Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Ab-initio study of electron transport in lead telluride QICHEN SONG, TEHUAN LIU, JIAWEI ZHOU, GANG CHEN, Massachusetts Inst of Tech-MIT — Nanostructuring has recently witnessed great success in improving material's thermoelectric efficiency. One key aspect of this method lies in the fact that mean free paths of phonons are typically larger than those of electrons, and therefore nanostructures with certain grain sizes can reduce the thermal conductivity while preserving the good electrical property. Despite recent computational and experimental progress on identifying the phonon mean free path spectrum, the quantitative electron mean free path spectrum has been mostly unknown, especially considering practical thermoelectric materials having complex structures. In this work, we perform a fully first-principles method to study the electron transport in a prototypical thermoelectric material - PbTe, which has shown to exhibit good thermoelectric performance and strong spin-orbital coupling. Such first-principles method enables us to study the electron transport mode by mode, providing detailed scattering mechanisms and mean free path spectrum. Specifically, we find that despite of the large dielectric constant of PbTe, the polar scattering is comparable with acoustic deformation potential scattering, with the electrical transport properties agreeing well with experiments. This work is supported by DOE EFRC (Grant No. DE-SC0001299).

Qichen Song
Massachusetts Inst of Tech-MIT

Date submitted: 13 Nov 2016 Electronic form version 1.4