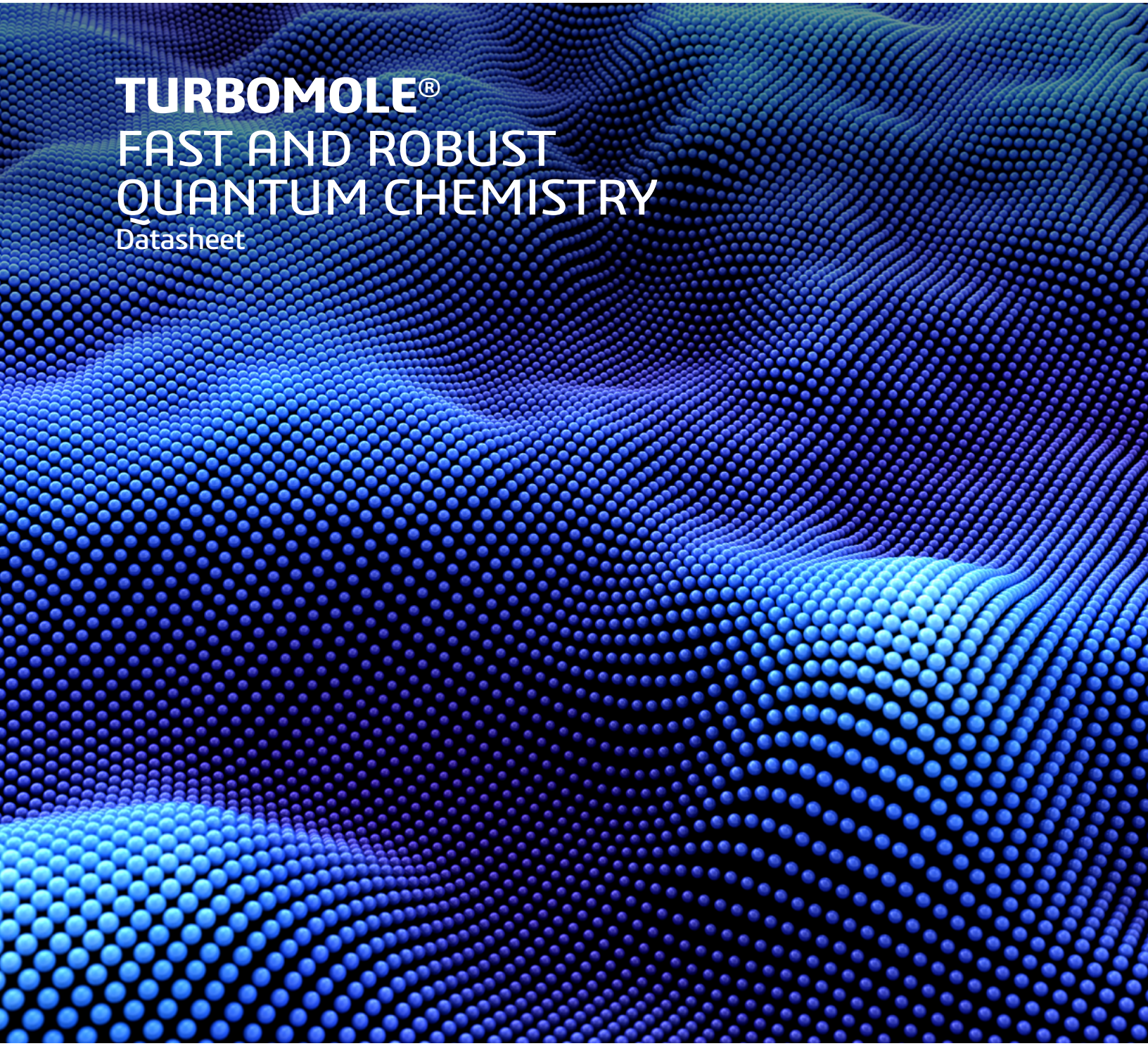
BIOVIA

3DEXPERIENCE

TURBOMOLE®
FAST AND ROBUST QUANTUM CHEMISTRY
Datasheet

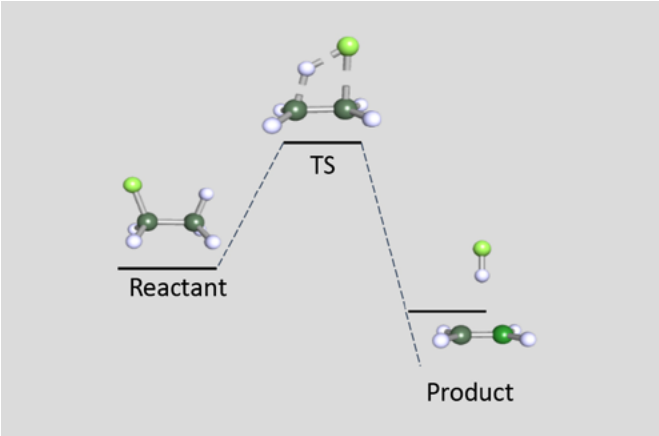


DASSAULT SYSTEMES

A QUANTUM CHEMICAL PROGRAM PACKAGE

TURBOMOLE[1] is a collaborative, multinational software development project owned and coordinated by the TURBOMOLE GmbH,[2] which provides highly efficient and stable computational tools for Quantum Chemical simulations of molecules, clusters, periodic systems, and solutions. It offers excellent tools for large systems and applications of all kinds:

- Energies
- Structures (minima and transition states)
- 2nd derivatives, vibrational frequencies
- Linear response properties



First order properties and spectra such as:

- IR, Raman, VCD
- UV-VIS, CD, OR
- NMR chemical shifts

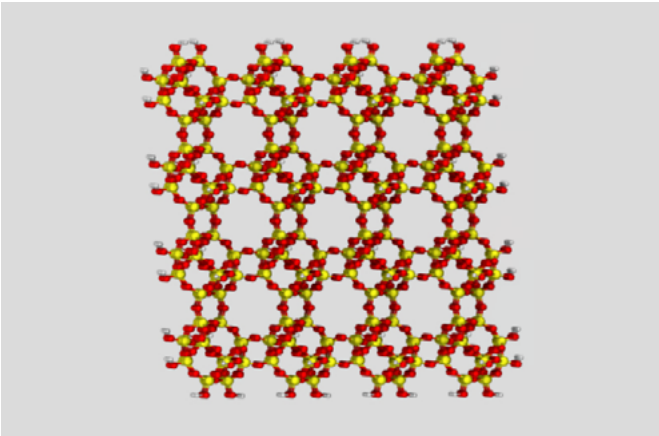


