Thermoelectric materials – electronic transport calculations and assessments of solubility and diffusivity

O. M. Løvvik[a),b)]
a) SINTEF Materials and Chemistry, 0314 Oslo, Norway
b) Dept. of Physics, University of Oslo, 0318 Oslo, Norway

Thermoelectric materials are solid state heat engines where electrons are the working fluid. They can be used to generate electric power from temperature gradients, or to provide efficient cooling or heating from electricity. They scale very well with size, and require virtually no maintenance, and are thus promising for a large range of potential applications.

It is a challenge to maximize the performance of thermoelectric devices. This requires simultaneous optimization of fundamental transport properties, which to a certain extent are interdependent. Parameter-free modelling studies can assist in the understanding of how this can be accomplished, as well as predicting novel materials with enhanced properties.

This presentation will demonstrate how band-structure calculations can be used to assess fundamental transport properties of Zn_4Sb_3. This is a promising material in this respect, due to its extraordinarily low thermal conductivity. This reduces Ohmic losses, and makes this material one of the most efficient ones for thermoelectricity.

One of the important transport properties of the material is the Seebeck coefficient α, which relates the voltage over a material ΔV with the temperature difference ΔT between the warm and cold end: $\Delta V = \alpha \, \Delta T$. We show how this can be calculated, and how it is strongly correlated with the geometric structure on the atomic scale. We also show how our calculations can be coupled with experimental data on the same system.