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Role of MoS2 and WS2 monolayers on photocatalytic hydrogen production and the pollutant degradation of monoclinic BiVO4: a first-principles study

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ABSTRACT:

The global dependence on exhaustible fossil fuel resources has made the search for an alternative renewable and sustainable fuel more urgent. Photocatalysis has gained increasing consideration as a promising technology to solve problems associated with solar energy conversion. Fabricated m-$BiVO_4$-based heterostructures have shown improved photocatalytic activity for hydrogen evolution and pollutant degradation; however, a deeper understanding of the photocatalytic mechanism and the role of the monolayers is still lacking. Moreover, no theoretical studies have been carried out on MS_2/m-$BiVO_4$(010) heterostructures. In the present study, the roles of MoS_2 and WS_2 monolayers loaded onto a m-$BiVO_4$ surface for active photocatalytic hydrogen production and pollutant degradation are explored using first-principle studies. Herein, hybrid density functional calculations and a long-range dispersion correction method were used to investigate the charge transfer, electronic properties, photocatalytic activity and mechanism of the MS_2/m-$BiVO_4$(010) heterostructures. The results showed a narrow band gap, built-in potential and a type-II band alignment for the MS_2/m-$BiVO_4$(010) heterostructures compared to pure m-$BiVO_4$, which favour the separation and transfer of charge carriers and visible-light-driven activity. The MoS_2/m-$BiVO_4$ heterostructure showed a suitable band edge for hydrogen production and pollutant degradation compared to the WS_2/m-$BiVO_4$ heterostructure. This improvement was attributed to the role of the MoS_2 monolayer as an electron donor, the many reactive sites on the MoS_2 surface and the enhanced electron/hole pair separation of charge carriers at the MoS_2/m-$BiVO_4$(010) interface. Considering that the MS_2 monolayer coupled with m-$BiVO_4$ can restrain the electron–hole recombination rate without lattice distortion indicates that the heterostructure approach is better than the doping approach. Based on the analysis of the electronic properties, the MS_2/m-$BiVO_4$(010) heterostructures were shown to fit within the acceptable band gap and built-in potential range. The proposed theoretical design paves a way

for the effective and large-scale fabrication of m-$BiVO_4$-based photocatalyst for solar energy conversion and environmental remediation applications.