Simulations of thermoelectric coefficients using DFT bandstructures and energy dependent scattering rates

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The discovery of efficient, cheap and non-toxic thermoelectric materials can be significantly promoted by predictive screening of novel compounds. The adopted computational scheme may dramatically impact the simulations outcomes.

The performance prediction for thermoelectric (TE) materials requires extracting DFT bandstructures and computation of TE coefficients using Boltzmann transport (BTE). The constant relaxation time approximation is commonly employed due to complexities in accurately computing scattering rates.

In this work, we describe the construction of an advanced simulator, which couples generic bandstructures (e.g. from DFT) with BTE, utilizing the full numerical energy/momentum/valley dependences of all states in the extraction of relaxation times. The method provides more predictive capabilities and accuracy, but also considers all scattering mechanisms (acoustic, non polar optic and polar phonons, ionized impurities) independently, as well as intra- and inter- band transitions.

We show that according to the scattering physics under consideration, the performance ranking between different materials, their doping and temperature dependence, the best materials descriptors, vary significantly compared to constant relaxation time consideration.

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