O.35 Thermoelectric properties of elemental metals from first principles

Bin Xu[1], Marco Di Gennaro[2] and Matthieu J. Verstraete[2]

[1] *Soochow University, Suzhou 215006, China*
[2] *Université de Liège, B-4000 Liège, Belgium*

The Seebeck coefficient is one of the key ingredients in thermoelectric properties, and it is often calculated based simply on the electronic band structure, within the frame of Boltzmann''s transport theory and the constant relaxation time approximation. Despite the simplicity and popularity of this approximation, its validity is not fully justified even in lightly doped semiconductors, and it breaks down completely in metals. On the other hand, more sophisticated first-principles approaches are available but require the computation of the full electron- phonon coupling. In this talk, I will discuss several simple (alkali and noble) metals viz., Li, Na, K, Cu, Ag, Au, and Pt, in which the variational approach based on *ab initio* couplings can reproduce experimental Seebeck coefficients quantitatively, whereas the constant relaxation time approximation yields significant quantitative discrepancies and often fails to predict the correct sign.