Phononic and electronic transport in nanostructures and complex materials

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Approximately two-thirds of all used energy is lost as waste heat [1]. Thermoelectrics are promising materials for waste-heat recovery. Efficient thermoelectric materials have very low thermal conductivity, high electrical conductivity (σ), and high Seebeck coefficient (S). Significant advances have been made to increase the efficiency of thermoelectrics via nanostructuring and band engineering. Nanostructuring promotes phonon scattering across a wide range of the spectrum, and can thus contribute significantly to lowering the thermal conductivity of materials. At the electron level, nanostructuring can be used to modulate electron transport, thus increasing the power factor (σS^2) [2,3]. Band engineering can also improve the performance of complex materials such as Heuslers, oxides, chalcogenides, etc., and provide guidance for rationally identifying novel chemical structures with desirable properties.

In our group we explore electronic and thermal transport at various length scales, from nano- to macro-, using various transport techniques that range from classical (e.g. molecular dynamics) and semi-classical (e.g. Monte Carlo) to fully quantum mechanical (e.g. non-equilibrium Greens functions). In all these, especially in the case of materials with complex bandstructures and complex geometries, accurate electronic properties, phonon properties, and electron-phonon scattering need to be considered. We have begun exploring the electronic properties of Heusler compounds using density functional theory, with an eye on next-generation thermoelectric materials, and using equilibrium molecular dynamics to study phonon transport in hierarchical structures. We focus here on introducing a map of the work we're performing on the latter topic, including some preliminary results for bulk crystalline Si with nanovoids, performed using the Green–Kubo formalism; and a qualitative analysis of how individual acoustic and optical modes are scattered, computed by means of a wavepacket approach.

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[3] Foster *et* al. Physical review B, 96, 195425 (2017)

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