2024-2025

Master 2 intrernship

Laboratoire des Solides Irradies
Ecole Polytechnique, route de Saclay, 91120 Palaiseau

Director: Michele Raynaud

Title: **COUPLED ELECTRON AND PHONON DYNAMICS IN GRAPHITE FOR POTENTIAL THERMOELECTRIC APPLICATIONS: EXTERNAL PHONON BATH EFFECTS**

Keywords: condensed matter, semiconductors, DFT, DFPT, electron-phonon, transport, thermoelectricity, interface, phonon drag, Boltzmann transport equations

Scientific description:

Today, in the context of climate change and the search for frugal numerical technologies, there is an urgent need to develop new routes in search for improved thermoelectric materials. This theoretical project aims at opening new ways to improve the thermoelectric efficiency of materials, by exploring the phonon drag effect, which arises from the momentum transfer (or drag) between the out-of-equilibrium phonon and electron populations, and which is responsible for the strong increase in Seebeck and Peltier coefficients of thermoelectric materials at low temperature. The concept we aim to explore is the use of substrate as an external phonon bath to provide additional out-of-equilibrium phonons, in order to enhance phonon drag effect and shift it to higher temperatures in the conducting channel. To this end, we aim to develop a numerical approach which would allow to describe the coupled transport of charge and heat carriers at the interface between a conducting system and a phonon bath, with the specific focus on phonon drag effect. In parallel, phonon drag effect will be studied experimentally by our collaborators.

In this theoretical project, we aim to describe the coupled dynamics of electrons and phonons via an approach based on Density Functional Theory and on the solution of coupled Boltzmann transport equations for electrons and phonons which was recently developed in our group[1] and to extend it by including the effect of interface and substrate. The study will first focus on phonon drag in graphite, in link with our new collaboration with experimentalists in the framework of ANR project DragHunt.

A successful internship can be followed by a PhD on related subject, financed by ANR DragHunt.

1. R. Sen, N. Vast, J. Sjakste, PRB 108, L060301 (2023).
https://doi.org/10.1103/PhysRevB.108.L060301

Techniques/methods in use: numerical methods based on DFT, QuantumEspresso code, Wannier code, EPW code.

Applicant skills: knowledge of solid state physics, interest in modelization, ability and/or willingness for programming

Industrial partnership: N

Internship supervisor(s) Jelena Sjakste, jelena.sjakste@polytechnique.edu; 0169334511

Internship location: LSI, Ecole Polytechnique, Palaiseau

Possibility for a Doctoral thesis: Yes, financed with ANR DragHunt