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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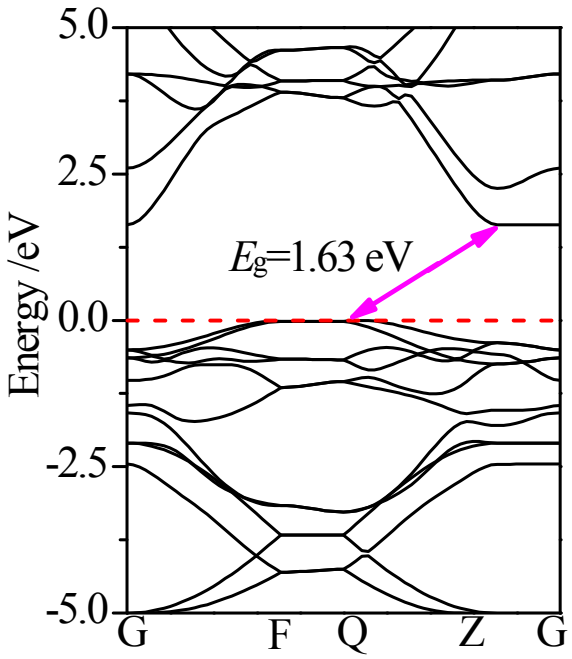

Figure S1. Energy band structure of bulk BiOI using PBE method.

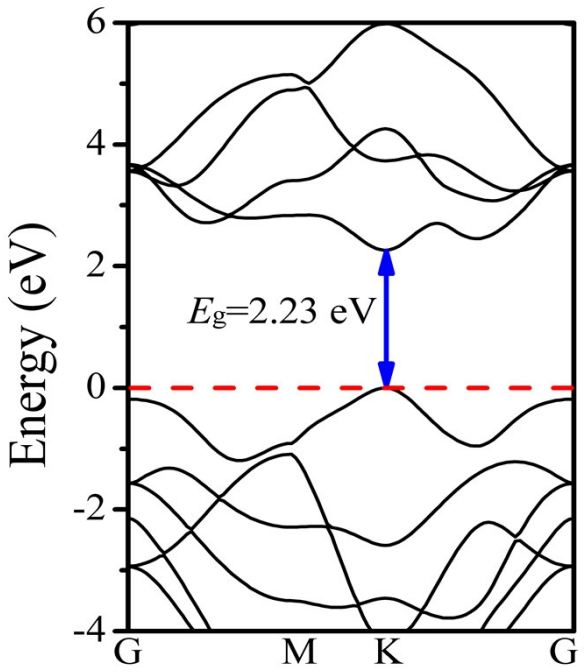

Figure S2. Energy band structure of monolayer MoS_2 using hybrid functional HSE06.

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 μ and the mixing parameter α 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]

[1] K. F. Mak, C. Lee, J. Hone, J. Shan and T. F. Heinz, Phys. Rev. Lett., 2010, 105, 136805.

[2] G. Eda, H. Yamaguchi, D. Voiry, T. Fujita, M. Chen and M. Chhowalla, Nano Lett., 2011, 11, 5111–5116.