Abstract

RTX compounds have gained an ambitious interest to the researcher for their wide applications in the field of optoelectronic, spintronics and thermoelectric applications. The research work presented in this thesis mainly highlights the theoretical study of half-Heusler semimetallic RPdBi (R = Gd, Dy, and Ho) compound by using Density Functional Theory (DFT) based on first principle technique within full potential linearized augmented plane wave (FPLAPW) method, LDA and GGA approximations are used for the exchange correlation calculation which are already employed in Wien2k-code. This theoretical study involves the exploration of structural, electronic, optical, magnetic and thermoelectric properties without considering spin-orbit coupling (SOC) and only measure the effect of SOC on electronic and optical properties of semimetallic compound GdPdBi, DyPdBi and HoPdBi. Our computed structural results are in good agreement with the literature work. In our study, *RPdBi* (*R* = Gd, Dy, and Ho) compound show semimetallic behaviour similar to other theoretical works. Thermoelectric behaviour are calculated by using BoltzTraP code at 100-800 K temperature reveals that DyPdBi shows a good electrical behaviour in comparison with the HoPdBi and GdPdBi. Results obtained from thermal conductivity show that GdPdBi would be a good thermoelectric material since it has the lowest value of thermal conductivity than the other two. Furthermore, comprehensive analysis of these compounds indicates that they are more feasible for Spintronics, magneto-electronics and optoelectronic devices.