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Electronic structure, elastic and transport properties of new Palladium-based Half-Heusler materials for thermoelectric applications

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ABSTRACT

Electronic structure with reference to bandgap energies play a significant role in deciding the dimensionless figure of merit (ZT), which in turn is used to identify the thermoelectric performance of a material. Slater Pauling arrangement of valence electrons and band orientations along k-space decide the effective mass of electrons/holes in the corresponding band valleys of PdMX (M= Sc, Y, and X = P, As, Sb) semiconductors. A detailed picture of the electronic structure and transport properties is rigorously established in this report. Calculations of elastic constant, phonon dispersion and formation (cohesive) energy reveal that these alloys are mechanically, dynamically, and chemically stable materials. Substantially, low lattice thermal conductivity is observed in the range 4.57 W/mK for PdScAs and 11.51 W/mK for PdYSb alloy. The relaxation time and effective mass are calculated with Deformation potential theory. The maximum calculated ZT value for PdScP, PdScAs, PdScSb, PdYP, PdYAs and PdYSb are 0.28, 0.33, 0.19, 0.43, 0.44 and 0.27 respectively.

1. Introduction

There is a large consumption of fossil fuels on a global scale and the waste generated from fossil fuel burning is not ecofriendly, which therefore contributes to global warming. The search for alternate energy sources is necessary due to high expense of fossil fuel and harmful gases by fossil fuels, which pollute the environment. There is one technique known as thermoelectricity which can convert waste heat into electrical energy. The thermoelectric conversion provides significant advantages such as flexibility, precise temperature control, long service life, no environmental pollution, etc. Furthermore, as compared to standard heat devices, the use of thermoelectric devices is still limited owing to their low conversion efficiency. The thermoelectric efficiency is calculated in form of a performance factor which is defined as [1].

$$\eta = \frac{T_H - T_c}{T_H}\left[\frac{\sqrt{1+ZT_a} - 1}{\sqrt{1+ZT_a} + \frac{T_c}{T_H}}\right] \quad (1)$$

here T_H and T_c are the temperature of the hot side and cool side respectively. T_a is average temperature $\left(T_a = \frac{T_H+T_c}{2}\right)$ of the material. At a particular temperature $(T_H - T_c)$, the thermoelectric efficiency is characterised by one parameter which is figure of merit (ZT= $\frac{S^2\sigma T}{k}$). In order to achieve a high ZT value, we need improve the power factor $(S^2\sigma)$ and decrease the overall thermal conductivity $(\boldsymbol{k})$. As a result, the main problem is how to improve ZT without affecting other factors.

From the last few decades, half Heulser's (HH) attract researcher's interest because of their significant properties such as eco-friendly, low expensive, thermal stability, non-toxic nature, low thermal conductivity, and high-power factor. Due to good thermal stability and mechanical strength, half Heusler system is well-suited material for thermoelectric applications. These materials are used in different fields

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