

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

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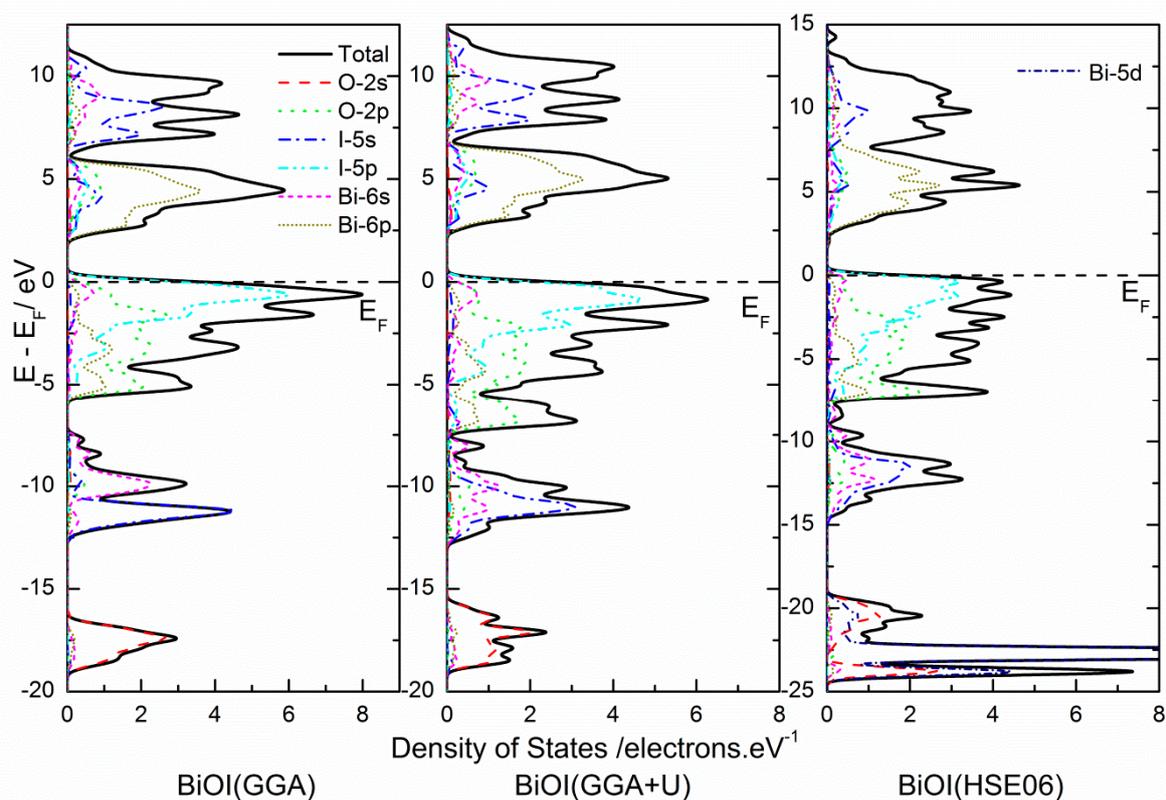


Figure S1. The comparison of total and partial density of states of BiOI by different density functional theory (DFT) methods.

