Bull. Mater. Sci. (2023)46:103
https://doi.org/10.1007/s12034-023-02945-z
© Indian Academy of Sciences

LiNbCoX (X = Al, Ga) quaternary Heusler compounds for high-temperature thermoelectric properties: a computational approach

JASPAL SINGH[1], TAVNEET KAUR[2,*], AMRIT PAL SINGH[3,4], MEGHA GOYAL[2], KULWINDER KAUR[5], SHAKEEL AHMAD KHANDY[6], ISHTIHADAH ISLAM[7], AADIL FAYAZ WANI[8], RAM KRISHAN[9], M M SINHA[2] and S S VERMA[2]

[1] Department of Physics, Mata Sundri University Girls College, Mansa, PB 151505, India
[2] Department of Physics, Sant Longowal Institute of Engineering and Technology (Deemed University), Sangrur, PB 148106, India
[3] Health Physics Unit, Nuclear Fuel Complex, Hyderabad 500062, India
[4] Homi Bhabha National Institute, Mumbai 400094, India
[5] Department of Physics, Mehar Chand Mahajan DAV College for Women, Chandigarh 160036, India
[6] Zhejiang University, Hangzhou 310027, China
[7] Department of Physics, Jamia Millia Islamia, New Delhi 110025, India
[8] Department of Applied Sciences, Punjab Engineering College (Deemed to be University), Chandigarh 160012, India
[9] Department of Computer Science, Mata Sundri University Girls College, Mansa, PB 151505, India
*Author for correspondence (tavneetkaur001@gmail.com)

MS received 14 November 2022; accepted 2 February 2023

Abstract. Researchers have looked into quaternary Heusler (QH) compounds for their potential use in futuristic gadgets like photovoltaic cells, optical fibres, thermoelectric modules and spintronic sensors. As per such motivations and research interests, here we are presenting two recently reported Li-based QH compounds LiNbCoAl and LiNbCoGa which are stabilized into face-centred cubic structure of space group F-43m with semiconducting nature. These compounds exhibit high melting temperatures, showing the p-type semiconducting nature and are found to have advantageous thermoelectric capabilities in the high-temperature range. Additionally, the dynamical stability and appropriate elastic and mechanical characteristics for the foundation of effective thermoelectric modules in the temperature range of 1600 K enhance their scientific and technical scope. The electronic band structure is discussed along with the density of states for the better understanding of the electrical properties. The thermodynamic response up to a temperature of 1600 K is also examined for understanding in terms of free energy, specific heat at constant volume and entropy. The special dependences in the two and three dimensions are applied and investigated to characterize the anisotropic nature. However all the required thermoelectric properties are calculated and presented, and the highest figure of merit value at 1600 K for both materials is 0.47 for LiNbCoAl and 0.56 for LiNbCoGa, respectively. As per their excellent practical properties, the current study asserts that both QH compounds should really be considered for energy conversion techniques in high-temperature environments. For the complete study prospectus, these materials are being disclosed for the first time here.

Keywords. Lattice thermal conductivity; phonons; thermoelectric characteristics; density functional theory; the figure of merit.

1. Introduction

The focus of current research is on ways for creating pollution-free energy that can considerably aid in solving the world's energy crisis. Thermoelectricity is a viable option for turning excess heat into usable electricity [1–5]. Since the functioning of thermoelectric modules (related to thermoelectric materials) produces no pollution, thermoelectricity has been named 'A Green Technology' for the future [6]. It is possible to evaluate the thermoelectric efficiency of a material using the relation utilizing a dimensionless measure known as the Figure of Merit (ZT) for measuring the thermoelectric efficiency of material:

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

Here the symbols have their conventional meanings. However the symbols k_e and k_l refer to the electronic and lattice portions of the thermal conductivity in this context, respectively, and their sum ($k_t = k_e + k_l$) denotes the

Published online: 19 May 2023