Hierarchical Nanostructuring for High Performance Thermoelectric Materials: A Simulation Prospective

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Thermoelectric (TE) materials convert heat from temperature gradients into useful electrical power. Over the last two decades, an enormous progress has been achieved, owning to the synthesis of complex bandstructure materials and their alloys, and nanostructured materials [1]. The figure of merit, $ZT=\sigma S^2T/\kappa$ where σS^2 is the power factor (PF) and κ the thermal conductivity, quantifies the efficiency. It has increased by 2-fold, to values above $ZT > 2$ across materials and operating conditions, with a maximum of $ZT=2.6$.

In this work, we describe a computational framework to compute the electronic and thermoelectric transport in materials with multi-band electronic structures of an arbitrary shape by coupling density function theory (DFT) bandstructures to the Boltzmann Transport Equation (BTE) [2]. We explain the computational complexities and the approximations made. We then show how 'real-space' methods, such as the non-equilibrium Green's function and the Monte Carlo methods can be used to design nanostructured materials with very high TE PFs [3, 4]. We show than careful design of potential well/barrier nanostructured materials and their interfaces can achieve over an order of magnitude increase in the TE power factor and overall performance, leading to extremely high *ZT* values.

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