the real part of the dielectric functions of BiOI along two polarization direction and polycrystalline model by on-site Coulomb interactions (GGA + U) method.