Electronic structures and related thermoelectric properties of Pb$_7$Bi$_4$Se$_{13}$ using first principle calculations and Boltzmann transport theory

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The electronic structure, optical and thermoelectric properties of Pb$_7$Bi$_4$Se$_{13}$ have been investigated using a combination of Density functional theory and Boltzmann transport theory. We applied the generalized gradient approximation as exchange-correlation energy functional added to the Coulomb energy (U Hubbard term). The existence of Bi and Pb has required the spin-orbit coupling. The intensity data for Pb$_7$Bi$_4$Se$_{13}$ were measured at 100 K and 300 K leading to consider Pb$_7$Bi$_4$Se$_{13}$ in two phases. The valence band maximum emerges predominantly from Se-$p$ state with admixture of Bi-$p$ and Pb-$p$ states, while the conduction band minimum comes from Se-$d$ states. The optical absorption shows the possibility of smaller multiple direct and indirect inter-band transitions in the visible region. We computed Seebeck coefficient, electrical and thermal conductivities, figure of merit and power factor, as function of temperature using the Boltzmann transport theory. Pb$_7$Bi$_4$Se$_{13}$ is a potential shielding material that can be used at visible and UV region for thermoelectric devices. The present results were validated by comparison with the available experimental measurements.