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Advanced simulation techniques for hierarchically disordered nanostructured thermoelectric materials

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Abstract: Hierarchical nanostructuring, where distortion is inserted in bulk materials at various length scales, can scatter phonons of different wavelengths. This strategy is now considered as one of the most promising ways to reduce a material's thermal conductivity and increase its thermoelectric performance. Nanostructuring not only affects the thermal conductivity, but also the electronic conductivity and the Seebeck coefficient as well, often in a negative way though. Due to the adverse interrelations of these quantities, is has been proven very difficult to achieve optimization of the thermoelectric properties of complex nanostructures. The large range of length scales (from a few, to hundreds of nanometers), the combination of disorder types (boundaries, pores, nanoinclusions, etc.), as well as the effect of non-uniformity in the parameters that define the disorder (distances, diameters, positioning, etc.), impose at the moment a significant barrier in understanding thermoelectric transport in such materials. This stresses the need for advanced simulation tools that can incorporate all necessary features and nanoscale transport details.

In this work, we describe the development of computational tools that describe electronic and phonon transport at various length scales (nanometers to micrometers) and transport regimes (from quantum mechanical to semiclassical). We use them within a multi-physics, multi-scale methodology to explore thermal and electronic transport in nanomaterials that combine superlattice-type barriers, nanoinclusions (quantum dots), voids, pores, etc. as indicated in the figures below. We discuss the features that degrade thermal transport, but also importantly the strategies that can be followed so that the power factor becomes not only resilient to degradation caused by nanostructuring (as is the common case), but exhibits significant improvements as well.

We believe that this work can provide design guidelines for the next generation thermoelectric materials and devices through not only thermal conductivity reductions, but also power factor improvements.

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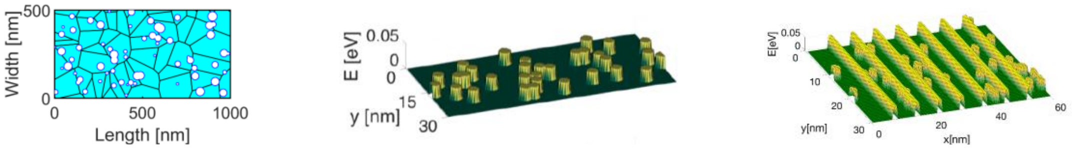

Example schematics of nanostructures we typically deal with: Nanovoids within nanocrystalline materials arranged randomly, quantum dots within a matrix material, and quantum dots within a superlattice material.