Heat transport in disordered systems: a computational study

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Context and Objectives:

Over the last fifteen years *ab initio* calculation methods, based on density functional theory, have become an essential component of research laboratories both academic and industrial. This success is explained by the predictive power of these methods. Indeed, it is possible to determine the physical characteristics of materials, such as the mechanical properties, the optical index, or the coefficient of thermal expansion, without providing any experimental information other than the crystallographic structure of the material. Consequently, this *in silico* approach to materials can save time and money for both manufacturers and scientists, and can lead to the discovery of new physics in conditions that are difficult to realize experimentally. This explains why a company like St Gobain supports this project.

Indeed, chemically or structurally disordered materials, such as vitreous compounds, remain difficult to study by these methods because their atomic structure is not known exactly. This prevents an in depth study of a large class of compounds encountered in our day to day life, and therefore the discovery of any new physics specific to those compounds. It is with this challenge that we are concerned in this project since our goal is to propose **a combined *ab initio*/parameterized strategy for the calculation of the thermal conductivity of glasses.**

To achieve this task, the successful candidate will have to perform density functional based simulations with existing codes and by developing the proposed method in this frame as well as classical molecular dynamics calculations.

A strong background in **solid states physics and chemistry**, **programming** and good skills in **mathematics** are needed.

The interested candidates should address their application to:

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P. Jund (philippe.jund@umontpellier.fr)

Useful references are:

[1] Computer Investigation of the Energy Landscape of Amorphous Silica
P. Jund and R. Jullien
Phys. Rev. Lett. 83, 2210 (1999)

[2] A direct solution to the phonon Boltzmann equation
L. Chaput
Phys. Rev. Lett, 110, 265506 (2013)

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