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Descriptors for the discovery of efficient thermoelectric materials

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The predictive performance screening of novel compounds can significantly promote the discovery of efficient, cheap, and non-toxic thermoelectric materials. Here we present the development of a set of descriptors that can be used in materials screening studies. We use Boltzmann transport simulations within the energy and momentum dependent relaxation time approximation, coupled to DFT bandstructures, and consider both electron-phonon scattering and electron-ionized impurity scattering as well. We compute the electronic transport and perform power factor optimization for a group of half-Heusler alloys. Then the material parameters that determine the optimal power factor based on this more advanced treatment are identified. Since we go beyond the constant relaxation time approximation, the set of descriptors we present are significantly more reliable, and offer deeper insights into the underlying nature of high performance thermoelectric materials. A combination of the number of valleys, dielectric constant, conductivity effective mass, deformation potential, and bandgap, forms a useful descriptor.