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A DFT insight into optoelectronics and transport phenomena in the monoclinic $BiGaIn_2S_6$ compound for applications in renewable energy

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ABSTRACT

The present study utilizes first-principles calculations grounded in density-functional theory (DFT) to examine the thermoelectric, electronic, elastic, optical, and structural properties of $BiGaIn_2S_6$. It is demonstrated that the approximated structural parameters (a, b, c, β, c/a, b/a), as well as atomic sites, correspond to the experimental data. Based on the measured elastic properties, it can be concluded that the investigated material possesses anisotropy and ductility. The computation of the electronic properties of our compound unveiled its semiconducting characteristics. The mBJ-LDA method was employed to ascertain that the compound exhibits an indirect band gap (Γ→Γ-E) of 2.711 eV. Based on the computational outcomes, it can be concluded that the real part of dielectric complex and refractive index exhibit a degree of anisotropy. The compound exhibits promising potential for optoelectronic applications due to its tolerable values of optical properties such as optical conductivity, absorption aspect, refractive index, and reflectivity. The positive Seebeck coefficient obtained from the calculation indicates that this compound can be classified as a *p*-type material. The semiconductor $BiGaIn_2S_6$ exhibits a maximum ZT value of 0.98741 when the charge carrier concentration is increased to $n = 0.14494 \times 10^{22}$ cm^{-3} or when the chemical potential lowers to 0.47499 Ryd. The material being studied demonstrates potential uses in the fields of thermoelectric and optoelectronic devices.

1. Introduction

There has been a significant increase in the need for energy in recent years, leading to heightened efforts in the pursuit of alternative energy sources that are independent of fossil fuels or traditional methods. The use of renewable energy sources has led to a shift in global attention [1, 2]. The conversion of thermal and electrical resources into useable energy through the process of thermoelectricity is a captivating approach for the production of renewable energy and the effective utilization of waste heat, as supported by previous scholarly works [3–5]. The assessment of the effectiveness of thermoelectric (TE) materials is conducted through the utilization of the figure of merit (ZT). The calculation is performed utilizing the formula $ZT = \frac{\sigma S^2 T}{k_L + k_e}$, in which S denotes the Seebeck coefficient, σ represents the electrical conductivity, T signifies the absolute temperature, and k_e and k_L refer to the electronic and lattice contributions to the total thermal conductivity k_T [1,6]. Achieving an ideal figure of merit (ZT) requires a substantial thermoelectric power factor (σS^2) and low total thermal conductivity (k_T). Presently, researchers are actively involved in endeavors aimed at enhancing the thermoelectric power factor and reducing the total thermal conductivity. These efforts are based on a comprehensive understanding of the principles underlying thermoelectricity [7–9]. The deployment of energy filtration and the incorporation of dislocations and point defects are effective strategies for reducing total thermal conductivity. Previous studies have demonstrated the efficacy of these tactics in augmenting multi-wavelength phonon scattering, and they have also been suggested as a means to raise power factor. Novel thermoelectric materials exhibiting favorable ZT values are now under development, leading to the emergence of revolutionary technological breakthroughs [9]. The determination of a material's suitability as a thermoelectric (TE) material is contingent upon its bandgap and stability, as evidenced by the extant body of literature [10]. Nevertheless, there has been a growing interest in bismuth-based compounds in the past few decades because of their remarkable thermoelectric figure of merit (ZT). Due to their wide range of physical, chemical, and catalytic properties, these compounds

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