Abstract

Half metallic materials have gained a keen interest to the scientist for their wide applications in the field of magneto-electronics and in spintronics devices. In this thesis, research work mainly focuses on the theoretical study of Half metallic materials $AMnTe_2$ (A=Li, Na, K). The theoretical study involves the investigation of structural, electronic, optical, magnetic and thermoelectric properties of half metallic compound $LiMnTe_2$, $NaMnTe_2$ and $KMnTe_2$ under the frame of Density Functional Theory (DFT). These calculations are based on first principle technique within Full Potential Linearized Augmented Plane Wave (FP-LAPW) method. Perdew-Burke-Ernzerhof Generalized Gradient Approximations (PBE-GGA) has been used for the exchange and correlation potential by employing Wien2K-code. Our calculated structural parameters are in good agreement with previous research work. In our study, these compounds have indirect band gap values in spin down channel. The calculated values of band gaps are in good agreement with other theoretical works. Half-metallicity in these compounds confirm by Electronic properties. Thermoelectric properties of these compounds are calculated by using BoltzTraP code at 200-800 K temperature. Moreover, the phonon dispersion curves are calculated by using the CASTEP Code to check the thermal stability of the materials. Furthermore, complete study of these compounds shows that they are more suitable for Spintronics and magnetoelectronics devices.