


# Structural, electronic, mechanical, and thermoelectric properties of LiTiCoX (X = Si, Ge) compounds

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## Summary

In the present work, we have used the first principles approach combined with semi classical Boltzmann Transport equations to calculate the structural, mechanical, electronic, and thermoelectric properties of LiTiCoX (X = Si, Ge). These materials are indirect band gap semiconductors with band gap 1.22 eV for LiTiCoSi and 1.09 eV for LiTiCoGe, respectively. Both materials are mechanically and dynamically stable. At room temperature, the value of Seebeck coefficient is 2016  $\mu\text{V}/\text{K}$  (1799  $\mu\text{V}/\text{K}$ ) for LiTiCoSi (LiTiCoGe) and the electrical conductivity is in the order of  $10^6$  S/m for both materials. The highest value of figure of merit recorded is 0.14 (LiTiCoGe) and 0.10 (LiTiCoSi) for p-type doping at 700 K temperature in both the materials. Hence, the theoretical results can be the compelling evidences to investigate the present materials experimentally in future.

## KEYWORDS

band structure, density functional theory, quaternary Heusler compounds, thermoelectric materials

## 1 | INTRODUCTION

The present era of research is oriented to introduce pollution free energy technologies especially, the transformation of waste heat into electrical energy. The waste heat is available everywhere, that is, in all the electrical and electronic devices, industrial regions, data centers, domestic appliances, furnaces, and in all kinds of the automobiles. This low-grade waste can be easily utilized by its conversion into electric energy with the aid of Thermoelectric Modules (TEM). These modules are based on the thermoelectric materials, which are capable of generating thermo e.m.f against any temperature gradient<sup>1-4</sup> that can be availed from the waste heat sources. Thermoelectric modules being free from moving parts, toxic materials and pollution, and their simple designing makes this technology to be regarded as the Green Technology<sup>5</sup> of energy generation. These materials can also be fabricated in nano-

dimensions to achieve chip sized TEM.<sup>6-9</sup> These robust applications of thermoelectric materials are in quest of a key to overcome the world energy crisis without any content of pollution. The performance of a thermoelectric device is characterized by the dimensionless figure of merit (ZT), which is defined as:

$$ZT = \frac{S^2 \sigma}{k_e + k_l} T \quad (1)$$

where T,  $\sigma$ , S,  $k_l$ , and  $k_e$  are absolute temperature, electrical conductivity, Seebeck coefficient, lattice thermal conductivity, and electronic thermal conductivity, respectively. To attain a better thermoelectric performance, the material should have high power factor ( $S^2 \sigma$ ) and low thermal conductivity ( $k = k_e + k_l$ ), which is a challenging task now a days. Even though the figure of merit (ZT) for some of the thermoelectric compounds like CoSb<sub>3</sub> and Bi<sub>2</sub>Te<sub>3</sub>