



Physics Colloquium

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Simulations of electronic and thermoelectric properties of materials from first principles

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ABSTRACT

Over the last decade a plethora of new thermoelectric materials, their alloys, and their nanostructures were synthesized, while their performance more than doubled. The ZT figure of merit, which quantifies the thermoelectric efficiency of these materials increased from values of unity to values consistently beyond two across material families [1]. At the same time, the need to understand their electronic transport properties, and the ability to identify and optimize such materials, has stressed the need for advanced numerical tools for computing electronic transport in materials with arbitrary bandstructure complexity and multiple scattering mechanisms. The convenient and arbitrary use of the constant relaxation time approximation offers limited predictive capabilities in this case, because the scattering processes are energy, momentum, and band dependent, $\tau(E,k,n)$. Fully ab initio electron-phonon scattering methods exist, but they are computationally prohibitive and rarely used.

In this talk I will describe the development of our recently deployed advanced electronic transport simulator ElecTra [2], which considers arbitrary DFT electronic structures of materials and allows for their full $\tau(E,k,n)$ dependence, providing accurate and reliable extraction of thermoelectric properties of materials. The electron-phonon scattering times considered are based on deformation potential scattering, for which however, deformation potentials are in general unavailable. For this, I will describe a novel method that we have developed to extract the necessary deformation potentials from first principles [3]. The new methods described, allow for the calculation of the thermoelectric properties of materials at the same accuracy as fully ab initio methods, but at a fraction of the computational cost, typically at less than 10%. Finally, a few examples of material performance evaluation studies are discussed [4, 5].

References:

- [1] Beretta, NN, et al., Materials Science and Engineer.: R: Reports, 138, 100501, 2019.
- [2] <https://github.com/PatrizioGraziosi/ELECTRA>
- [3] Li, Graziosi, NN, PRB, 104, 195201, 2021.
- [4] Graziosi, NN et al., J. Applied Physics, 126, 155701, 2019;
- [5] Graziosi, NN et al., ACS Appl. Energy Mater., 3, 6, 5913–5926, 2020.

ZOOM Link: <https://zoom.us/j/99382967643?pwd=Z0ZmSERObkNNbWt2bTVXVWx0aG1EQT09>