ABSTRACT

Thermoelectric materials are functional materials capable of directly converting thermal energy into electrical energy, making them highly promising for waste heat recovery and the development of sustainable energy systems. The performance of thermoelectric materials is strongly governed by their electronic structure and charge transport properties, highlighting the importance of atomistic-level understanding. One material that has attracted significant attention in recent years is tin selenide (SnSe), which is known for its high thermoelectric performance. In this study, a computational investigation based on Density Functional Theory (DFT) was carried out to analyze the effect of nickel doping on the electronic and thermoelectric properties of SnSe. The calculations were performed on unit cell structures, supercell structures, and nickel-doped SnSe, with particular emphasis on band structure, projected density of states, Seebeck coefficient, electrical conductivity, and power factor at temperatures of 300 K and 600 K. The results show that pristine SnSe, both in the unit cell and supercell models, exhibits an indirect semiconducting band gap with values of 0.566 eV and 0.496 eV, respectively. The formation of the supercell does not alter the fundamental electronic properties of the material but only introduces minor adjustments to the band structure. Substitution of tin atoms with nickel induces significant changes in the electronic structure, characterized by the emergence of nickel 3d impurity states near the Fermi energy, leading to band gap closure and enhanced electrical conductivity, as supported by the projected density of states analysis. From a thermoelectric perspective, pristine SnSe shows relatively high Seebeck coefficient values at both temperatures. In contrast, nickel doping results in a pronounced reduction in the Seebeck coefficient due to the increased charge carrier concentration and the reduced asymmetry of the density of states around the Fermi energy. Although nickel doping enhances electrical conductivity, this increase is insufficient to compensate for the reduction in the Seebeck coefficient, causing the power factor of nickel-doped SnSe to remain lower than that of pristine SnSe. This indicates that, at the doping configuration and concentration considered in this study, the enhancement of the thermoelectric performance of SnSe has not yet been fully achieved, as the electronic structure modifications predominantly favor conductive behavior rather than thermoelectric response. Overall, this study confirms that SnSe remains a material with significant thermoelectric potential and demonstrates that further optimization of dopant type and doping concentration is required to achieve improved thermoelectric performance.

Keywords*: SnSe, Nickel doping, Density Functional Theory, electronic properties, band gap, thermoelectric properties, Seebeck coefficient, Boltzmann transport*