Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

Ab Initio Electron Relaxation Times and Computational Screening of Thermoelectric Materials BORIS KOZINSKY, GEORGY SAMSONIDZE, Bosch Research, Cambridge MA — We report recent progress in development of an efficient approximation scheme for computing electron relaxation times in bulk crystalline materials from first principles. This technique takes into account electron-phonon coupling and opens up the possibility for ab initio calculations of electronic transport coefficients: electrical conductivity, the electronic part of thermal conductivity, and Seebeck coefficient. We find that electron relaxation times and transport coefficients are very sensitive to carrier concentration, and their accurate prediction is necessary for computational optimization of thermoelectric material composition. For a given thermoelectric material, we are able to determine the optimal carrier concentration which maximizes ZT at a target temperature. With this methodology at hand, systematic computational screening is performed in the compositional space of half-Heusler materials selected from materials databases and consisting of cheap earth-abundant elements. Good agreement is found with the available experimental data for previously synthesized half-Heusler compounds, and several new promising candidates for thermoelectric applications are identified, which have been synthesized and validated by experimental collaborators. Based on the results of our calculations, we also discuss the validity and applicability limits of the Wiedemann-Franz law for thermoelectric materials.

Boris Kozinsky
Bosch Research, Cambridge MA

Date submitted: 14 Nov 2014 Electronic form version 1.4