Ph.D. in theoretical physics/chemistry

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 to apply contact eduardo.fabiano@nano.cnr.it before **July 15th, 2015.**

Research Project: Development of kinetic energy functionals for nanoscience: application to orbital-free, hydrodynamic and subsystems' density functional theory.

With the constant development of nanoscience there is an increasing need to perform accurate electronic structure calculations on very large systems (e.g. biomolecules, nanocrystals,...). However, since most of the state-of-the-art computational methods are implemented in a wave-function or orbital framework, they have a very unfavorable scaling with system's dimensions, so that they cannot be applied in practice to large systems even using the most advanced computing facilities. Alternative methods which are attracting increasing interest in the last years are the orbital-free DFT methods (OF-DFT), including the hydrodynamic model to describe the absorption spectra of nanoparticles, which is based on the use of the electron density as only main input ingredient, and the embedding methods (e.g. frozen-density embedding, partition DFT), which divide the system into smaller interacting fragments.
A common feature of all these methods (and many others) is the fact that they need a density-functional expression for the kinetic energy of electrons. This expression is however unknown from fist principles and needs to be approximated. The development of accurate and efficient density-functional kinetic energy functional models is therefore a crucial topic with many possible applications in condensed-matter physics, theoretical chemistry, and nanoscience.

The Ph.D. project aims at the development of advanced kinetic-energy density-functional models, with minimal empiricism. The reference framework for theoretical development will be the density functional theory and the exploitation of known exact properties of the kinetic energy functional. The developed methods will be implemented in state-of-the-art simulation codes and applied to different problems in nanoscience.
The main goals are: (1) Development of kinetic energy functionals for orbital-free applications (OF-DFT, hydrodynamic model); (2) Development of non-additive kinetic energy funcitonals for embedding calculations; (3) Application of the developed method for the study of the electronic and optical properties of metal nanoparticles, isolated and interacting with molecules, complex molecular aggregates.

Main References from the group:
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