MAR16-2015-003903 C

Abstract for an Invited Paper
for the MAR16 Meeting of
the American Physical Society

Ab initio phonon limited transport

MATTHIEU VERSTRAETE, Univ de Liege

We revisit the thermoelectric (TE) transport properties of two champion materials, PbTe and SnSe, using fully first principles methods. In both cases the performance of the material is due to subtle combinations of structural effects, scattering, and phase space reduction. In PbTe anharmonic effects are completely opposite to the predicted quasiharmonic evolution of phonon frequencies and to frequently (and incorrectly) cited extrapolations of experiments. This stabilizes the material at high T, but also tends to enhance its thermal conductivity, in a non linear manner, above 600 Kelvin. This explains why PbTe is in practice limited to room temperature applications. SnSe has recently been shown to be the most efficient TE material in bulk form. This is mainly due to a strongly enhanced carrier concentration and electrical conductivity, after going through a phase transition from 600 to 800 K. We calculate the transport coefficients as well as the defect concentrations ab initio, showing excellent agreement with experiment, and elucidating the origin of the double phase transition as well as the new charge carriers. AH Romero, EKU Gross, MJ Verstraete, and O Hellman PRB 91, 214310 (2015) O. Hellman, IA Abrikosov, and SI Simak, PRB 84 180301 (2011)