

DFT investigation of Janus MoSSe/Ga₂SSe heterostructures for photocatalysis

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ABSTRACT

The two-dimensional Janus van der Waals heterojunctions, as novel asymmetric materials, have become highly promising photocatalysts due to their superior electronic structure and optical properties. In particular, the electronic properties of the type-2 band arrangement enable them to effectively separate photogenerated electrons and holes as Z-type photocatalysts [1], and to transport the charge carriers along different pathways [2], maintaining strong reduction and oxidation abilities, similar to green observations of plant photosynthesis [3,4].

In this work, we have systematically investigated the electronic structure and photocatalytic performance of MoSSe/Ga₂SSe heterojunctions using density functional theory (DFT). Considering the interlayer van der Waals interaction, two exchange-correlation functionals (PBE and HSE06) have been used. By screening different interlayer distances and stacking patterns, multiple stable configurations have been ultimately obtained. Based on these stable configurations, the HSE06 functional appears to be superior to the PBE one with a more accurate bandgap. Subsequently, we have calculated with the HSE06 functional a series of properties, including band structures, density of states, electrostatic potentials, charge density differences, optical absorption coefficients. After analysis, these heterojunctions exhibit strong absorption performance in the visible and ultraviolet light ranges.

References

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