Name:
Neophytos Neophytou

Title:
Advanced quantum transport simulations for the design of nanostructured thermoelectric materials

Preferred choice:
ORAL presentation

Abstract:
N. Neophytou, S. Foster, D. Chakraborty, V. Vargiamidis, and L. de Sousa Oliveira
School of Engineering, University of Warwick, Coventry, UK,
*n.neophytou@warwick.ac.uk

Nanostructured materials have shown great potential to achieve extremely low thermal conductivities, and thus, improve thermoelectric performance. Hierarchical nanostructuring, where phonons of different wavelengths scatter on features of different sizes have resulted in ZT>2. Less attention has been paid, however, in the possibility of designing nanostructured materials for improving the thermoelectric power factor. For effective reduction in thermal conductivity and power factor improvements, advanced simulations, which can capture all transport physics and nanoscale geometry details, are needed.

In this work, we present our simulations efforts to address both electronic and phononic transport in nanostructured materials. With regards to electronic transport, we have developed the fully quantum mechanical electron transport non-equilibrium Green's function method (NEGF) for nanocomposites of arbitrary geometries. We present simulations for thermoelectric power factor in materials with embedded nanoinclusions (NIs) and hierarchical geometries where nanoinclusions are placed within nanograins. The NEGF formalism captures all important effects that relate to the different and non-uniform geometrical features extending from a few to hundreds of nanometers. With enough computational power, electron-phonon interactions is also included, which allows treatment from fully quantum mechanical to semiclassical, and from fully ballistic to diffusive transport regimes. With regards to phonon transport, we present our newly developed phonon Monte Carlo simulator and our simulation work on highly disordered nanostructured materials. Finally, we discuss our efforts to include bandstructure, atomistic, and coherent effects, that would allow more accurate treatment of electrothermal transport at the nanoscale compared to continuum semiclassical methods.