Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

Quasiparticle band structures and thermoelectric transport properties of p-type SnSe GUANGSHA SHI, EMMANOUIL KIOUPAKIS, Materials Science and Engineering, University of Michigan — We used density functional and many-body perturbation theory to calculate the band structure and electronic transport parameters of p-type SnSe both for the low-temperature Pnma and high-temperature Cmcm phases. The Pnma phase has an indirect band gap of 0.829 eV while the Cmcm has a direct band gap of 0.464 eV. Both phases exhibit multiple local band extrema within an energy range comparable to the thermal energy of carriers from the global extrema. We calculated the electronic transport coefficients within the constant relaxation time approximation as a function of doping concentration and temperature for single-crystal and polycrystalline materials to understand experimental measurements. The electronic transport coefficients are highly anisotropic and are strongly affected by bipolar transport effects at low doping and high temperature. Our results indicate that SnSe exhibits optimal thermoelectric performance at high temperature when doped in the 10^{19}–10^{20} cm^{-3} range. This work was supported in part by the National Science Foundation (DMR-1254314) and in part by CSTEC, an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science. Computational resources were provided by the DOE NERSC facility.

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Date submitted: 13 Nov 2014 Electronic form version 1.4