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ELECTRICAL, OPTICAL, AND THERMAL PROPERTIES OF SnSe-BASED MATERIALS WITH HIGH THERMOELECTRIC PERFORMANCES

by
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Abstract

This thesis conducts a thorough exploration of the characteristics and prospective applications of Tin Selenide (SnSe), a pivotal semiconductor for advancing contemporary electronics and optoelectronics. The investigation mainly focuses on comprehending the alterations in SnSe's properties when doped with elements such as Hafnium, Zinc, Bismuth, Germanium, Sodium, Iodine, and Silicon. 2D-SnSe allotropes, when doped with Hafnium, have exhibited remarkable optical characteristics, especially in the δ-SnSe allotrope, rendering it adaptable for varied optical uses like solar cells and LEDs. Additionally, evaluations of elasticity show improved resilience and augmented in-plane stiffness owing to Hf doping, occasionally reducing ductility. The work uniquely emphasizes the properties of Zinc-doped α-SnSe, revealing semiconductor traits conducive for deep ultraviolet applications and capacitors, primarily due to a reduction in the dielectric constant in monolayer structures. The exploration further delves into the impacts of Silicon-doping on α-SnSe, identifying both diminished thermal conductivity and amplified electronic conductivity. The exploration of this thesis broadens to include the co-doping of SnSe, incorporating combinations like Bismuth and Zinc, Germanium and Zinc, and Sodium and Iodine. Introducing both Bismuth and Zinc to SnSe led to enhancements in electrical conductivity and exhibited elevated mechanical durability, underlining its potent thermoelectric capabilities. In contrast, structures co-doped with Germanium and Zinc showcased stability and heightened thermoelectric efficiency due to their p-type semiconductor properties. SnSe, when amalgamated with Sodium and Iodine, manifested a modified triclinic auxetic formation with a minimized bandgap, showing a high probability for uses in capacitors and solar cells owing to its elevated static dielectric constant and stability. Moreover, the attributes of π-SnSe have been scrutinized, highlighting its capabilities in various photovoltaic and thermoelectric applications due to its distinctive lattice constant and optical bandgap.

Keywords: Tin Selenide; Thermoelectric material; Density-functional theory; Ab initio calculations; Electronic properties; Optoelectronic properties; Mechanical properties; 2D materials.