

### Key features of TURBOMOLE:

- Robustness
- Applicable for very large systems and a wide range of chemistry
- Excited states are treated as efficiently as ground states for both, energy and gradient calculations
- Fast and robust COSMO implementation for molecules in solvents
- Very efficient integral evaluation
- **High efficiency for all methods.** The usage of the RI approximation for DFT and MP2/CC2 and low scaling techniques allow for **DFT and MP2 calculations with several thousands of basis functions**
- Full use of all (including non-abelian) point groups
- Low memory and disk space requirements
- Available for Linux, Windows, MacOS, HP-UX, AIX, SGI Altix, and SUN Solaris systems

### Implemented Methods:

- Energy calculation:
  - Ground state: HF, DFT, MP2, CC2, SCS-MP2, SOS-MP2, and UFF
  - Excited state: TDDFT, CIS, TDHF, CC2, CIS(D), ADC(2)
- Ground & excited state gradients: HF, DFT, MP2, TDDFT, CC2

- Geometry optimization:
  - Minima and transition states in cartesian or internal coordinates
  - Excited states for TDDFT and CC2 (analytical gradients)
- Force constants, vibrational frequencies, and IR intensities:
  - Analytical calculation for HF and DFT
  - Numerical calculation for MP2, TDDFT, CC2
- Molecular dynamics for all methods
- Relativistic ECPs for heavy elements
- Balanced basis sets for the elements H to Rn of types SV, TZV and QZV (plus polarization sets)
- External electric field and field gradient
- QM/MM interface
- Properties:
  - Electric and magnetic moments and polarizabilities
  - UV/VIS and CD spectra
  - IR and Raman spectra
  - NMR shieldings on HF, DFT, and MP2 level
  - ESP fit
  - Population analysis
- Interface to external visualization programs:
  - Structures, Geometry opt., and vibrational modes
  - Molecular orbitals
  - Densities (total, spin, difference)
  - Electrostatic potentials and fields

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Cover picture: difference density of Au<sub>146</sub> and Au<sub>146</sub><sup>-</sup>

**COSMOlogic** GmbH & Co. KG

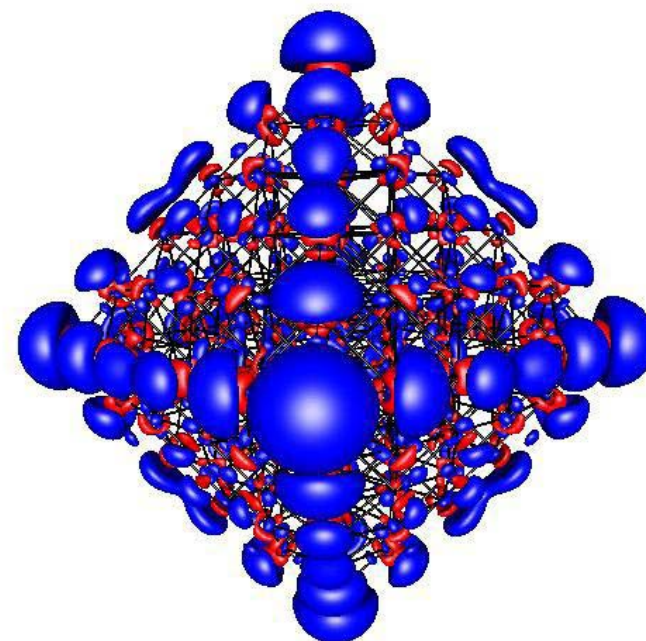
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# TURBOMOLE

A Quantum Chemistry Program Package



It's a tool not a toy!

Get a free Demo Version at:  
<http://www.cosmologic.de/turbomole.html>

TURBOMOLE is a standard Quantum Chemistry program package, developed in the group of Prof. Ahlrichs at the University of Karlsruhe, and now by the Turbomole GmbH, covering a wide range of research areas from both academia and industry. With more than 15 years of development, TURBOMOLE has become a powerful tool

for chemists, physicists and engineers. The philosophy behind the development of the code was, and still is, its usefulness for applications: "Applications to molecules with more than 100 atoms -of all kinds- are mainly carried out in connection with experiments to check, correct, and predict properties of molecules and their existence." (Prof. Ahlrichs). Because of its robustness and speed, TURBOMOLE is an excellent tool for large systems and applications of all kinds, including standard organic and inorganic chemistry (including transition metals), catalysis, biochemistry, and nano sciences. TURBOMOLE is the workhorse for quantum chemical calculations in the leading German chemical companies for more than a decade. The TURBOMOLE package consists of several modules and scripts that facilitate its usage, and provide interfaces to standard visualization programs.

#### Ground state chemistry:

Optimization of structures, transition state searches, and molecular dynamics can be treated very efficiently by using the RI method for DFT and MP2 calculations, without loss of accuracy for large systems (Fig. 2, Fig. 3, and Fig. 4). A set of highly optimized basis functions for the elements H to Rn is available in three qualities (double, triple, and quadruple zeta). The energy calculation of crambin (Fig. 4) took only 7 hours on a single 1.5 GHz HP Itanium workstation; the gradient calculation took 2 hours. The COSMO solvation model is implemented at the DFT and HF level, allowing a very efficient treatment of solvation effect in the

continuum solvent framework. HF and DFT frequencies can be calculated analytically, a lowest eigenvalue search that determines only a certain number of frequencies allows a very efficient check for minima and transition states without the need of calculating the full Hessian. Numerical frequency calculations are available for all levels of theory.

