**Thermoelectric properties of AgSbTe$_2$ from first-principles calculations**

HADI AKBARZADEH, Department of Physics, Isfahan University of Technology, NAFISEH REZAEI, S. JAVAD HASHEMIFAR, Isfahan University of Technology, KEIVAN ESFARJANI, Rutgers University — Recently, novel thermoelectric materials are extensively investigated for providing sustainable energy resource. In this regard, AgSbTe$_2$ as a p-type semiconductor is widely investigated due to its low lattice thermal conductivity and relatively large Seebeck coefficient. We study electronic, vibrational, and thermoelectric properties of FCC and rhombohedral structures of AgSbTe$_2$ by first-principles calculations. The hybrid HSE03 functional is employed to correct wrong prediction of semimetal behavior in GGA and obtain a band gap of about 0.5 eV. The Seebeck coefficient, electrical conductivity, and electronic part of thermal conductivity are calculated by using a combination of maximally localized Wannier functions and semi-classical Boltzmann equation. By matching the calculated Seebeck coefficient with the experimental data, we predict the carrier concentration and band gap of several experimental samples. Our results indicate that the band gap and hole concentration of pure samples should be in the range of 0.2-0.5 eV and $2-5 \times 10^{19}$ holes/cm$^3$. Finally, we use the experimental electrical conductivity and the constant relaxation time assumption to estimate the relaxation time of this compound.

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