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Quantum transport simulations of thermoelectric power factor in materials with hierarchical nanostructuring

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Abstract

The need for multiscale hierarchical nanostructuring in increasing phonon scattering in bulk thermoelectrics is emphasized as one of the most promising routes to increase the ZT figure of merit [1]. Such materials contain macroscale grain boundaries, nanoinclusions, and atomic defects, each responsible for scattering phonons of different wavelengths. However, the power factor in materials with such complexities is usually overlooked and is much less theoretically studied, as it imposes the difficulty in accurately estimating both the conductivity and the Seebeck coefficient under such large degree of disorder.

In this work we employ the fully quantum mechanical non-equilibrium Green's function (NEGF) electronic transport method, which is particularly suitable for treating details of material geometrical features as well as electron-phonon scattering [2]. We investigate the thermoelectric power factor of nanocomposite materials with hierarchical nanostructuring; namely, embedded nanoinclusions, superlattice/nanocrystalline barriers, voids, and combinations of all within the same material. We identify cases, and present the conditions under which the power factor in these structures is: i) either resilient to the density of the embedded nanostructuring, ii) or even exhibits gains. Thus, we demonstrate how the materials can retain a high power factor in addition to the targeted suppressed thermal conductivity. Finally, we describe our efforts to relate our conclusions to real recently developed nanostructured material systems, which will prove experimentally useful and potentially further improve ZT.

References:

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