First-Principles Simulation of Electronic Structure of Bulk and Surfaces SnS

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Tin mono-sulfide (SnS) is an IV-VI group semiconductor with a narrow band gap. SnS is a favorable candidate for photovoltaic applications due to its band gap, high absorption coefficient, low cost, low toxicity, abundance, ease of processing, and stable chemical and physical properties. An understanding of the thermodynamics and electronic properties of SnS would be helpful in designing high-performance photovoltaic devices. In this context, the influence of native surface defects and their electronic structures of SnS was calculated using the first-principles density functional theory.

In this study, we adopted the GGA-PBE exchange-correlation functional and the projector augmented wave (PAW) method. Our DFT simulations were performed using the Vienna *Ab Initio* Simulation Package (VASP). We performed the geometrical optimization of the surface and found that the surface reconstruction occurs. For the optimized geometries, we performed the *ab initio* electronic structure analysis.

It was found that a smaller band gap occurs from the surface electrical structure of the SnS (111) surface (0.23 eV) compared to its bulk SnS (0.92 eV) as shown in Fig 1. Furthermore, the electronic structure of the SnS surface with the presence of various native surface defects including vacancy, interstitials, and antisites was analyzed. The impurity on the surface caused a change in the electronic structure and metallic behavior in some cases. In this talk, we will demonstrate our analysis in more detail.

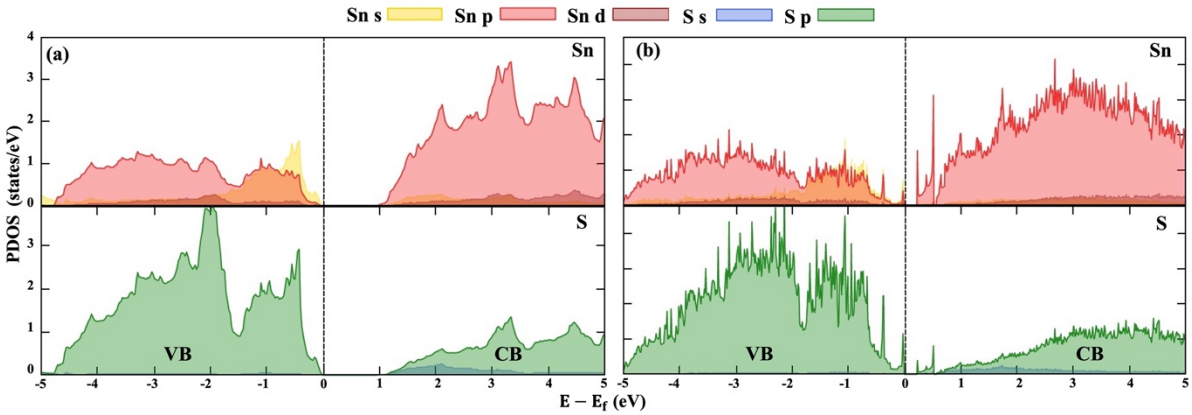

Fig. 1 Partial density of states of (a) bulk and (b) surface SnS, where the Fermi level (E_F) was set to zero on the energy scale.

Reference:

1. R. Dahule, C. C. Singh, K. Hongo, R. Maezono, and E. Panda. Anomalies in the bulk and surface electronic properties of SnS: effects of native defects. J. Mater. Chem. C 10, 5514 (2022).