Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

Thermoelectric properties of FeSb2: A first principles study MOMAR DIAKHATE, MATTHIEU VERSTRAETE, Universite de Liege — The development of new types of thermoelectric materials with a large figure of merit is strongly driven by the need for sustainable and clean energy. In this respect first-principles study of thermoelectric properties can help to achieve a better understanding of microscopic mechanisms in transport, which provides insight for discovering new materials. To study the thermoelectrical properties, we combine the well known Boltzmann transport theory with the predictive power of density functional calculations. With the exception of the lattice thermal conductivity, all of the required transport coefficients can be obtained using the BoltzTrap code, based simply on the electronic band energies. With a constant relaxation time, we predict the Seebeck coefficient of bulk FeSb2, which showed colossal negative value at 12K experimentally. The calculated peak position is consistent with the observation, while the amplitude is underestimated. The inclusion of contributions from phonon drag effect and the exact calculation of the electronic density of states around Fermi level may better describe the experimentally observed phenomena.

Momar Diakhate
Universite de Liege

Date submitted: 20 Nov 2012 Electronic form version 1.4