Thermoelectric power from first principles

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Thermoelectricity can be used to convert heat directly to electricity, without any working fluid or moving parts. The voltage created by a given temperature difference is defined by the Seebeck coefficient, which thus should be maximized in order to create large output. At the same time, heat conductivity should be minimized to avoid large losses through the structure, and the electrical conductivity should be maximized to allow for efficient transport of electric current.

Optimization of these transport coefficients requires fundamental insight into basic materials properties which are governed by the electronic structure, phonon interactions, defect structure, etc. Much of this can now be calculated atomistically, using an approach without any adjustable parameters. As an example, semiclassical Boltzmann theory can be employed to predict the transport parameters above using a calculated electronic band structure as the only input (in addition to a few assumptions). In this talk, different thermoelectric materials will be described and examples of using first principles calculations for predicting transport properties will be presented.