

Charge transport, interfacial interactions and synergistic mechanisms in BiNbO₄/MWO₄ (M = Zn and Cd) heterostructures for hydrogen production: insights from a DFT+U study

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ABSTRACT:

In the 21st century, the growing demand of global energy is one of the key challenges. The photocatalytic generation of hydrogen has attracted extensive attention to discuss the increasing global demand for sustainable and clean energy. However, hydrogen evolution reactions normally use the economically expensive rare noble metals and the processes remain a challenge. Herein, low-cost BiNbO₄/MWO₄(010) heterostructures are studied for the first time to check their suitability towards photocatalytic hydrogen production. A theoretical study with the aid of density functional theory (DFT) is used to investigate the synergistic effect, ionisation energy, electron affinities, charge transfer, electronic properties and the underlying mechanism for hydrogen generation of BiNbO₄/MWO₄(010) heterostructures. The experimental band gaps of bulk ZnWO₄, CdWO₄ and BiNbO₄ are well reproduced using the DFT+U method. The calculated band edge position shows a type-II staggered band alignment and the charge transfer between BiNbO₄ and MWO₄ monolayers results in a large interfacial built-in potential, which will favour the separation of charge carriers in the heterostructures. The effective mass of the photoinduced holes is higher compared to the electrons, making the heterostructures useful in hydrogen production. The relatively low ionisation energy and electron affinity for the heterostructures compared to the monolayers make them ideal for photocatalysis applications due to their small energy barrier for the injection of electrons and creation of holes. The BiNbO₄/MWO₄(010) heterostructures are more suitable for photocatalytic hydrogen production due to their strong reducing power relative to the H⁺/H₂O potential. This study sheds light on the less known BiNbO₄/ZnWO₄(010) heterostructures and the fully explored electronic and optical properties will pave way for future photocatalytic water splitting applications.