

To Symposium I: Recent Developments in thermoelectric materials and applications

Title

Quantum transport simulations in hierarchically disordered nanostructures for high thermoelectric power factors

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Abstract (1500)

Nanostructuring is a promising approach for the next generation thermoelectric materials yielding ultra-low thermal conductivities. More specifically, some of the lower thermal conductivities in materials have been achieved by the inclusion of hierarchically sized structures, at the atomic size, the nanoscale, and mesoscale, which can scatter phonons of various wavelengths and reduce phonon transport throughout the spectrum. Less attention has been paid, however, to the power factor (PF), which in most cases is reduced.

In this work, we present our recent simulation results on the thermoelectric PF of hierarchically nanostructured materials that include nanocrystalline potential barrier boundaries, nanoinclusions and voids. We employ a fully quantum mechanical simulator based on the Non-Equilibrium Green's function method, including electron-phonon interactions, which allows robust treatment of nanoscale transport physics, and includes all geometrical and scattering details without the need of approximations.

We discuss the conditions under which the PF is less affected due to the presence of nanostructuring, and conditions under which the PF is even enhanced. We further couple our results with Molecular Dynamics simulations to compute the reduction in thermal conductivity in our structures and compute ZT. Our findings can complement the large volume of work on reducing thermal conductivity, and point to design directions that further increase the ZT figure of merit.