Research project title : Theoretical *prediction of stable B and N-doped C_{60} and their synthesis pathways*
Supervisor's name: Pascal Pochet

Lab : L_Sim**;** http://inac.cea.fr/Pisp/pascal.pochet/

Key words to describe the project: Fullerene and graphene-like materials; Density fonctional theory; Potential energy surface exploration

Description of the considered work (aims, experimental techniques, recommended background):

The raise of nano-science has promoted a lot of research efforts to find alternative fullerene materials that might be used as building block in the so-called bottom-up approach. In this study we will focus on N-doped C_{60} fullerene that have been synthesised 10 years ago [1] and on their boron counterpart as well. The attendee will perform an exhaustive exploration of the potential energy surface for this fullerene in order to check their synthesizable character using the proposed criterion in our last publication [2]. The second step will be to used the ART method [3] in order to find possible growth routes for the identified building block as recently proposed for boron cages [4]. The exploration will be performed at the DFT level using the BigDFT package [5] developed in Grenoble. Besides these important studies in cluster science, the attendee will have the possibility to develop experience in *ab initio* simulations on massive parallel supercomputers, which is a powerful investigation tool widely used both for basic or applied research.

The key of success for the training in the lab is twofolds:

- computer friendly (including some programing/scripting skills)
- curiosity and knowledge in condensed matters physics

[1] L. Hultman *et al.* Phys Rev Lett. **87** 225503 (2001).
[2] S. De *et al.* Phys. Rev. Lett. **106**, 225502 (2011).
[3] E. Machado *et al.* J. Chem. Phys. **135**, 034102 (2011)
[4] P. Pochet *et al.* Phys. Rev. B **83**, 081403(R) (2011)
[5] http://bigdft.org/