Supplementary Information (SI)

Insights into the mechanism of the enhanced visible-light photocatalytic activity of MoS$_2$/BiOI heterostructure under interfacial coupling

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Figure S1. Energy band structure of bulk BiOI using PBE method.
The state-of-the-art hybrid DFT approach based on the Heyd-Scuseria-Ernzerhof functional (HSE06) was used to calculate the electronic structures of MoS$_2$ after geometric optimization. In the default hybrid functional HSE06, the screening parameter $\mu$ and the mixing parameter $\alpha$ are set as 0.21 Å$^{-1}$ and 0.25, respectively. And norm-conserving pseudopotentials were used for all-electron HSE06 calculations. The calculated band gap of monolayer MoS$_2$ is 2.23 eV at the high symmetry K point, which is larger than the experimental band gap of about 1.9 eV$^{1,2}$.