Abstract

Cubic perovskites have boosted a potential interest to the researcher for their wide applications in the field of optoelectronic devices. For the last decades, lead based perovskites compounds have a remarkable impact in the photovoltaic applications. However, it is observed that lead is toxic to the environment and organisms for a long time and is hard to excrete from the body. Therefore, it is essential to find environmentally-friendly metal ions to replace lead for the further development of Perovskites Solar Cells (PSCs). In our work, we doped Ge with a different percentage that could be used as alternative ions in perovskite configurations to form a new environment-friendly lead free perovskites.The research work presented in this thesis mainly highlights the theoretical study of perovskite $CsPbI_3$, $CsGe_{0.25}Pb_{0.75}I_3$and $CsGe_{0.5}Pb_{0.5}I_3$ compounds. The theoretical study also involves the investigation of structural properties as well as optoelectronics and thermal properties of perovskite compounds using Density Functional Theory. These calculations based on first principle technique within the full-potential linearized augmented plane wave (FPLAPW) method. For exchange-correlation effects, GGA approximation is employed in WIEN2k code. Our computed structural parameters for structural, electronic, thermal and optical properties are in good agreement with the literature work. In our work $CsPbI_3$, has direct bandgap with values 1.6eV and $CsGe_{0.25}Pb_{0.75}I_3$ and $CsGe_{0.5}Pb_{0.5}I_3$ have indirect bandgap values of 0.91 eV and 1.2 eV respectively. Computed band gaps are in good agreement with other research works. Thermoelectric behaviour is calculated by using BoltzTraP code at 100-800 K temperature which shows that $CsPbI_3$, has good electrical behaviour in comparison with the $CsGe_{0.25}Pb_{0.75}I_3$ and $CsGe_{0.5}Pb_{0.5}I_3$.. Results derived from thermal conductivity show that $CsGe_{0.25}Pb_{0.75}I_3$and $CsGe_{0.5}Pb_{0.5}I_3$ are good thermoelectric materials since they have the lowest value of thermal conductivity than $CsPbI_3$. Moreover, comprehensive analysis of these compounds indicates that they are more feasible for optoelectronic devices.