Advanced thermoelectric transport simulations in complex bandstructure and nanostructured materials

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Abstract

Nanostructured materials materials are a promising direction for new generation thermoelectric materials as they offer thermal conductivities close or below the amorphous limit, as well as improved power factors in some cases through energy filtering. Specifically, incorporation of disorder at various (hierarchical) length scales using a combination of alloying, grains, surfaces, etc., seems to be a very successful strategy. In addition, current efforts involve a plethora of complex bandstructure materials, that offer multiple opportunities for tuning the parameters that control the ZT figure of merit. For proper performance optimization and identification of new design directions, however, advanced simulations are needed, which can capture the geometrical complexity of the nano-features, the local material properties and material variations, carrier scattering events, etc.

Advanced simulations can also be employed to extend the simpler, analytical models that are commonly employed, but break down when the structures become complex, or when the feature sizes become similar to the characteristic length scales of the heat/charge carriers. This work, describes the development of advanced simulators related to the extraction of thermoelectric transport properties of nanostructures and complex bandstructure materials. Quantum and semiclassical transport studies related to thermoelectric performance optimization in materials with embedded nanoinclusions, voids, and superlattice-type barriers are discussed. Band alignment studies on the thermoelectric properties of complex bandstructure materials based on DFT studies coupled with Boltzmann transport are also discussed. In both cases, the aim is to provide deeper understanding in thermoelectric transport, that could not have been reached from simplified considerations, and then be able to design guidelines that capture those details.