



## MOLCAS Workshop Intro

Roland Lindh

*Department of Chemistry - Ångström  
the Theoretical Chemistry Programme  
Uppsala University  
Sweden*

December 15, 2011

## Once upon a time...



## Status late 1980'ies

- Björn Roos: CASSCF / multi configurational methods
- Jan Almlöf: MOLECULE / 2-electron integrals
- Per Siegbahn: MRCI / dynamic electron correlation
- Ulf Wahlgren: Relativistic effects



- From only point energy calculations (MOLECULE/CASSCF/MRCI)
- MOLCAS Version 1 ('89), 2 ('91), 3 ('93), 4 ('97), 5 ('00), 6 ('03), and 7 ('07)
- Parallelization
- More general (DFT, CC, Opt., Freq., exc. states, and SO)
- 2006 1st MOLCAS workshop, Valencia
- 2007 2nd MOLCAS workshop, Villars
- Cholesky decomposition and RI technique for all wfn models
- Version 7.6 fall, 2010

- GUI, fall 2010
- CD gradients for DFT, HF, MP2 and (SA-)CASSCF spring 2012

# What is MOLCAS?

## Software for Quantum Chemistry

- for ground and excited states,
- for molecular structure, chemical and photochemical reactions,
- for solution chemistry, chemical bonding, and much more,
- for all elements of the periodic table.

Developed by quantum chemists at the Lund and Uppsala Universities  
+ many external developers

- Electronic structure methods
  - Hartree-Fock and DFT for closed and open shell systems.
  - Møller-Plesset second order perturbation theory.
  - Multiconfigurational SCF: CASSCF and RASSCF.
  - Multiconfigurational second order perturbation theory CASPT2.
  - Multi-reference CI MRCI.
  - Coupled-cluster methods CCSD, CCSD(T).

- Geometry optimization
  - Analytical gradients for SCF/DFT and RASSCF.
  - Numerical gradients for CASPT2, Coupled-Cluster methods
  - Automatic geometry optimization of equilibrium geometries, transition states, intersystem crossing, conical intersections, etc.
  - Vibrational frequencies and thermodynamic quantities.



- Excited States and Electronic Spectra
  - Electronic Spectroscopy with vibrational resolution.
  - Photochemical reactions, locating conical intersections.
  - Geometries and vibrational frequencies for excited states.
  - Spin-orbit coupling and spin-forbidden transitions and reactions.

- Environmental Effects

- Solvent effects using the Onsager spherical cavity model or the Polarizable Continuum Model (PCM).
- Combined QM and molecular Mechanics (MM) calculations.
- The NEMO procedure for creating intermolecular force fields for MC/MD simulations.

## Typical applications with MOLCAS



- Accurate Potential Energy Curves
- Molecular spectroscopy
- Reaction mechanisms
- Biochemistry
- Heavy element chemistry
- Molecular trajectories

# WELCOME to the 7th MOLCAS workshop!



We are pleased to see you here. We hope that both you, the students, and we, the teachers, will learn from this experience.

We will be using MOLCAS 7.6!

Diploma and Evaluation.