Introduction

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Durée du module : 1h30

Objectifs

Improve familiarity with the potentialities and limitations of *ab-initio* lattice thermal conductivity calculations for crystalline compounds. Provide attendees with practical knowledge enabling them to combine software elements to perform these calculations end to end. Explain the role of *ab-initio* lattice thermal conductivity calculations in materials design, review some landmark achievements and discuss open challenges.

Contenu - programme

The lattice thermal conductivity is a key property for many important applications of materials. Hence it is extremely desirable to have workflows available that yield predictive, parameter-free estimates of this variable using only basic information about the chemical structure of the crystal. Alas, historically the development of such approaches has been hindered both by methodological difficulties and by CPU time constraints.

The first part of this presentation will be devoted to a discussion of the theoretical foundations of *ab-initio* approaches to this problem. A particular emphasis will be put on the features that set these methods apart from phenomenological approaches. The historical development of solutions to the Boltzmann transport equation (BTE) for phonons will be used as a guiding thread. More specifically, the emergence of direct solutions starting in the mid-1990s will serve to show how new theoretical tools and improved computers were needed to cope with the difficulties inherent to the problem.

Next, the practical aspects of assembling a workflow such as the one referred to in the first paragraph will be addressed. It will be shown how to go from an atomistic description of an arbitrary crystal to the value of its lattice thermal conductivity. This kind of calculation relies on an electronic structure code (usually a DFT program) to perform atomistic calculations, and on higher-level code to generate the required inputs. The final step is the solution to the BTE itself. The first publicly available BTE solver for phonons, ShengBTE, has been developed at CEA Grenoble and will be presented here.

Finally, a selection of published *ab-initio* lattice thermal conductivity calculations for systems of practical interest will be reviewed. The purpose is to highlight the usefulness of this kind of approach. It will also serve as a prelude for a presentation of the remaining challenges in this area, as well as of some of the most promising possibilities to overcome them.