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First principles calculations to investigate Li-based quaternary Heusler compounds LiHfCoX (X = Ge, Sn) for thermoelectric applications

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Tavneet Kaur[1], **Jaspal Singh**[2,*], **Megha Goyal**[1], **Kulwinder Kaur**[3], **Shakeel Ahmad Khandy**[4,*], **Muzzammil Ahmad Bhat**[5], **Utkir Bahodirovich Sharopov**[6], **Shobhna Dhiman**[3], **Aadil Fayaz Wani**[3], **Bindu Rani**[3], **M M Sinha**[1] and **S S Verma**[1]

[1] Department of Physics, Sant Longowal Institute of Engineering and Technology (Deemed University), Longowal-148106, Sangrur (Pb), India
[2] Department of Physics, Mata Sundri University Girls College, Mansa-151505, Punjab, India
[3] Department of Applied Sciences, Punjab Engineering College (Deemed to be University), Chandigarh (160012), India
[4] ZJU-Hangzhou Global Scientific and Technological Innovation Center, School of Micro-Nano Electronics, Zhejiang University, 311200-People's Republic of China
[5] Department of Physics, Islamic University of Science and Techonology, Awantipora, Jammu and Kashmir 192122, India
[6] Solar Thermal and Power Plants Laboratory, Physical-Technical Institute, Uzbekistan Academy of Sciences, Chingiz Aitmatov St., 2,100084 Tashkent, Uzbekistan
* Authors to whom any correspondence should be addressed.

E-mail: jaspalsliet@gmail.com **and** shakeelkhandy11@gmail.com

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Abstract

In the last few decades, varieties of semiconductors have been explored for electronic and thermoelectric applications. As a result of these motivations, the current research work investigates the structural, electronic, vibrational, elastic, mechanical, thermodynamic, and thermoelectric properties of two quaternary Heuslers (QHs), namely LiHfCoGe and LiHfCoSn (both of which are semiconducting in nature), within the computational framework of DensityFunctional Theory (DFT) and Boltzmann transport equations. Both alloys display the p-type semiconductivity, dynamical stability and crystallize in the FCC cubic structure within F-43 m space group. The high Seebeck coefficient values pronounce an excellent and fundamental thermoelectric character. The large melting points expose their scope in the high-temperature regions. However, all of the thermoelectric characteristics are also measured in terms of the estimated relaxation time using deformation potential theory. Even though the figure of merit (ZT) is in the middle of the pack yet better than many compounds of the same sort. The impact of spin–orbit coupling on the thermoelectric characteristics is also examined. The practical utilization of the materials can be evaluated from the elastic and mechanical properties that are favorable in manufacturing efficient and reliable Thermoelectric Modules at high-temperatures.

1. Introduction

The pollution-free energy generation technologies always attract the researchers for the future prospectus. Thermoelectricity is such a reliable technology to utilize waste heat by conversion into electrical energy [1–5]. Due to the pollution-free operation of the thermoelectric modules (concerned with thermoelectric materials), for future generations, thermoelectricity has been dubbed 'A Green Technology' [6]. Figure of Merit (ZT), a dimensionless metric used to measure a material's thermoelectric efficiency, using the relation:

$$\mathrm{ZT} = \frac{S^2\sigma}{k_e + k_l}\mathrm{T} \tag{1}$$

Where the Seebeck coefficient, electrical conductivity, and absolute temperature are represented by S, σ, and T, respectively. The symbols k_e and k_l in this context refer to the thermal conductivity's electronic and lattice