MOLCAS Workshop 2006

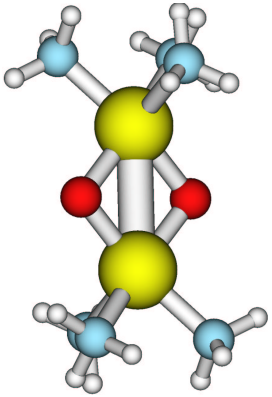
Training Workshop on Computational Quantum Chemistry

April 20th–23rd, 2006

Valencia, Spain

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, to more versatile procedures applied to systems of large size.

The workshop is addressed to users and potential users of the MOLCAS suite. The workshop will consist of 8 hours of lectures and 17 hours of practical sessions. Researchers interested in using MOLCAS as a platform to implement their own software are also welcome.



$Cu_2O_2(NH_3)_6$

- **4-day training workshop**
- **Novice to experienced users**
- **Problem oriented**
- **8 hours of lectures**
- **17 hours of exercises**
- **Bring your own project**

Contents of the Workshop

The Workshop is designed on a practical training basis. 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.
- Multiconfigurational approaches.
- Structure optimizations.
- Calculation of properties.
- Solvent effects in quantum chemistry.
- Handling scientific problems in MOLCAS.
- Case studies: bring your own problem.
- MOLCAS as a development platform.

Most of the Workshop will make use of computers, where simple calculations will be run. Participants must bring their own portable computer.

Lectures and computer sessions will be given by different MOLCAS authors from the Department of Theoretical Chemistry of Lund University, Sweden, and the Institute of Molecular Science of the University of Valencia, Spain. Prospective teachers will be: Björn O. Roos, Roland Lindh, Per-Åke Malmqvist, Valera Veryazov, and Luis Serrano-Andrès.

The number of participants is restricted to 20, therefore early registration is highly encouraged.

Deadlines and costs

The deadline for the registration is December 15th 2005.

	Registration only	With lodging
Academic prices	400 Euro	650 Euro
Company prices	800 Euro	1050 Euro

For further information and on-line registration access
`http://www.teokem.lu.se/molcas/wsh`