Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

Thermoelectric properties of $AgSbTe_2$ from first-principles calculations[1] 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.

[1]This work was supported jointly by the Vice Chancellor for Research Affairs of Isfahan University of Technology, Center of Excellence for Applied Nanotechnology, and ICTP Affiliated Centre

Hadi Akbarzadeh
Department of Physics, Isfahan University of Technology

Date submitted: 27 Oct 2012 Electronic form version 1.4