Abstract

The full potential linearized augmented plane wave (FP-LAPW) based on the density functional theory used to calculate structural, electronic, magnetic, thermoelectric and elastic characteristics theoretically of $X_{0.9375}Ti_{0.0625}Te$ (X = Ca, Sr, and Ba) with 6.25% doping of Ti concentration in a host material (CaTe , SrTe , BaTe) by-Wu-Cohen generalize gradient approximation (Wu-GGA) method used to find the potential Exchange correlation of the structural characteristics, GGA is used to calculate electronic and magnetic characteristics and the recently developed Tran-Blaha-modified-backe Johnson (TB-mBJ) approximations. Properties of these materials are calculated, in which including the investigation spin polarize electronic band structure and spin polarize density of state and spin polarization 100% around the fermi-level depicted half metallic ferromagnetic character. Further, the studied materials depict direct bandgap in spin down channel which indicate that these materials may have a potential candidate for best performance of spintronics devices. In addition, the ferromagnetic nature stability of $X_{0.9375}Ti_{0.0625}Te$ (X = Ca, Sr, and Ba) with 6.25% doping of Ti can be shown by crystal field energy E_{cry} along with john-teller distortion, magnetic moment, direct exchange energy $\Delta_x(d)$, exchange splitting energy $\Delta_x(pd)$ exchange constants (Noα and Noβ) respectively. Boltztrap code is used to calculate the thermoelectric characteristics of understudied materials.