#### Excited states:

One of the key features of TURBOMOLE is the efficient treatment of excited states. Geometry optimizations with analytical gradients can be performed at the TDDFT and CC2 levels of theory. These levels allow the user to apply two different branches of quantum chemistry and therefore to check the validity and stability of the methods for the given problem. UV/VIS and CD spectra (see Fig. 2 and 3) are ready for calculation with both methods.

#### Properties:

A variety of additional properties are available, such as IR- and Raman spectra, NMR chemical shielding, ESP fits, and population analysis. Orbitals and densities can be plotted using external and free visualization tools.

#### Parallel version:

The parallel TURBOMOLE version is based on the already extremely fast serial code using standard MPI routines, allowing parallel calculation of ground state structural optimization on all supported systems at the DFT, MP2, and CC2 level.

### Graphical User Interface TmoleX included

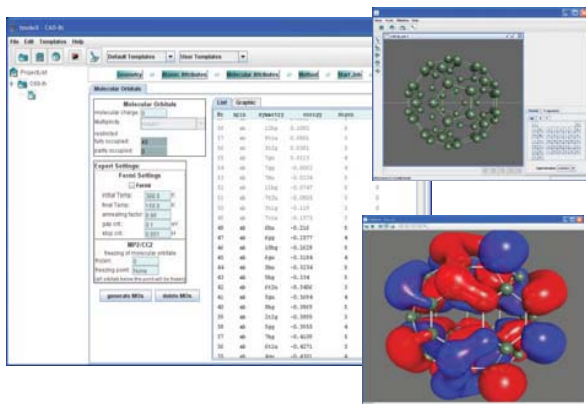


Fig. 1. TmoleX screen shots of coming TmoleX 2 [1]

### Excited state UV/VIS spectra with RI-CC2

#### The UV/VIS Spectrum of Free-Base Porphyrin

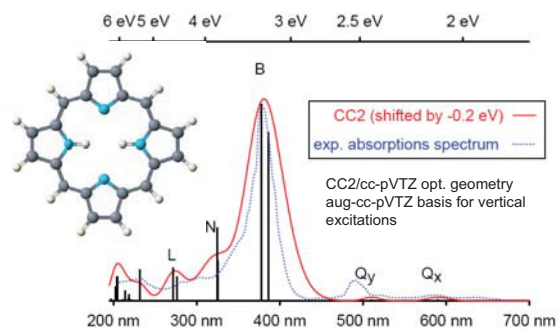


Fig. 2. RICC2 calculation of the Porphyrin UV/VIS spectrum [2].

### Excited state CD spectra with TDDFT.

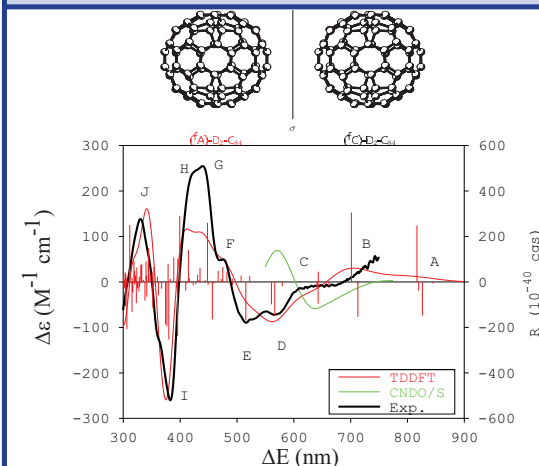


Fig. 3. Determination of the absolute configuration of C(84) by comparison of the exp. and the TDDFT CD spectrum [3].

### RI-DFT timings: an example.

Crambin (645 atoms)  
SV(P) basis (5500 functions)

1.5 GHz HP Itanium workstation  
(single processor)  
4GB core memory  
MARI-J approximation  
SCF convergence 1  $\mu$ H

Total time in hours:minutes

	BP86	TPSS
Energy	6:52	7:40
Gradient	1:54	1:58

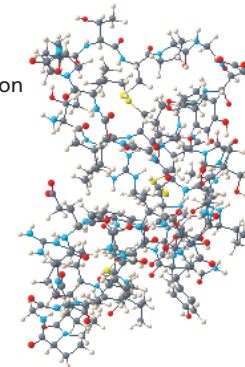


Fig. 4. DFT timings [4].

#### References

- 1) TmoleX 2 beta version
- 2) Seminar talk: "Calculations of Energies and Structures of Excited States using the Approximated Coupled-Cluster Singles-and-Doubles Model CC2", C. Hättig, University of Bochum.
- 3) F. Furche, R. Ahlrichs, *J. Am. Chem. Soc.* 124 (2002), 3804.
- 4) F. Furche, J. P. Perdew, *J. Chem. Phys.* 124 (2006), 44103.