Master 2: *International Centre for Fundamental Physics*

<u>INTERNSHIP PROPOSAL</u>

(One page maximum)

Laboratory name: Laboratoire de Physique des Solides
CNRS identification code: UMR8502
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Internship location: University Paris Saclay, Bat. 510, 91405 Orsay Cedex

Thesis possibility after internship: YES
Funding already obtained for a PhD: NO If YES, which type of funding:

Title: Prediction of charge density wave states under biaxial strain

Charge density waves (CDWs) are exotic states of matter in which electrons form a standing wave pattern different from the periodic crystal. These states are actively researched because they represent a fundamental theoretical quantum physics problem of interactions between electrons and ions. Understanding CDW states is also important for applied physics, where they could be used for nano-transistors. The family of materials RTe3, where R is a rare earth element, hosts multiple CDW states [1,2], as well as other quantum interacting phenomena such as superconductivity, and it is therefore an important challenge to understand the physics of these materials.

A new experiment [3], designed at the LPS, allows for the first time the full exploration of the phase diagram of RTe3 materials under biaxial strain, a deformation of the material along two independent directions. Using strain, one precisely controls the microscopic parameters of geometry and interactions in the material, and one may access parameter values otherwise impossible in unstrained materials, thus creating exciting research questions. Multiple experimental techniques, such as scattering and transport, are giving complementary information on the CDW states, so it is key to advance the theory which can interpret all the observed phenomena. Multiple theoretical approaches are necessary for making predictions which can guide experimentalists in the exploration of the huge phase diagram.

In this internship, the candidate will calculate charge density wave properties of electrons in models of RTe3 under biaxial strain, using multiple theoretical approaches: analytical and numerical solutions of tight-binding lattice models, and microscopic numerical predictions from first-principles techniques such as density functional theory. The models will be matched to experimental systems, and the theoretical results, such as the CDW periodicity as function of temperature and biaxial strain, will be directly used to interpret the experimental data. This internship is a great opportunity to work closely with experimentalists and learn about the theory of quantum matter and the rich physics of charge density waves.

[1] J. J. Hamlin *et al.*, Phys. Rev. Lett. 102, 177002 (2009)
[2] V. Brouet *et al.*, Phys. Rev. B 77, 235104 (2008)
[3] A. Gallo-Frantz *et al.*, arXiv:2306.15712 (2023)

Please, indicate which speciality(ies) seem(s) to be more adapted to the subject:

Condensed Matter Physics: YES
Soft Matter and Biological Physics: NO
Quantum Physics: YES
Theoretical Physics: YES