

Evaluating the effect of crystal structure on thermoelectric performance of promising $\text{Cu}_2\text{FeSnS}_x\text{Se}_{4-x}$ diamond-like materials for sustainable applications

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Thermoelectric technologies are attracting more and more attention as a sustainable solution to overcome the global energy challenge and reduce greenhouse gas emissions. [1] By enabling the direct conversion of heat into electricity, thermoelectric materials are promising for power generation and solid-state cooling. [2]. The most common thermoelectric materials, such as Bi_2Te_3 and PbTe or GeTe tellurides, often contain rare and toxic elements, and therefore the development of highly efficient and eco-friendly TE materials for energy conversion remains a significant challenge. [3]. Diamond-like chalcogenides, such as $\text{Cu}_2\text{FeSnS}_x\text{Se}_{4-x}$, are prospective due to their content of earth-abundant and non-toxic elements, high thermal stability and their tunable properties.

This study focuses on investigating a new promising eco-friendly material, $\text{Cu}_2\text{FeSnS}_x\text{Se}_{4-x}$ ($x = 0, 1, 2, 3, 4$) with enhanced thermoelectric performance achieved by tuning the sulfur (S) and selenium (Se) content. Using this approach, we can enhance the crystal structure and improve thermoelectric performance. The material shows structural stability, inherently low thermal conductivity ($\sim 0.7 \text{ W}\cdot\text{m}^{-1}\cdot\text{K}^{-1}$ at 773 K), combined with a promising value of Seebeck coefficient 212 – 300 $\mu\text{V K}^{-1}$ at , and optimal value of carrier concentration $\sim 1.38 \times 10^{20} \text{ cm}^{-3}$ making it a potential candidate for thermoelectric applications. Rietveld refinement revealed that the material belongs to the tetragonal crystal structure system (space group $I4_2m$), and shows no significant presence of secondary phases. The single-phase structure provides structural homogeneity and is reliable to estimate the intrinsic thermoelectric properties of the material. The substitution of selenium leads to an improvement in the power factor (PF), which consequently results in an enhancement of the dimensionless figure of merit (ZT).

The significance of this work lies in introducing a new perspective on diamond-like structure (DLS) materials and demonstrating their potential as efficient and environmentally friendly candidates for thermoelectric energy conversion. By leveraging compositional tuning and structural optimization, we reveal promising pathways to enhance their performance and sustainability.

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