High throughput multi-scale modelling of the thermal conductivity

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Since the last few years, it is possible to perform multi-scale ab initio computations of the lattice thermal conductivity of semiconductors and insulators. In this research project, the basic idea is to perform quantum mechanical computations of the physical properties [1] at the atomic scale, and then transfer those properties at the meso and macro scale to study heat transport in an real device [2].
At the device scale, the transport equations are solved using a Monte Carlo method to include the effects of boundary conditions and to study the dependence of thermal conductivity with device size and shape. To perform such calculations, materials properties are needed, and those are obtained through quantum mechanical calculations, within the framework of density functional theory (DFT).
The goal of the present project is to make the above-mentioned procedure fully automatic, and to use it to perform high-throughput computations and AI-based optimization of thermal transport in devices.
To achieve this goal, in the first part of the project the Monte Carlo solver [3] will be improved, a step which include its parallelization. The second part of the project will focus on DFT calculations of materials properties. A database of inputs for the Monte Carlo solver will be filled and this database will then be used to optimize heat transfer in selected simple devices.

Considering the above challenges, the recruited candidate should have strong background in solid state physics and numerical computing.

Applications should be sent to laurent.chaput@univ-lorraine.fr before June 15, 2024

[1] Distributions of phonon lifetimes in Brillouin zones
A. Togo, L. Chaput, and I. Tanaka
Phys. Rev. B 91, 094306 (2015)

[2] Ab initio based calculations of the thermal conductivity at the micron scale
L. Chaput, J. Larroque, P. Dollfus, J. Saint-Martin, D. Lacroix
Appl. Phys. Lett. 112, 033104 (2018)

[3] Monte Carlo simulation of phonon transport from ab-initio data with Nano-κ
B.H. Silva and D. Lacroix and M. Isaiev and L. Chaput
Comp. Phys. Comm. 294, 108954 (2024)