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Comprehensive DFT study of $ZnGe_{1-x}Si_xAs_2$ alloys: Insights into structural, electronic, optical, and thermoelectric properties

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ABSTRACT

The substitution of Ge with Si in the $ZnGeAs_2$ chalcopyrite semiconductor and its impact on structural, electronic, optical, and thermoelectric properties have been systematically studied using density functional theory. This study demonstrates the tunability of material properties through alloying, revealing novel insights into the $ZnGe_{1-x}Si_xAs_2$ (x = 0–1) system. The exchange-correlation energy was evaluated using the local density, generalized gradient, and modified Becke-Johnson schemes, ensuring accurate predictions. The calculated structural parameters and band gap energies for $ZnGeAs_2$ and $ZnSiAs_2$ exhibit excellent agreement with experimental data, validating the reliability of our approach.

Both $ZnGeAs_2$ and $ZnSiAs_2$ exhibit semiconductor characteristics with a direct band gap at the Γ point, making them promising for optoelectronic applications. The alloys show anisotropic optical behavior, with $ZnGe_{0.25}Si_{0.75}As_2$ demonstrating the highest refractive index and energy loss, making it a strong candidate for UV-shielding and optoelectronic devices. Thermoelectric analysis identifies $ZnGe_{0.75}Si_{0.25}As_2$ as the optimal composition, achieving a maximum Seebeck coefficient of 228.26 μV/K at 800 K. Moreover, by tuning the carrier concentration to $n = 4.87 \times 10^{18}$ cm^{-3}, the Seebeck coefficient can be significantly enhanced to 449.44 μV/K. These findings highlight the potential of Si substitution to enhance material performance and provide a roadmap for tailoring the structural, optical, and thermoelectric properties of chalcopyrite semiconductors.

1. Introduction

The rapid advancements in renewable energy technologies have amplified the need for high-performance materials with tailored properties for specific applications. Among these, chalcopyrite compounds have emerged as some of the most promising materials, primarily due to their remarkable electrical, optical, and thermoelectric properties [1]. These properties make chalcopyrites highly versatile, enabling their use in various technological domains, including photovoltaic detectors, multijunction solar cells, light-emitting diodes (LEDs), modulators, and nonlinear optics [2–5]. Furthermore, their tunable band gaps position them as excellent candidates for infrared detectors, opening avenues for their use in optoelectronics and energy harvesting applications [6].

Within the ternary chalcopyrite family, compounds with the general formula A-B-C_2 (where A = Mg, Zn, Cd; B = Si, Ge, Sn; C = P, As, Sb) have gained significant attention due to their direct band gaps and highly adjustable properties. In particular, pnictide-based chalcopyrites like $ZnGeAs_2$ and $ZnSiAs_2$ stand out for their favorable electronic and optical behaviors. Their ability to balance good electronic conductivity with low thermal conductivity further enhances their potential for thermoelectric applications, especially in energy conversion and waste heat recovery systems.

Significant progress has been made in the study of these materials through both experimental and theoretical approaches. Experimentally, $ZnGeAs_2$ has been investigated for its structural and optoelectronic properties by Drahokoupil et al. [7], Solomon et al. [8], and Shah et al. [9], while related compounds such as $ZnSiAs_2$, $ZnGeP_2$, and $CdGeP_2$ have been explored by Masumoto et al. [10]. On the theoretical front,

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