## DFT study of Structural, Mechanical, Thermodynamical, Electronic and Thermoelectric properties of PdTiZ (Z = Ge and Pb) half Heusler compounds

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## Abstract

A first principle investigation of structural, mechanical, thermodynamical, electronic and thermoelectric properties of PdTiZ (Z = Ge and Pb) was carried out using plane wave pseudopotential (PP-PW) method. The exchange-correlation was considered with the generalized gradient approximation of Perdew-Burke-Ernzerhof (PBE-GGA). The energy band structure of the sample material exhibited semiconducting energy band structure with indirect energy band gaps of 0.66 eV and 0.387 eV in PdTiGe and PdTiPb respectively with density of states being mainly dominated by the p state of Z and d states of Ti atom around the vicinity of the Fermi energy level. The sample compounds were found to be mechanically stable in their non-magnetic cubic phase. PdTiGe was found to be harder and stiffer than PdTiPb. The positive phonon modes of the compounds predicted their dynamical stabilities. Thermodynamic study revealed that pressure has a negative effect on heat capacity whereas Debye temperature increases with enhanced pressure in both the sample compounds. The thermoelectric properties of the sample compounds predicted that p-type nature of the sample compounds possess better thermoelectric performance. The room temperature Seebeck coefficient values are found to be 98.73  $\mu$ V/K at 1200 K at n = 1021 cm-3. The lowest value of lattice thermal conductivity (K\_L) of 2.28 W/m-K and 0.98 W/m-K was observed for PdTiGe and PdTiPb respectively. The optimum dimensionless figure of merit of 0.66 (1200 K) and 0.64 (1000 K) were found for p-type PdTiGe and PdTiPb, respectively at optimum carrier concentration.

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