The Non-Equilibrium Green's Function method for quantum transport in disordered thermoelectric nanomaterials

Neophytos Neophytou* and Vassilios Vargiamidis

School of Engineering, University of Warwick
**n.neophytou@warwick.ac.uk*

New generation thermoelectric materials involve complex bandstructure materials which are nanostructured in a hierarchical manner in order to scatter phonons across the spectrum. Although this results in the favourable situation of extremely low thermal conductivities, it also degrades the electronic conductivity. It is possible, however, to have nanostructured materials engineered in a way not to only retain their electrical conductivity, but allow for Seebeck coefficient improvements as well, all of which improve the thermoelectric performance of materials. For this, however, advanced electronic transport simulations are needed, that account for all relevant nanoscale features.

Here, we present the development of a fully quantum mechanical electronic transport simulator for hierarchically nanostructured thermoelectric materials based on the Non-Equilibrium Green's Function (NEGF) method, including the effect of electron-phonon scattering. We show that nanomaterials can indeed be designed such that the power factor (the product of the electrical conductivity and the square of the Seebeck coefficient) can be made resilient to the presence of nanoinclusions, independently of their density. We also show how such simulations provide a better way to understand and optimize thermoelectric transport in nanostructures. Finally, we explain the 'ingredients' for designs that can reach more than an order of magnitude performance improvements.