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Intrinsic thermoelectric performance enhancement of $Bi_2Al_4S_8$ via carrier concentration and chemical potential engineering

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ABSTRACT

This study presents a comprehensive computational analysis of the structural, electronic, optical, elastic, and thermoelectric properties of $Bi_2Al_4S_8$, a metastable tetragonal compound with promising applications in optoelectronics, photovoltaics, and thermoelectric energy conversion. Density functional theory (DFT) calculations, employing both the LDA and the mBJ potential, were used to determine the optimized structural parameters, electronic band structure, density of states, optical response, elastic constants, and thermoelectric transport coefficients. $Bi_2Al_4S_8$ exhibits an indirect bandgap of 2.589 eV (LDA) and 3.234 eV (mBJ), making it suitable for photovoltaic applications. Optical property analyses reveal strong visible-light absorption, a static dielectric constant of 6, and a refractive index of 2.4, indicating its potential for efficient light-harvesting devices. The mechanical stability of $Bi_2Al_4S_8$ is confirmed by its elastic constants, with a bulk modulus of 70.1896 GPa and low anisotropy.

Furthermore, thermoelectric performance evaluations indicate that $Bi_2Al_4S_8$ exhibits an improved thermoelectric figure of merit (ZT), increasing from 0.6412 at $n_0 = 65.7670 \times 10^{19}$ cm^{-3} to 0.9524 at $n = -29.26049 \times 10^{21}$ cm^{-3} or when the chemical potential shifts from 0.20424 eV to 0.3117 eV. This enhancement is achieved through intrinsic tuning of the carrier concentration and chemical potential, without the introduction of extrinsic dopants. These findings highlight $Bi_2Al_4S_8$ as a non-toxic, mechanically robust, and multifunctional material, encouraging further experimental validation and advancing its prospects for integration into next-generation renewable energy and thermoelectric technologies.

1. Introduction

Over the past two decades, quasi-binary systems incorporating sesqui-chalcogenides (M_2X_3), where M denotes group 13 or 15 elements and X represents chalcogens, have attracted substantial attention due to their remarkable physical properties. These materials exhibit high piezoelectricity, ferroelectricity, and ferroelasticity, making them indispensable for various advanced technological applications [1–4]. Among these properties, thermoelectric performance has emerged as a particularly promising area of research, driven by the growing demand for efficient energy conversion technologies.

Thermoelectric materials, which can directly convert heat into electricity, are critical for waste heat recovery, sustainable energy generation, and advanced cooling systems. The efficiency of thermoelectric materials is quantified by the dimensionless figure of merit $ZT = \frac{\sigma S^2 T}{(k_l)}$, where S is the Seebeck coefficient, σ is the electrical conductivity, T is the absolute temperature, and k_T is the total thermal conductivity (comprising electronic and lattice contributions). Achieving a high ZT requires a delicate balance between these parameters, often pursued through strategies such as band engineering, nanostructuring, and defect engineering.

For instance, Bi_2Te_3-based materials are well-known for their excellent thermoelectric performance at near-room temperatures. In particular, $Bi_{2-x}Sb_xTe_3$ samples exhibit high ZT values: 1.04 at 440 K for MW-Bi_2Te_3 and 0.76 at 523 K for MW-$Bi_{0.5}Sb_{1.5}Te_3$, while MA-Bi_2Te_3 and MA-$Bi_{0.5}Sb_{1.5}Te_3$ samples achieved maximum ZT values of 0.74 at 460 K and 0.27 at 300 K, respectively, as n- and p-type materials [5].

Additionally, $PbTe$ and other lead chalcogenide-based compounds (e.g., $PbSe$, PbS) are prominent thermoelectric materials, particularly effective in the mid-temperature range (600–800 K). Single-phase $PbTe$

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