



Exploring thermoelectric properties and stability of half-Heusler PtXSn (X = Zr, Hf) semiconductors: A first principle investigation

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ABSTRACT

Half-Heuslers (HH) have found ever-increasing popularity as high temperature thermoelectric (TE) materials. In this paper, the electron and phonon transport equations are solved to understand the thermoelectric character of the PtXSn (X = Zr, Hf) compounds. Here, we have elucidated the phonon stability, electronic properties, thermoelectric response from lattice thermal conductivity, and phonon dependent parameters. The PtXSn compounds reveal an indirect bandgap semiconducting nature with a gap of 1.23 eV and 0.94 eV for PtZrSn and PtHfSn, respectively. At room temperature, a low magnitude of lattice thermal conductivity (κ_L) for PtZrSn (16.96 W/mK) and PtHfSn (10.04 W/mK) compounds is observed. The calculated maximum value of ZT is 0.57 and 0.24 observed for PtHfSn and 0.24 PtZrSn, respectively. Our present investigation demonstrate that the PtHfSn compound is potentially a favorable candidate for high-temperature power generation.

1. Introduction

Growing fame and necessity for renewable energy has led to extensive research works in the various forms of energy storage technologies over the past decades. Rising demand for renewable energy resources is thus encouraging the usage of thermoelectric materials that can directly transform waste heat into usable electricity [1]. Using the Seebeck effect, thermoelectrics can pursue the direct conversion of thermal energy into electric energy to meet the growing demand for novel sustainable energy technology. The efficiency of thermoelectric device can be understood by the dimensionless figure of merit (ZT) of TE material, which can be expressed as: $ZT = S^2\sigma T / (\kappa_e + \kappa_L)$, where S , σ , T , κ_e and κ_L represents the Seebeck coefficient, electrical conductivity, the absolute temperature and the electronic and lattice components of total thermal conductivity [1,2]. Thus, a high value of ZT would be greatly helpful to enhance the conversion efficiency of any TE material. Probing for high ZT materials is a thought-provoking process, and such type of material requires high power factor ($S^2\sigma$) alongside low thermal conductance. Thus, an optimum balance among these coefficients needs to be

established in order to furnish a good thermoelectric response of the material. Until now, broad varieties of thermoelectric materials (TE) have been scrutinized for various temperature regimes. Exceptionally, the layered structure of Heuslers is primarily being considered for various functional applications in photovoltaic materials, thermoelectric energy conversion, solar cell devices, catalysis, and fuel cells, etc. [3,4]. This class comprises of half Heuslers (XYZ) [5,6], full Heuslers (X_2YZ) [7,8], quaternary Heuslers (XXYZ) [9,10], double ($X'X''Y_2Z_2$, $X_2Y'Y''Z_2$, $X_2Y_2Z'Z''$), triple ($X'_2X''Y_3Z_3$) and quadruple ($X'_3X''Y_4Z_4$) half-Heusler compositions [11]. The X- and Y-site atom is mainly have its place in the transition metals (pre and post) group elements, while the Z-site atoms are p-block (post-transition metal) elements. Hence, the compositional complexity finds a huge scope in chemistry of such structures. The main group element in Heusler alloys plays a vital role to adjust their physical properties for desired applications. Such materials display an interesting overview of electronic properties with semi-conducting, spin-semi metallic, metallic, spin gapless, half-metallic, and topological or superconducting properties etc. [12–14]. However, half-Heuslers (HH) with narrow bandgap energies display a wide range of

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