Abstract

Cubic perovskites have gained a potential interest to the researcher for their wide applications in the field of optoelectronic devices. The research work presented in this thesis mainly focuses on the theoretical study of perovskite stannates $ASnO_3$ (A = Ba, Sr, and Cs). The theoretical study also involves the investigation of structural properties as well as optoelectronic and thermal properties of perovskite compound $BaSnO_3$ $SrSnO_3$ and $CsSnO_3$ using Density Functional Theory. (DFT) calculations based on first principle technique within full potential linearized augmented plane wave (FPLAPW) method. For exchange correlation effects, GGA approximation is employed in Wien2k-code. Our calculated structural parameters for structural, electronic, optical and thermal properties are in good agreement with the literature work. In our study, $BaSnO_3$ and $SrSnO_3$ have indirect bandgap values of 2.08 eV and 2.12 eV respectively showing semiconducting behavior while $CsSnO_3$ has direct bandgap of 0.1 eV and show metallic behavior. Calculated band gaps are in good agreement with other theoretical works. The thermoelectric properties were calculated by solving the Boltzmann transport equation reveals that that $CsSnO_3$ is a good electrical in comparison with the $BaSnO_3$ and $SrSnO_3$. Results obtained from thermal conductivity show that $SrSnO_3$ would be a good thermoelectric material since it has the lowest value of thermal conductivity than the other two. The positive value of the Seebeck coefficient for all investigated perovskite compounds reveals that each of the compounds has p-type conductivity. Moreover, comprehensive analysis of these compounds indicates that they are more feasible for optoelectronic devices.