deMon2k and deMon-nano tutorial

Date & place: 15-20 juin 2015, Orsay, France
Website: under construction
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PRESENTATION

Computational biology, materials science, and nanoscience often benefit from quantum chemical modeling giving quantitative information on large and complex systems including, for example, energy changes, accurate microscopic structures, ligand binding energies and spectroscopic parameters. This task demands programs that can perform calculations with a reasonable accuracy in a reasonable amount of time.

The *deMon* family of programs constitutes a system of programs developed around density-functional theory (DFT) for calculations on atoms, molecules, clusters, and solids. *deMon2k* is an efficiently parallelized program for solving the Kohn-Sham equations based on Gaussian-type atomic orbitals. It makes intensive use of variationally-fitted densities to speed-up the calculations of DFT energies and of molecular properties. *deMon-nano* is dedicated to the density-functional tight-binding (DFTB) method with or without self-consistent charges (SCC), whose efficiency comes from the use of parameterized integrals.

The tutorial will be organized at Orsay (France), a few months after the releases of new public versions of the programs. The tutorial divides into two parts, namely (i) a set of theoretical courses emphasizing key concepts needed to understand how to use the programs and (ii) a hands-on part of the course consisting partly of a tutorial and partly of group projects chosen from a list. Although the students will have access to powerful computers, each student who completes the *deMon* licence will receive a USB flash drive with a copy of the *deMon* programs which they can install on their laptop computers. We plan to welcome around 50 participants, essentially PhD, although postdocs and academic may also be accepted depending on the number of applications. Participants from all nationalities will be welcome.

PROGRAM

The objective of this tutorial is to train new potential users to the use of deMon2k and deMon-nano. It will last 6 days. Morning lectures on the most important topics will be given by internationally renowned experts. In the afternoons the participants will put this knowledge into practice during hands-on tutorials and to work of specific projects. The theoretical lectures will cover a consistent arrays of topics that are necessary for an efficient use of the programs. Each point will take

[1]. Generalities and historic of DFT (Hohenberg and Kohn theorems, Kohn-Sham approach...). (*Dennis Salahub*). Modern methodologies for solving the KS equations (Resolution of the Identify, variational density fitting, parallelization techniques...) (*Andreas Köster*)

[2]. Auxiliary Density Perturbation Theory (ADPT); application to the calculation of molecular properties (*Andreas Köster*). Calculation of NMR and EPR parameters by DFT (*Vladimir Malkin*)

[3]. Time-Dependent DFT for simulating electronic spectra (*Mark E. Casida*). Inner-shell spectroscopies (NEXAFS, XES) (*Lars G.M. Pettersson*)

[4]. *Ab initio* molecular dynamics simulations (Born-Oppenheimer MD, Car-Parrinello MD, thermostats for NVT simulations). (*Patrizia Calaminici*)

[5] Modeling complex molecular systems:

5.1 DFT/MM approaches (subtractive and additive schemes, embedding techniques, treatments of QM-MM boarders, type of DFT/MM calculations available with deMon2k…) (*Isabelle Navizet*)

5.2 DFTB (basic theory, self-consistent-charge, DFTB-CI…) (*Thomas Heine*)

ORGANIZING COMMITTEE

Fabien Cailliez (Univ. Paris-Sud, Orsay), Mark Casida (Univ. J. Fourier, Grenoble), Aurélien de la Lande (Univ. Paris-Sud, Orsay), Jean-Philip Piquemal (UPMC, Paris), Tzonka Mineva (Institut C. Gherardt, Montpellier), Eve Ranvier (Univ. Paris-Sud, Orsay), Mathias Rapacioli (Univ. P. Sabatier, Toulouse) and Eve Ranvier (Univ. Paris-Sud, Orsay).