MOLCAS Workshop 2007
Training Workshop on Computational Quantum Chemistry
July 1-5, 2007
Villars, Switzerland

MOLCAS is a quantum chemistry package for first-principle structure calculations on atomic and molecular systems. The philosophy behind MOLCAS is to provide the user methods covering from very accurate ab initio treatments of general electronic structure problems in small molecules in both ground and excited states (with an emphasis on multiconfigurational approaches), to more versatile procedures (density-functional theory for instance) applied to systems of large size.

The workshop is addressed to users and potential users of the MOLCAS suite, and it is not intended as a course on electronic structure theory but a practical approach to the use of the MOLCAS program. Some knowledge on quantum chemical methods is desirable, but no previous experience with MOLCAS is required. The workshop will consist of 25% lectures and 75% practical sessions. People interested in using MOLCAS as a platform to implement their own software are also welcome.

Main topics to be covered include:

- Overview of MOLCAS, its possibilities, capabilities, and easy ways to handle installation, run calculations, and interpret results.
- How to design a quantum chemical calculation with MOLCAS: geometries, basis sets, input building.
- Overview of single-reference methods for closed- and high-spin open-shell molecules: Hartree-Fock and Kohn-Sham calculations. Other correlated approaches using perturbative and coupled-cluster theory.
- Multiconfigurational approaches for ground and excited states.
- Structure optimizations in ground and excited states: minima, hessians, transition states, reactivity, constrained optimizations, minimum energy paths, and electronic states crossings.
- Calculation of transition and state properties: oscillator strengths, spin-orbit couplings, and radiative lifetimes.
- Solvent effects in quantum chemistry.
- Handling problems in MOLCAS: selection of active spaces, convergence problems, etc.
- Case studies: bring your own problem.
- MOLCAS as a development platform: implement your own code.

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Lecturers

Lectures and computer sessions will be given by different MOLCAS authors from the Deartment of Theoretical Chemistry of the University of Lund, Sweden (Björn O. Roos, Roland Lindh, Per-Ake Malmqvist, Valera Veryazov) and from the Institute of Molecular Sciences of the University of Valencia (Luis Serano-Andrés)

Location

The workshop will be held at the Eurotel Victoria in Villars, Switzerland (http://www.eurotel-victoria.ch/, click on "Villars"), a four-star hotel situated on a sunny terrace at 1300 m overlooking the lower Rhone valley (see: http://www.villars.ch)

Villars is accessible by a local train from Bex or by bus from Aigle. Intercity trains from Geneva (airport) - Lausanne usually stop at one or both of these stations. Intercity trains from Bern / Basel / Zürich connect in Lausanne (use: http://www.sbb.ch/en/ to find connections from your place of origin to Villars).

Equipment

All participants must bring a laptop computer (running Linux, Mac OS X or Windows, plus an Ethernet port) onto which the latest version of the MOLCAS program and other material will be loaded at the workshop, via a local network.

Cost

The cost of the workshop is CHF 750 (€ 480) in double rooms, CHF 800 (€ 520) in single rooms. This includes accommodation and all meals between dinner on Sunday, July 1, until lunch on Thursday, July 5, and all the course material. Students from the Universities of Geneva, Fribourg, Bern, Basel, and from the EPF Lausanne obtain a reduction of CHF 550 through support from the CUSO organization.

Participants have the possibility to purchase a copy of the textbook of the European School of Quantum Chemistry (ESQC), where a lot of the theory behind the methods coded in MOLCAS is explained, for the special price of SFr 110 / € 70.

Registration

Registration for the workshop is to be effected on the Website

http://www.teokem.lu.se/molcas/wsh/2007/

Once registration is confirmed by the organizers, the appropriate fee (see Cost, including the ESQC book if desired) should be paid to:

Banque Cantonale de Fribourg, Account No., 25 01 024.422.09
(IBAN CH05 0076 8250 1024 4220 9) "MOLCAS Workshop 2007"

Registration will only become definitive once the fee has been received. If this is not the case a month after registration has been confirmed, it will be cancelled and the next person on the waiting list shall be invited to register by paying the fee (Attendance to the workshop is strictly limited to 30 participants).

Thomas Bally
(Univ. of Fribourg)

Laura Gagliardi
(Univ. of Geneva)

Roland Lindh
(Univ. of Lund)

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