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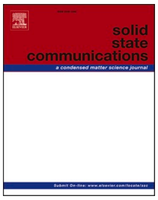

# Pursuit of stability, electronic and thermoelectric properties of novel PdVGa half heusler compound

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## ABSTRACT

In this work, we have explored structural, electronic, and thermoelectric properties of novel PdVGa half Heusler compound. PdVGa is chemically, mechanically, dynamically stable and a direct bandgap semiconductor with a bandgap of 1.012 eV. At 300 K, the maximum value of Seebeck coefficient, electrical conductivity and lattice thermal conductivity are 763 μV/K, 28.61 × $10^4$ S/m and 4.60 W/mK respectively. The computed value of ZT is 0.048 at 700 K. This compound has been designed as a thermoelectric material for the first time, and it may be useful in thermoelectric material experimental research.

## 1. Introduction

Due to contemporary living styles and rising population needs, the globe has experienced an energy problem in all commercial, household, technological, health, space, and research sectors in recent years. Traditional energy sources, such as power plants are damaging the environment significantly and should be changed to preserve the world and future generations. Thermoelectric materials which can convert waste heat into power are now being investigated [1–3]. Furthermore, developments in thermoelectric materials have resulted in the creation of multistage Peltier coolers that may be utilized to produce efficient cooling and heating. The efficiency of thermoelectric devices is calculated by a figure of merit (ZT) [4], which is a dimensionless quantity and can be defined as (see Table 4)

$$ZT = \frac{S^2\sigma T}{k} \tag{1}$$

where S is Seebeck coefficient, $\sigma$ is electrical conductivity, T is absolute temperature, k is total thermal conductivity respectively. The total thermal conductivity of the crystal is the sum of lattice thermal conductivity ($k_L$) and electronic thermal conductivity ($k_{el}$) [5]. Half Heusler (HH) compounds have gained significant attention in research because of their application in spintronics [6–8], thermoelectrics [9–16], anti-ferromagnetism, ferromagnetism [17–19], and topological insulators [20–23]. Also, Half-Heuslers compounds attract researchers' interest for the intriguing thermoelectric properties because of their high seebeck coefficient and electrical conductivity [24]. MNiSn (M = Ti, Zr, Hf) are the most reliable half Heusler compound due to their ZT value which is lying between the range 0.7 to 1.5[10]. Thermoelectric properties of KBiX (X = Ba, Sr) are investigated by Z. F. et al. using ab inito principle and found values of ZT = 2.68 (1.56) for KBiBa (KBiSr) [25]. J. Nagura and his co-workers using the first principle calculations explored the thermoelectric and mechanical properties of XHfSn (X = Ni, Pd, Pt) materials [26]. FeNbSb based half heusler compound has been explored and their value of ZT is > 1 [14], [27]. M. K. bamgbose has investigated XIrSb(X = Ti, Zr, Hf) HH compounds and found that ZT = 0.87, 0.95, 0.90 for TiIrSb, TrIrSb, HfIrSb at 800 K respectively [9]. XCoSb (X = Ti, Zr, Hf) compound gain attention because of their ZT value which is equal to 1.0 at 1097 K in p-type doping [13,28]. K. Jia et al. have explored that CuLiX(X = Se, Te) are good thermoelectric material due to their high ZT value which is equal to 2.65 (1.7) for CuLiTe (CuLiSe) [29]. Fang et al. [23] have reported that due to large band degeneracy and low effective mass, the value of ZT = 1.5 at 1200 K for RuTaSb half Heusler. Bi based Half Heusler compounds have investigated by A. Dey et al. using first principle calculations and reported ZT = 0.7 at room temperature [30].

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