Abstract Submitted
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**First principles calculations of Thermoelectric properties of Bi2Te3 and PbTe**[1] HYO SEOK KIM, WON BO LEE, Seoul Natl Univ — We presented first-principle calculations of electron and phonon transport in Bi2 Te3 and PbTe. We focused on the several thermoelectric properties; Seebeck coefficient, electrical conductivity, electrical thermal conductivity and lattice thermal conductivity. The electronic transport is calculated using the projector augmented wave (PAW) method implemented in Vienna Ab-initio Simulation Package (VASP) and Boltzmann transport equation (BTE). From electronic transport, the Seebeck coefficient can be estimated by simple expression containing band-gap energy. From phonon transport, we calculated the interatomic force constants (IFCs) along with a fully iterative solution of phonon-BTE. This approach allows both harmonic and anharmonic interatomic forces to be contained into the result. The calculated lattice thermal conductivity was found to be in good agreement with experimental data. We discussed that the first-principle methodology can be a tool to understand the transport details in many solid-state devices.

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