From deformation potential extraction to thermoelectric transport simulations: an efficient and practical approach

Authors: Zhen Li, Patrizio Graziosi, and Neophytos Neophytou

School of Engineering, University of Warwick, Coventry, UK

Abstract

Thermoelectric transport is traditionally computed by coupling density-functional theory (DFT) bandstructures with the Boltzmann Transport Equation (BTE), commonly using the constant relaxation time approximation (RTA), which introduces an arbitrary error [1, 2]. More recently, methods for computing relaxation time using first-principles are developed, which, however are computationally very expensive. In this work, we present a first-principles framework to compute the thermoelectric properties of materials based on the extraction and use of deformation potentials and then the corresponding scattering rates. This method would be the middle ground computationally between the constant RTA and first-principles relaxation time extraction.

Based on DFT and density-functional perturbation theory (DFPT), we compute the electronic bandstructures, phonon dispersion relations, and electron-phonon matrix elements. Within the polar Wannier interpolation scheme, we consider the short-range interactions between electrons and long-wavelength phonons, and the long-range optical interactions. From the short-range electron-phonon matrix elements, we derive the acoustic deformation potential (ADP) and optical deformation potential (ODP) for long-wavelength phonons. The electronic structures and deformation potentials are taken as inputs to compute the charge transport coefficients (electrical conductivity (σ), Seebeck coefficient (S), thermoelectric power factor (σS^2), and electronic part of the thermal conductivity (κ_e)). For this we use an advanced, home-developed numerical simulator, which allows not only for the incorporation of electron-phonon scattering,

but also for other (even more) important scattering mechanisms, such as ionized impurity scattering, alloy scattering, etc.

References:

[1] P. Graziosi, C. Kumarasinghe, and N. Neophytou, , *Journal of Applied Physics* 2019, 126, 155701

[2] P. Graziosi, C. Kumarasinghe, and N. Neophytou, *ACS Appl. Energy Mater.* 2020, 3, 6, 5913–5926