

Job offer: PhD position in Theoretical Physics and Chemistry
Place: Institut des Sciences Moléculaires (ISM), University Bordeaux I, France
Starting date: 1st September 2013
Duration: 3 years

Applications are invited for a PhD position in the Theoretical Chemistry group of the Institute of Molecular Sciences (ISM), University of Bordeaux I, under the supervision of Dr. Lionel Truflandier and Prof. Alain Fritsch, in linear-scaling electronic structure methodologies and implementations. The project aims to extend the effort initiated for linear-scaling density functional theory (see: D. R. Bowler and T. Miyazaki *Reports on Progress in Physics*, **75** 036503, 2012) to linear-response calculation for spectroscopic observables.

The project involves the:

- Derivation of a methodological framework for the linear-response function(s) calculation, using density matrix perturbation theory.
- Development of a robust linear scaling algorithm and its implementation within the CONQUEST code (<http://www.conquest.ucl.ac.uk>). This part of the work will be realized in collaboration with Dr. David Bowler, Department of Physics & Astronomy, University College London (UCL), UK.
- Application to large-scale systems, such as IR differential spectroscopy applied to proteins, solid state NMR spectroscopy in glasses, or UV-Vis spectroscopy applied to functionalized materials.

The candidate will join a dynamic group, which includes 17 researchers, covering various theoretical chemistry/physics aspects, from ultra-cold collisions and electron molecule scattering to the simulation of macroscopic observables in condensed phases. The candidate will also have the opportunity to work in close collaboration with developers from UCL in UK, and NIMS (National Institute for Materials Science) in Japan within the CONQUEST consortium.

We seek highly motivated candidates with a MSc degree in Physics/Chemical-Physics, or related expertise, interested in contributing to the development and implementation of new approaches in a cutting-edge electronic structure code. Candidates should have a solid background in quantum chemistry/physics and knowledge in numerical sciences. Good communication skills in English are required. Previous experiences with (either) quantum chemistry, condensed matter theory, density functional theory, and LINUX environment/scientific programming will be appreciated (but not mandatory).

Applications should include a detailed CV, a brief description of motivations, and the contact information of at least two referees. Inquiries and applications should be sent to l.truflandier@ism.u-bordeaux1.fr (Subject: PhD position). Consideration of candidates will begin immediately and continue until the position is filled. The gross monthly salary is roughly 1685 € (up to 2025 € if teaching & other tasks are also performed).

Contact:

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