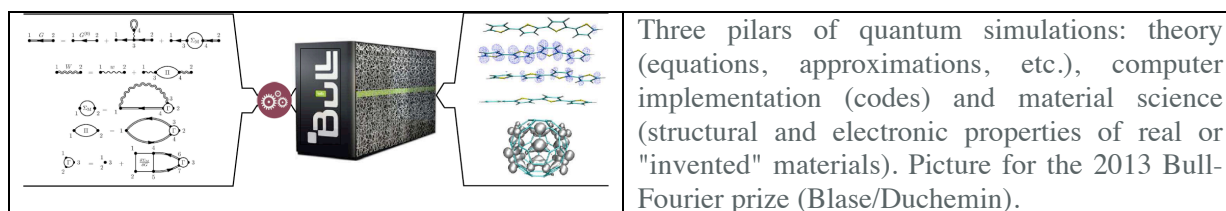


Proposition de stage Master 2 - Année universitaire 2014-2015

Title: "From photovoltaics to photosynthesis: Novel theoretical approaches and quantum simulations."

Cadre général (General background): Photovoltaics and photosynthesis, namely natural but complex phenomena that transform sun light into electrical or chemical energy, are attracting increasing fundamental and applied research interest worldwide in relation with the crucial search for alternative energy sources. From a theoretical stand point, the basic mechanisms controlling the efficiency of innovating devices, based on organic or hybrid organic/inorganic systems, such as semiconductors, nanotubes or graphene combined with optically active molecules, are still poorly understood, since they rely on a complex interplay between photons, excited electrons (excitons) and vibrations in inhomogeneous disordered systems. Our group has pioneered novel theoretical and quantum simulation approaches, implementing "many-body perturbation theories" into a massively parallel code (the Fiesta initiative) revealing unprecedented accuracy for the electronic and optical properties of organic and hybrid systems.



Sujet et moyens disponibles (Joining our group): Opportunities to join our group at the Master 2 level are now opening to start learning the fundamental theories and apply the existing codes to simple practical cases of experimental interest. We are developing in particular an hybrid "quantum mechanical"/"standard electrostatics" approach to allow the study of the electronic and optical properties of a finite number of "active molecules" surrounded by a complex dielectric medium and first tests on simple photoactive and/or biological molecules are an important and timely subject. Néel institute is equipped with a large cluster (>256 cores) on which calculations will be performed, together with a limited, but comfortable, access to national and European supercomputing centers.

Interactions et collaborations éventuelles (Collaborations): this project is developed in strong interaction with the L_sim group at CEA Grenoble. Active connections with groups in France, Belgium, England, US and Canada can serve as a basis for visits or subsequent research programs.

Opportunité de thèse (Ph.D opportunities): YES. Depending on the abilities and interest of the candidate, continuation into a Ph.D thesis is possible for pushing forward the theoretical and/or code developments, together with related applications.

Formation / Compétences (Required skills) : The ideal candidate should have an excellent background and strong interest in quantum mechanics with possibly some experience with computers.

Période envisagée pour le début du stage (Training period): 4-6 months within the first semester of 2015.

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