

Full band energy-dependent scattering rate simulation approach for complex thermoelectric materials

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The predictive screening of novel compounds can significantly promote the discovery of efficient, cheap and non-toxic thermoelectric materials. The adopted computational scheme for the extraction of the transport coefficients dramatically affects the simulation outcomes.

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

We present an advanced simulator that couples generic bandstructures (e.g. from DFT) with BTE, utilizing the full numerical energy/momentum/band dependence of all the states to extract the relaxation times. The method provides more predictive capabilities and accuracy, and considers all the important scattering mechanisms (acoustic, non polar and polar optical phonons, ionized impurities) independently.

We show that metrics such as the performance ranking between different materials, their doping and temperature dependence, and the appropriate materials descriptors, are very different compared to the constant relaxation time approximation. We believe this novel simulator will provide the thermoelectric community with the means to improve the search for high performance materials.