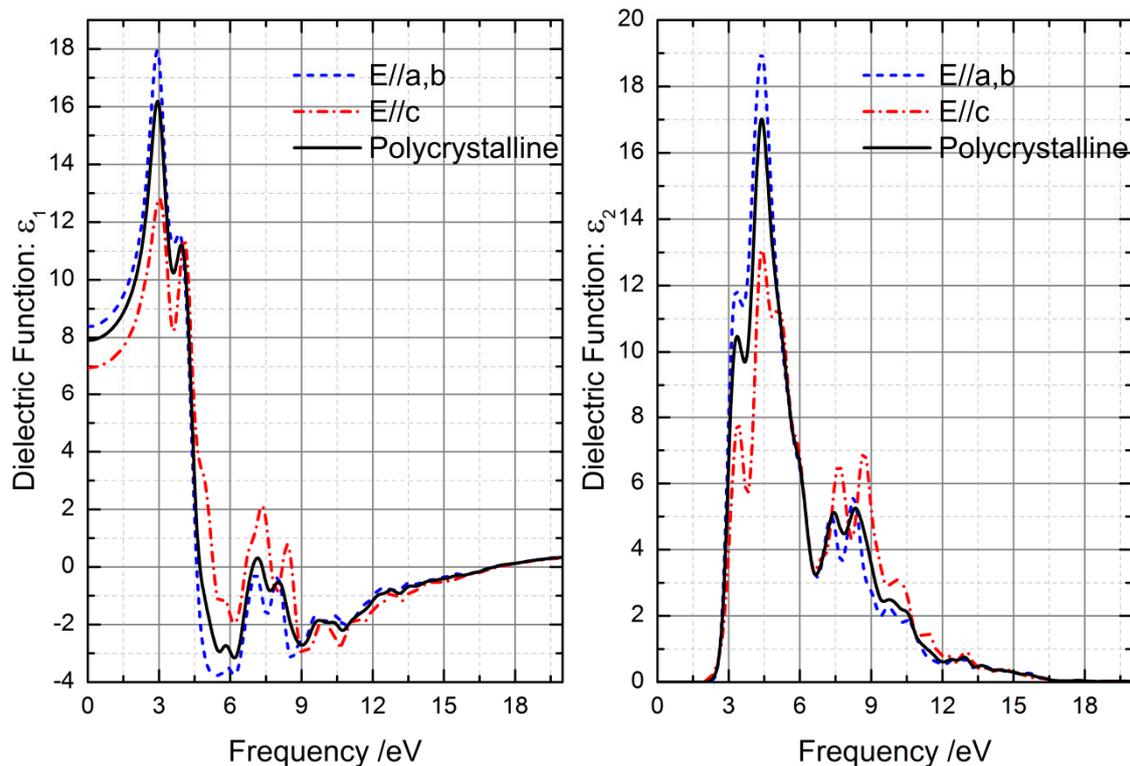


Figure S2. The imaginary part and the real part of the dielectric functions of BiOI along two polarization direction and polycrystalline model by generalized-gradient approximation (GGA) method.

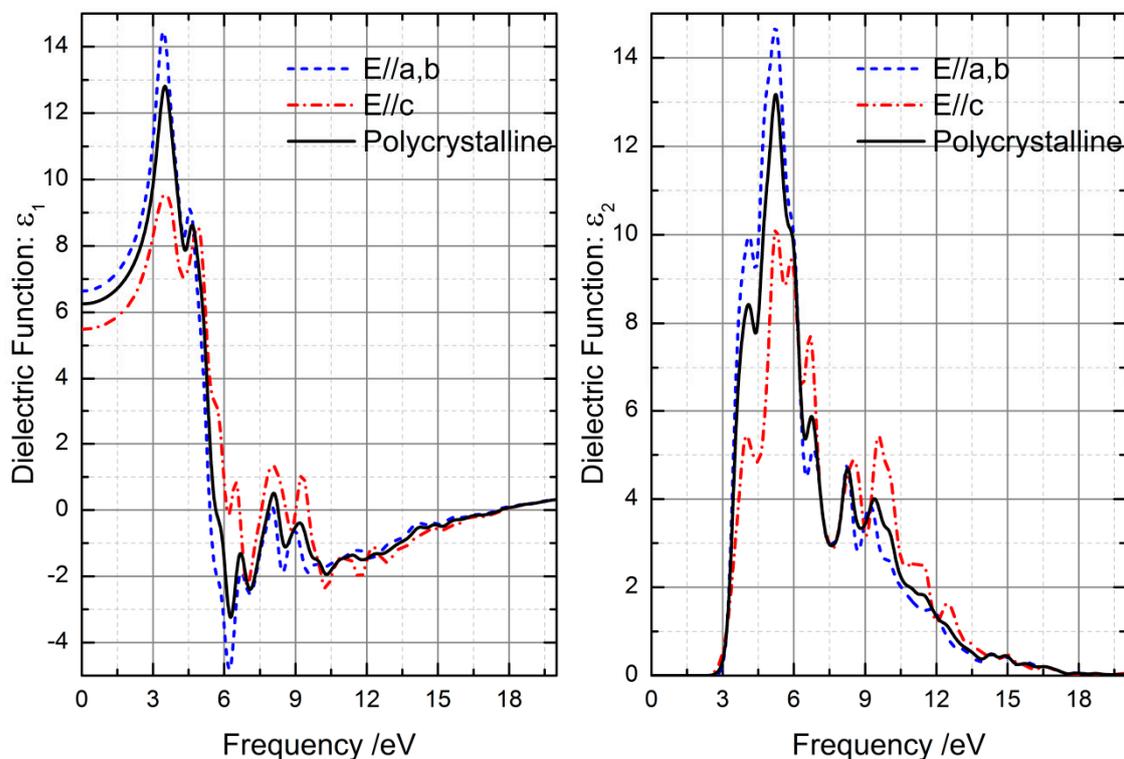


Figure S3. The imaginary part and the real part of the dielectric functions of BiOI along two polarization direction and polycrystalline model by on-site Coulomb interactions (GGA + U) method.