MASTER DE PHYSIQUE ET APPLICATIONS - 2ème année
Spécialité Sciences des Matériaux et Nano-objets
International Nanomat Master Program

Internship proposal 2011-2012

Laboratory : IMPMC

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Title for the scientific project

Magnetic properties of acenes and graphene nanoribbons

Scientific project:

One of the sources of magnetism proposed in literature for carbon materials is related to the formation of edge states in graphene nanoribbons with monohydrogenated zig-zag configurations, that turn out to be spin-polarized in density functional theory (DFT) calculations. This scenario was further studied by our group, that showed the monohydrogenated zig-zag configurations are thermodynamically more reactive and less stable than the armchair edges for hydrogen concentrations reachable in normal experimental conditions. On the other hand, armchair edges are nonmagnetic and usually metallic. The energetics would disfavor the edge states as a way to create and exploit the magnetism in the carbon materials in normal conditions. Anyway, the small energy difference between the armchair and zig-zag configurations opens the possibility for the correlation to shift the relative order of the structures. Therefore, a study with a highly correlated method would be desirable to definitely assess this question.

In this project we want to tackle this problem by starting from the "parent molecules", that share the same resonating properties as the zig-zag and armchair graphene nanoribbons, namely the acene-type and the phenanthrene-edge-type hydrocarbons, respectively. The acene family is known to be a challenge for any quantum chemistry method, as the excitations around its open-shell singlet ground state require a multiconfigurational description.

Here, we plan to study them by quantum Monte Carlo (QMC) calculations, and set up the numerical approach to tackle the more difficult problem of graphene nanoribbons. By carrying out this study, we will have also the chance to compare directly the QMC accuracy with the DFT one for this type of physics.

Techniques in use :
First-principles calculations based on Density Functional Theory and Quantum Monte Carlo

Applicant skills :
Condensed matter theory, quantum mechanics

Granted internship : yes (400.00 €/month)
C'nano IdF laboratory (France only) : yes
Possibility for a thesis : yes (type of grant : Ecole doctorale UPMC, Labex Matisse)