High figure of merit in Half Heusler semiconductor RhNbZ with(Z = Ge, Sn)

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Abstract

Using the Full Potential Linearized Augmented Plane Wave FP-LAPW, as implemented in the Wien2k package. The structural, electronic, magnetic and elastic properties of the Half Heusler (HH) RhNbGe and RhNbSn were investigated. The Generalized Gradient Approximation (GGA) and the Tran-Blaha-modified Becke-Johnson exchange potential method (TB-mBJ) was applied to model the exchange correlation potential. Our results show that the both compounds studied are mechanically stable. Moreover, RhNbZ (Z:Ge,Sn) presents a semiconductor behavior obeying the Slater-Pauling rule. The thermodynamic properties, in particular the Bulk modulus, the heat capacity, the Debye temperature and the thermal expansion coefficients of the two alloys are investigated using the quasi-harmonic Debye model. The semi-classical Boltzmann theory, as implemented in the BoltzTraP code, is used to study thermoelectric properties. The high values obtained figures of merit ZT of RhNbGe and RhNbSn compounds make them promising candidates for thermoelectric applications at low and high temperatures.

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