Post-doc offer

Laboratory: C2N – Center of Nanosciences and Nanotechnologies
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Topology and low dimensionality for thermoelectricity

Scientific project:
Technologies exploiting solar and thermal energies are promising avenues that could help realize 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, providing a quick and inexpensive way to verify device designs and processes.

Topological insulators (TIs), possess novel symmetry-protected electronic and optical properties that make them promising candidates as future highly efficient quantum materials for energy conversion [1].

By exploiting first principles simulation techniques from theoretical physics and chemistry, this project aims to understand the correlation between the topology of electrons/phonons, low dimensionality of materials and their applications in the field of thermoelectricity (i.e. that is to say the direct conversion of heat flow into electricity) and propose new interesting materials.

In 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 an effective decoupling of the two types of transport [3] and thus an independent means for simultaneous optimization of electronic and thermal conductivity, which can also be improved by reducing the dimensionality of the system [4].

[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

Job profile: characterization of topological invariants in topological insulators (quasi-1d), depending on pressure, doping, substitutions and heterostructures and the development of effective Hamiltonians for the description of transport properties (electronic and thermal) . He/she will be hired to work full-time on the analysis of the interaction between topological properties of bands and thermoelectricity. He/she will also be required to supervise the work of master and doctoral students.

Candidate profile: We are looking for young candidates (<3 years) who have a PhD in physics, materials science or equivalent. The applicant should show experience in research using electronic structure calculations (such as Quantum Espresso, CRYSTAL, VASP, etc.) with publications in scientific journals. We are also looking for those with programming experience (preferably MATLAB, FORTRAN, C++ and Python) and Shell scripting. Previous experience on wannier interpolation of electronic band structures and software development is considered a merit. Preference will be given to candidates with a strong background in at least one of the following areas: modelling of topological materials, simulation of transport properties in materials via NEGF or quantum montecarlo techniques.

Contract length: 1 year, renewable

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Start of the contract: From fall 2024

Applications should be sent to davide.romanin@universite-paris-saclay.fr and should include:
- Motivation letter
- detailed CV, list of publications and a short description of the most relevant past achievements
- contact details of at least two researchers that can provide recommendation letters for the candidate

Applications will be accepted and reviewed until the position is filled.