Calculating the thermoelectric properties of zinc-antimonides

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The electronic structure and transport properties of the 1:1 phase of Zn-Sb will be discussed based on the boltzmann transport equation. It will be shown how the conduction band of ZnSb has several minima stemming from increased bonding between distant neighbors at special k-points. from literature, the carrier concentrations, band gaps, and relaxation times of the compounds are determined. The thermodynamic stability of intrinsic defects in ZnSb are studied. It is shown that the low formation energy of negatively charged Zn defects limit pins the chemical potential to the valence bands, thereby explaining the experimentally observed p-type behavior. Finally, we introduce a simple Klemens-Callaway like model of the thermal conductivity and use it to explain the low thermal conductivity of the 1:1 and especially the 4:3 phase.