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Electronic structures and related thermoelectric properties of $Pb_7Bi_4Se_{13}$ using first principle calculations and Boltzmann transport theory MOHAMMED BENALI KANOUN, Al Faisal University, college of science — The electronic structure, optical and thermoelectric properties of $Pb_7Bi_4Se_{13}$ 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 $Pb_7Bi_4Se_{13}$ were measured at 100 K and 300 K leading to consider $Pb_7Bi_4Se_{13}$ 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. $Pb_7Bi_4Se_{13}$ 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.

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