Computational Envision of Structural, Electronic, Mechanical and Thermoelectric Properties of PdXSn (X=Zr, Hf) half Heusler compounds

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Abstract

Half heusler compounds have gained attention due to their excellent properties and good thermal stability. In this paper, using first principle calculation and Boltzmann transport equation, we have investigated structural, electronic, mechanical and thermoelectric properties of PdXSn (X=Zr,Hf) half Heusler materials. These materials are indirect band gap semiconductors with band gap of 0.52 (0.44) for PdZrSn (PdHfSn). Calculations of elastic and phonon characteristics show that both materials are mechanically and dynamically stable. At 300K the magnitude of lattice thermal conductivity observed for PdZrSn is 15.16 W/mK and 9.53 W/mK for PdHfSn. The highest ZT value for PdZrSn and PdHfSn is 0.32 and 0.4 respectively.

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