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Photocatalytic Properties of Intrinsically Defective Undoped Bismuth Vanadate (BiVO_4) Photocatalyst: A DFT Study

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Abstract

Monoclinic clinobisvanite BiVO_4 is one of the most promising photocatalyst due to its stability, low cost, narrow band gap, and suitable valence band maximum (VBM) position. The valence band maximum of about -7.10 eV at vacuum level was observed, which is well below the redox potential of water. However, the conduction band minimum, CBM of about -4.86 eV at vacuum level, which was responsible for its low efficiency. The presence of metal (Bi or V) vacancy changed the charge density and VBM of pristine BiVO_4 . Our calculated results revealed that 0.04% of the intrinsic Bi or V defects enhanced p-type conductivity and hence improved photocatalytic activity than O-interstitial in pristine BiVO_4 . The optical properties of both pristine and intrinsically defective BiVO_4 were calculated and analyzed with perspective of their photocatalytic properties. Conclusively, the role of Bi or V (metal) vacancies in pristine BiVO_4 was found to be significant than O interstitials in enhancing the photocatalytic properties regarding the solar water splitting.

Keywords: BiVO_4 , doping, vacancies, water splitting, conductivity, DFT

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