Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

Temperature dependent phonon properties of thermoelectric materials[1] OLLE HELLMAN, Department of Applied Physics and Materials Science, California Institute of Technology, Pasadena, California 91125, USA, DAVID BROIDO, Department of Physics, Boston College, Chestnut Hill, Massachusetts 02467, USA, BRENT FULTZ, Department of Applied Physics and Materials Science, California Institute of Technology, Pasadena, California 91125, USA — We present recent developments using the temperature dependent effective potential technique (TDEP) to model thermoelectric materials. We use ab initio molecular dynamics to generate an effective Hamiltonian that reproduce neutron scattering spectra, thermal conductivity, phonon self energies, and heat capacities. Results are presented for (among others) SnSe, Bi_2Te_3, and Cu_2Se proving the necessity of careful modelling of finite temperature properties for strongly anharmonic materials.

[1]Supported by the Swedish Research Council (VR) project number 637-2013-7296.

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Date submitted: 14 Nov 2014 Electronic form version 1.4