Advanced simulations of thermoelectric coefficients using DFT bandstructures and energy dependent scattering mechanisms

Patrizio Graziosi, Neophytos Neophytou

School of Engineering, University of Warwick, United Kingdom

patrizio.graziosi@gmail.com

The predictive performance screening of novel compounds can accelerate the discovery of efficient, cheap, and nontoxic thermoelectric (TE) materials. Large efforts to couple machinelearning techniques and materials databases are currently undertaken, but the adopted computational methods can dramatically affect the outcome. Typically, thermoelectric transport calculations employ the constant relaxation time approximation to reduce computational complexity. However, such simplifications fail to capture the details of bandstructure features and to give accurate results, especially for complex bandstructures. We show that depending on the scattering treatment, different material performance rankings, different optimal doping regimes, and different temperature dependent trends are found. We also give an indication of single relaxation time for half-Heusler materials for different doping concentrations, useful in interpreting data. We then present a set of new descriptors that we have identified as the most useful and generic: a combination of the number of valleys, the dielectric constant, the conductivity effective mass, and the deformation potential for the dominant electron–phonon process. The proposed descriptors can boost the discovery of new efficient and environment-friendly TE materials in a much more accurate and reliable manner.

References

[1] P. Graziosi et al. , J. Appl. Phys. 2019, 126, 155701

[2] P. Graziosi et al., ACS Appl. Energy Materials, 10.1021/acsaem.0c00825