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Hierarchical design of nanomaterials for improving the power factor

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-abstract-

Hierarchically nanostructured thermoelectric materials, where nanoinclusions are inserted at various length scales (grain boundaries, embedded quantum dots, atomistic defects), have shown the potential to provide much larger thermoelectric performance compared to pristine materials. This is to-date being attributed to drastic reductions in the thermal conductivity, but less on power factor improvements. In this work we combine Molecular Dynamics simulations for the thermal conductivity and Non-Equilibrium Green’s Function simulations for electronic transport to study thermoelectric transport through materials with hierarchically embedded nanoinclusions, namely sperlattice-type barriers with quantum dots and voids in between them. We show that beyond the drastic reductions in thermal conductivity, the nanomaterials can be designed such that the power factor: i) is resilient to the presence of nanoinclusions, and ii) is even improved compared to pristine materials, independently of the density of the distorting nanoinclusions.

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