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Computational Design of Nanostructured Thermoelectrics

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Creating nanostructures within alloyed bulk thermoelectric materials can greatly decrease the lattice thermal conductivity of the material and thereby increase the thermoelectric efficiency of these materials. However, the rational design of thermoelectric alloys with even larger figures of merit will require a quantitative knowledge of the electronic and thermal properties and phase stability of nanostructured semiconductor materials. Here, we show how first-principles based calculations can reveal the intricate but tractable relationships between properties for optimization of thermoelectric performance. The integrated optimization includes a multipronged strategy: 1) significant reduction of the lattice thermal conductivity with multi-scale hierarchical architecturing, 2) large enhancement of Seebeck coefficients with intra-matrix electronic band convergence engineering, and 3) control of the carrier mobility with band alignment between host and second phases. These techniques can simultaneously enhance the power factor and reduce the lattice thermal conductivity, thereby leading to high efficiency thermoelectric materials.