Master Physics of Complex Systems

Internship offer 2023/2024

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Theoretical Investigation of Topological Insulators for Thermoelectric Applications

Scientific project: Technologies harnessing solar and thermal energies are promising avenues that could help achieving sustainable and alternative energy sources. However, it is essential to find suitable materials and then evaluate their performance by simulating them from the material to the device level, offering a fast and inexpensive way to check device designs and processes.

Topological insulators (TIs), possess novel, symmetry-protected electronic and optical properties (e.g. long-lifetime quasi-particles with decoherence-free internal states) that make them promising candidates as future highly efficient quantum materials for energy conversion [1].

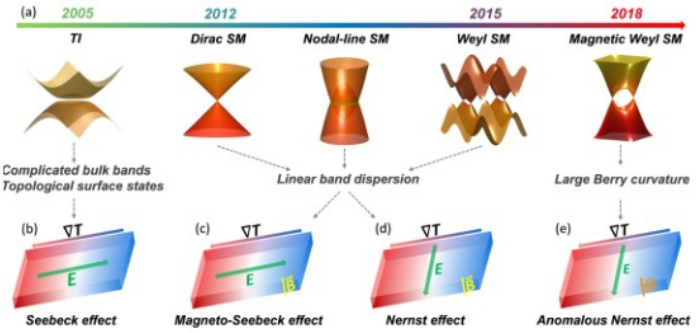

Fig. 1 : Evolution of topological materials' understanding over the years and their application to thermal transport [9]

By exploiting first-principles simulation techniques from theoretical physics and chemistry, this master project aims at understanding the correlation between the topology of electrons/phonons, low dimensionality of materials and their applications in the field of thermoelectricity (i.e. direct conversion of thermal flow into electric current) and to propose new interesting materials.

As a matter of fact, TIs exhibit intrinsic properties that are "topologically protected" [2], allowing electrons not to suffer from backscattering due to impurities and defects (unlike phonons). This allows for efficient decoupling of the two types of transport [3] and thus an independent way for a simultaneous optimization of the electronic and thermal conductivity, which can also be improved by reducing the dimensionality of the system [4].

The aim of the student will be to use state-of-the art ab-initio techniques to investigate the effect of low-dimensionality and topological phase transitions on the electronic structure of quasi-1D semiconductors, as function of pressure, doping, substitutions and/or heterostructures.

[1] K. Behnia, “Fundamentals of Thermoelectricity” (Oxford University Press, 2015)
[2] N. Xu, et al., npj Quantum Materials 2, 51 (2017)
[3] K. Pal, S. Anand, and U. V. Waghmare, J. Mater. Chem. C 3, 12130 (2015).
[4] Y. Ichinose, et al., Phys. Rev. Mat. 5, 025404 (2021)

Methods and techniques: Density Functional Theory (DFT), Density Functional Perturbation Theory (DFTP), Wannier Functions, Boltzmann Transport Equation

Student profile: We are looking for master students with a strong background in solid state physics as well as knowledge of electronic structure theory and computataional languages (Fortran, C++, Python, Julia). Previous experience of DFT codes (e.g. Quantum ESPRESSO) would be advantageous.

Possibility to go on with a PhD ? Yes, with funds from Agence Nationale de la Recherche (ANR)