Abstract

Thin-film solar cells utilizing tin sulfide (SnS) and zinc sulfide (ZnS) represent a promising avenue for advancing photovoltaic technologies. This research investigates the stability and electronic properties of bulk, surface, and interface structures between SnS and ZnS, addressing the critical need to enhance semiconductor interface efficiency and stability. A comprehensive approach employs first-principles calculations and advanced high-throughput interface structure search techniques to explore the structural and electronic characteristics of SnS and ZnS heterostructures.

The analysis begins with an examination of the bulk and surface properties using density functional theory (DFT). Results indicate that bulk SnS has a bandgap of 0.92 eV, while ZnS demonstrates a wider bandgap of 2.08 eV. The evaluation of surface stability reveals that SnS (100) and ZnS (110) exhibit lower surface energies than other low-index surfaces, establishing them as the most stable surfaces. Additionally, the assessment shows slight decreases in bandgap for surface structures, with SnS (100) at 0.91 eV and ZnS (110) at 1.87 eV, attributed to surface reconstructions and atomic rearrangements.

The pristine SnS/ZnS interface structure, modeled from SnS (100) and ZnS (110) surfaces, exhibits a staggered type-II band alignment that facilitates spatial separation of electron and hole states, significantly reducing charge recombination. This energy offset is crucial for optimized photovoltaic performance, with the electronic structure featuring a conduction band offset of 0.18 eV, a valence band offset of 1.28 eV, and a bandgap of 0.857 eV. These findings highlight the potential of the SnS/ZnS interface to enhance thin-film solar cell efficiency.

To investigate the effects of defects on the SnS/ZnS heterostructure, various interface compositions were analyzed by incorporating ad-atoms such as Sn, S, and Zn. Six distinct configurations were generated to simulate realistic defect conditions. Results show that interfaces with balanced atomic distributions from both SnS and ZnS retained their semiconducting properties, with a bandgap of 0.43 eV. Conversely, configurations dominated by a single element whether Sn-rich, S-rich, or Zn-rich exhibited metallic behavior characterized by overlapping valence and conduction bands near the Fermi level. This metallic behavior adversely affects device performance by increasing recombination rates and hindering effective charge transport. Additionally, introducing ad-atoms significantly alters the electronic structure, leading to reduced bandgaps in certain configurations. For instance, (Sn,S)-rich and (Zn,S)-rich interfaces displayed bandgaps of 0.27 eV and 0.32 eV, respectively, due to additional electronic states introduced within the bandgap.

In summary, this research underscores the importance of interface engineering in the development of SnS/ZnS heterostructures for solar energy applications. By tailoring interface compositions and reducing defect-induced alterations in electronic properties, the structural and operational stability of SnS/ZnS-based solar cells can be improved. These results contribute to advancing the understanding of interface phenomena, providing insights that are essential for the development of reliable and sustainable photovoltaic technologies.

Keywords: Thin-film solar cells, SnS, ZnS, Interface stability, First-principles calculations, Electronic properties