Master 2: *International Centre for Fundamental Physics*

INTERNSHIP PROPOSAL

(One page maximum)

Laboratory name:**Laboratoire des Solides Irradiés**
CNRS identification code: **UMR7642**
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Internship location: **Laboratoire des Solides Irradiés, Ecole Polytechnique Palaiseau**

Thesis possibility after internship: YES
Funding: NO If YES, which type of funding:

From spectra to total energies: a new approach to the ground state

This internship is part of a research line that has the ambition to build a new theoretical approach, aimed at describing efficiently and precisely a wide range of properties of so-called « strongly correlated » materials. These are materials for which the effects of the Coulomb interaction between electrons are particularly important.
Density Functional Theory (DFT), for which Walter Kohn was awarded the Nobel prize in 1998, is a formidable tool to understand and predict many properties of materials. DFT allows one to determine crystal structures and lattice parameters, vibration frequencies, the charge density, and much more, reliably and for a broad range of materials. However, whereas it is known that the knowledge of the charge density is in principle sufficient to obtain observables, this is not true in practice, since the corresponding functionals are not known. Therefore DFT has many shortcomings, even to describe ground state properties, for which it has originally been designed. For example, the weak van der Waals bonding that occurs in many biological systems cannot be described by simple functionals. DFT also often fails to correctly describe phase transitions, such as the volume collapse that occurs between two different phases in Cerium, or the correct density at which the Wigner transition happens, where a homogeneous electron gas crystallizes. For this reason, it is interesting to search for routes that constitute promising alternatives to DFT, and/or that could inspire new functionals.

Over the last years, we have proposed a non-perturbative approach for the calculation of many-body Green's functions to predict electronic excitations [1]. It is based on the approximate solution of a functional differential equation and has already led to a revival of the study of signatures of correlation in electronic spectra, such as plasmon satellites in photoemission [2]. In the present project the student will explore the same idea, but in order to access also ground state properties. He/she will combine mathematical tools with physical intution in order to push the frontiers of this approach, starting from simple models and moving towards real materials.

[1] G. Lani, P. Romaniello, and L. Reining, New Journal of Physics 14, 013056 (2012).
[2] M. Guzzo et al., Phys. Rev. Lett. 107, 166401 (2011).

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

Condensed Matter Physics:	YES	Macroscopic Physics and complexity:	NO
Quantum Physics:	YES	Theoretical Physics:	YES