Abstract

We will discuss in detail the structural, electronic, elastic, and thermoelectric properties of half-Heusler-like PtTiSn and PdLaBi ternary transition metals compounds using the first-principles density functional theory (DFT) and semi-classical Boltzmann transport theory. Our results revealed that these alloys are stable as well as ductile in nature. The Seebeck coefficient's contributions to both electrons and holes in these two materials would also be revealed. Where available, our results are in good agreement with few existing results.