INTERNSHIP PROPOSAL

Laboratory name: Laboratoire des Solides Irradiés

CNRS identification code: UMR7642

Internship director'surname: Sjakste Jelena

e-mail: jelena.sjakste@polytechnique.edu

Phone number: 0169334511

Web page: https://portail.polytechnique.edu/lsi/fr/research/theorie-de-la-science-des-materiaux

Internship location: Ecole Polytechnique, Palaiseau

Thesis possibility after internship: YES

Funding: to be confirmed

COUPLED ELECTRON AND PHONON DYNAMICS IN 1D AND 2D MATERIALS FORPOTENTIAL THERMOELECTRIC APPLICATIONS: QUANTUM CONFINEMENT AND EXTERNAL PHONON BATH EFFECTS

Today, in the context of climate change and the search for frugal numerical technologies, there is an urgent need to develop a portfolio of thermoelectric materials offering thermal stability, especially for the temperature range 300-400 K, where a large amount of heat is wasted into the environment. Compared to bulk materials, low-dimensional materials, such as nanowires and thin films, offer interesting possibilities for improvement of their thermoelectric properties. **I**ndeed, due to dimensionality, confinement, surface and interface effects, nanostructured materials exhibit the electrical and thermal transport properties which largely differ from their pristine forms.

In this theoretical project, we aim to describe the coupled dynamics of hot electrons and phonons via an approach based on Density Functional Theory and on the solution of coupled Boltzmann transport equations for electrons and phonons[1]. In the case of 1D and 2D materials, the focus of the project will be to describe main effects of reduced dimensionality on the electronic, vibrational properties, the electron-phonon scattering channels as well as the electronic and thermal transport coefficients, and identify the main changes with respect to bulk materials. Another important aspect in this study is the effect of interface and substrate on thermoelectric transport in low dimensional materials.

The choice of materials is motivated by the potential applicability in the field of next generation energy harvesting, as well as by the ongoing collaborations with experimentalists. Recently, GEEPS researchers (M. Boutchich) have demonstrated that 2D Bi_2O_2Se allows to achieve a high power factor of ~ 0.86 $mWm^{-1}K^{-2,}$ which is 6-fold larger and closer to room temperature operation than that measured in a recent work[2] on the same system. This preliminary result is very encouraging and, at the same time, raises fundamental questions on the physical reasons which led to such outstanding power factor. This is what our theoretical project aims to elucidate.

1. R. Sen, N. Vast, J. Sjakste, PRB 108, L060301 (2023).
https://doi.org/10.1103/PhysRevB.108.L060301
2.F. Yang *et al.*, *Adv. Mater.* **33**, 2004786 (2021).
https://onlinelibrary.wiley.com/doi/abs/10.1002/adma.202004786.