Abstract

The cubic perovskite structures have enlarged the potential for their wide applications for the purpose of hydrogen storage.The present research work aims at undergoing the theoretical study of perovskite type hydrides $LiXH_3$ (X = Ba, Sr and Cs). The study includes the investigation of structural, electronic and thermal and thermodynamic properties using full potential linearized augmented plane wave (FP-LAPW) method under the frame work of Density Functional Theory (DFT) by employing WIEN2K code. The calculated parameters for structural, electronic and thermal properties are in good agreement with the literature work. Results reveal that all the compounds have indirect band gaps of values of 1.48eV, 1.35eV and 1.73eV for $LiBaH_3$, $LiCsH_3$ and $LiSrH_3$, respectively and these calculated band gaps are in good agreement with other theoretical work. In addition, the thermoelectric properties calculated by solving the Boltzmann transport equation reveal that $LiBaH_3$ possesses superior electrical properties in comparison with the $LiSrH_3$ and $LiCsH_3$. Using density functional perturbation theory, we have also calculated the phonon dispersion curves and phonon density of states with the help of CASTEP code. Various thermo-dynamical properties, such as, heat capacity, Debye temperature, Enthalpy, Entropy and free energy have been calculated with the help of thermodynamic functions by using phonon density of states and results reveal that $LiBaH_3$ is more stable as compared to $LiSrH_3$. Moreover, results also exhibit that $LiCsH_3$ is unstable compound in cubic phase.