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Electronic structure, phonon stability, mechanical and high-temperature thermoelectric properties of Li-based quaternary Heusler alloys

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ABSTRACT

This paper presents a detailed discussion of thermoelectric and electronic properties of newly designed Li-based Heusler compounds (LiScPtGe, LiYPtSn, LiYPdPb) using Boltzmann transport theory alongside the first-principles calculations. Our investigations predict that these materials exhibit band gaps 0.76 eV (for LiScPtGe), 0.67 (for LiYPtGe) and 0.21 eV (for LiYPdPb), respectively. All the reported materials are indirect band gap semiconductors; mechanical and dynamical stability is also confirmed. At 300 K, the lowest value of lattice thermal conductivity is observed in LiYPdPb (21.64 Wm^{-1} K^{-1}), which is very small as compared to the other two materials. The perceived value of the figure of merit (ZT) is 0.61 (for LiScPtGe), 0.52 (for LiYPtSn) and 0.35 (for LiYPdPb) respectively, and probably ensure a considerable thermoelectric efficiency of these newly designed materials.

1. Introduction

The world energy crisis is a blazing challenge due to the demand and consumption reliance of the present lifestyle. The researchers are focusing on pollution-free energy generation techniques in comparison to the traditional energy sources; later being responsible for the huge pollution and difficult to use or handle. In the present scenario, the demand for pollution free and easily available energy sources is related everywhere and anywhere. Thermoelectricity is one of the techniques that fulfills these specific energy requirements. The idea of direct energy conversion from heat to electrical energy [1,2] is the foundation of thermoelectricity. The parameter known as a Figure of merit ($ZT = \frac{S^2\sigma}{k_e+k_l}T$) evaluates the performance of thermoelectric materials. Here, S, σ, and T arethe Seebeck coefficient, electrical conductivity, and absolute temperature respectively. In denominator, $k_e + k_l$ is defined as total thermal conductivity summed up as combination of electronic and phononic thermal conductivity. There are few efficient thermoelectric materials such as Bi_2Te_3 and $CoSb_3$ etc. where the figure of merit approaches unity (ZT ≈ 1) [3–5]. Motivated by these materials, researchers are exploring other efficient materials of different categories. In 1903, Friedrich Heusler introduced a novel class of materials conceded as Heusler materials which are stable in the F-43m space group and structure is face-centered cubic (FCC).

Heusler compounds are intermetallic compounds in nature. Due to their semiconducting behavior, these materials display transpiring applications in the field of optical, photovoltaic, and thermoelectrics. These materials augmented with mechanical stability and 2D exfoliation properties play a specific role in thermoelectric generation devices [6–8]. Full and half-Heuslers have been familiar as effective components for topological devices, spintronics, superconductor applications, and ferromagnetism [9–12]. Striking characteristics of Heusler compounds such as the presence of non-toxic elements, semiconductor nature, thermodynamic and mechanical stability, and availability at low cost gained attraction in the research community [13–17].

The materials belonging to this category such as TiCoSb, Fe_2XY (X = V, Ti, Y=Al, Si), TiNiSn and FeVSb whose elements are easily available

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