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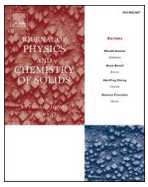

Enhancing the thermoelectric performance of $BiGa_2X_4$ (X=S, Se) P-type semiconductors by optimizing charge carrier concentration or chemical potentials

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ABSTRACT

We present an extensive analysis of the structural, electronic, optical, elastic, and thermoelectric properties of $BiGa_2X_4$ compounds, where X represents either sulfur (S) or selenium (Se). Our approach employed the all-electron full potential linearized augmented plane wave (FP-LAPW) technique, offering a comprehensive understanding of these materials' characteristics. The calculated lattice constants (a), the unit cell height (c), and the c/a ratio closely match experimental data, affirming the accuracy of our calculations. A pivotal focus of our study was on the electronic properties, including the indirect bandgaps (A → M − Γ) and (M → A). We found that $BiGa_2S_4$ exhibited an indirect bandgap (E_g) of 2.504 eV, while $BiGa_2Se_4$ possessed a slightly lower value of 1.878 eV. This variation was primarily attributed to the intricate interactions among bismuth, sulfur, and selenium atoms, particularly involving $p-p$ orbital interactions. Additionally, we explored the optical characteristics of these compounds, determining their maximum absorption wavelengths. $BiGa_2S_4$ exhibited an absorption peak at 4.476 eV, whereas $BiGa_2Se_4$ displayed a slightly lower maximum absorption at 3.741 eV. Moreover, $BiGa_2Se_4$ showcases a higher dielectric constant, which augments its potential for optoelectronic applications. A critical aspect of our research is the assessment of the elastic properties, elucidating that both compounds exhibited fragility and anisotropy. We observed that at 300 K, the lattice thermal conductivity (k_L) for $BiGa_2S_4$ and $BiGa_2Se_4$ was measured at 1.57 W/mK and 1.14 W/mK, respectively, indicating low thermal conductivity. At 1000 K, both $BiGa_2S_4$, and $BiGa_2Se_4$ exhibit significant ZT values of 0.8389 and 0.8722, respectively. The ZT values of the p-type semiconductors are notably higher than those of the n-type. At T = 900 K, the optimized ZT values for $BiGa_2S_4$, and $BiGa_2Se_4$ are found to be 0.82909 and 0.90548, respectively. Achieving these values requires either increasing the concentration of charge carriers to $n = 0.11715 \times 10^{22}$ cm^{-3} for $BiGa_2S_4$ and $n = 0.0812 \times 10^{22}$ cm^{-3} for $BiGa_2Se_4$, or reducing the chemical potentials by 0.40151 Ryd and 0.38001 Ryd, respectively.

1. Introduction

Perovskites and inorganic quantum dot solar cells are currently among the most popular and efficient photovoltaic (PV) technologies [1]. These technologies have garnered significant attention due to their potential for cost-effectiveness, compact size, and higher efficiency across a wider spectrum of light intensities compared to existing or emerging technologies. As a result, they are considered as promising

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