Ph. D. in theoretical chemistry/physics

The Center for Biomolecular Nanotechnology (CBN, www.cbn.iit.it) of the Italian Institute of Technology (IIT, www.iit.it) in collaboration with the University of Salento (http://www.matfis.unisalento.it) invites applications for Ph.D. positions in theoretical physics/chemistry in the group of Dr. Fabio Della Sala. Positions are **3-years** long. Successful candidates must have a master degree in physics, chemistry or related disciplines.
For information on how to apply contact lucian.constantin@iit.it **before July 15th, 2015.**

Research project: Quantum mechanics under strong spatial electronic confinement: towards accurate theoretical modeling of quasi-low-dimensional systems.

Quantum confinement of electrons is a main paradigm in modern nanoscience, being at the base of numerous of the most important and famous nanotechnological advances of the last decades. However, despite the scientific interest of the topic, most of the studies and practically all applications so far have concerned solid-state and/or extended systems, while the quantum mechanics under strong spatial electronic confinement still an almost unexplored field.

The Ph.D. research project aims at starting the exciting exploration of this field by developing and applying advanced computational methods to study the properties of atoms and molecules subject to a strong spatial confinement. Thus, a theoretical analysis of the whole crossover between the full-dimensional (3D) and quasi-low-dimensional (2D or 1D) regimes will be carried on for different atomic and molecular system to investigate the dependence of different chemical and physical properties on the confinement strength and type. The main goals are: (1) Extension of quantum chemistry methods to study quasi-low-dimensional systems, application of the different methods to interesting tests cases to study chemical physics under confinement, and creation of a database of reference data; (2) Development of density-functional methods to describe chemical systems under strong spatial confinement.

Main References from the group:
L. Chiodo, L.A. Constantin, E. Fabiano, F. Della Sala, **Phys. Rev. Lett.** 108 , 126402 (2012)
F. Della Sala, E. Fabiano, L. A. Constantin, **Phys. Rev. B** 91, 035126 (2015).
E. Fabiano, L.A. Constantin, P. Cortona, and F. Della Sala, **J. Chem. Theory Comput.** 11, 122, 2015.
E. Fabiano and L.A. Constantin, **Phys. Rev. A** 87, 012511 (2013).
L.A. Constantin, **Phys. Rev. B** 78, 155106 (2008).