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Ternary Germanide Li_2ZnGe: A New Candidate for High Temperature Thermoelectrics

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Abstract

Experimentally studied F-43m structured Li_2ZnGe ternary germanide is investigated theoretically by evaluating the electronic structure, thermodynamic stability and thermoelectric efficiency using the full-potential method. The calculated lattice parameter and structural characterization agree well with the experimental results. The thermoelectric properties are calculated within the temperature range of 0-1200 K. The computed value of figure of merit is 0.40 at 1200 K and Seebeck coefficient is 150 μV/K specifying n-type nature. The electrical conductivity is high mainly due to high carrier mobility, while total thermal conductivity is moderate due to low lattice thermal conductivity. The estimated figure of merit projects it as a potential thermoelectric material for high temperature power generation.

Keywords: Ternary germanide; Electronic structure; Band structure; Thermoelectric properties; Thermodynamic properties.

I. Introduction

Applications of thermoelectric materials at cryogenic as well as thermogenic temperatures has given rise to considerable interest from the scientific community probably due to the severe exploitation of fossil fuels and an ever-increasing demand for a sustainable supply of energy [1-3]. They are envisaged with the ability to directly convert thermal and electrical energy to provide an alternative route for power generation and refrigeration. The factor establishing the efficiency of conversion is defined by dimensionless figure of merit (zT) [4-9]

$$zT = \frac{S^2 \sigma T}{\kappa_{electronic} + \kappa_{lattice}} \qquad (1)$$