Figure 1: Zeolite, 2592 atoms, 37632 basis functions 3D periodic

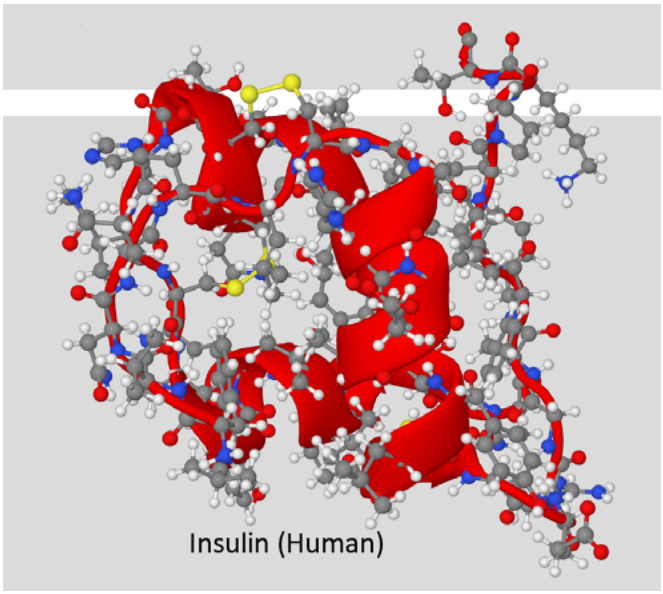
It has outstanding speed and robustness for:

- DFT, DFT-D3, TD-DFT (with and without RI)
- RI-MP2 and RI-CC2
- SCF (with and without RI)
- High symmetry (including non-abelian point groups)
- Balanced basis sets: SV[P], TZVP[P], QZVP[P] for elements H-Rn

New feature: DFT with **periodic boundary conditions in 1D, 2D, and 3D** using Gaussian type basis sets, with k-points, band structures, cell optimization, ...

Key Methods

- Fast DFT, MP2, CCSD(T), TDDFT, CC2, F12, RPA, ...
- Solvent effects with COSMO
- Optical properties and spectra
- Scalar relativistic and spin-orbit coupling effects



RI-DFT Example

Insulin: 784 atoms, **6450 basis functions** def-SV(P) basis set PBE functional

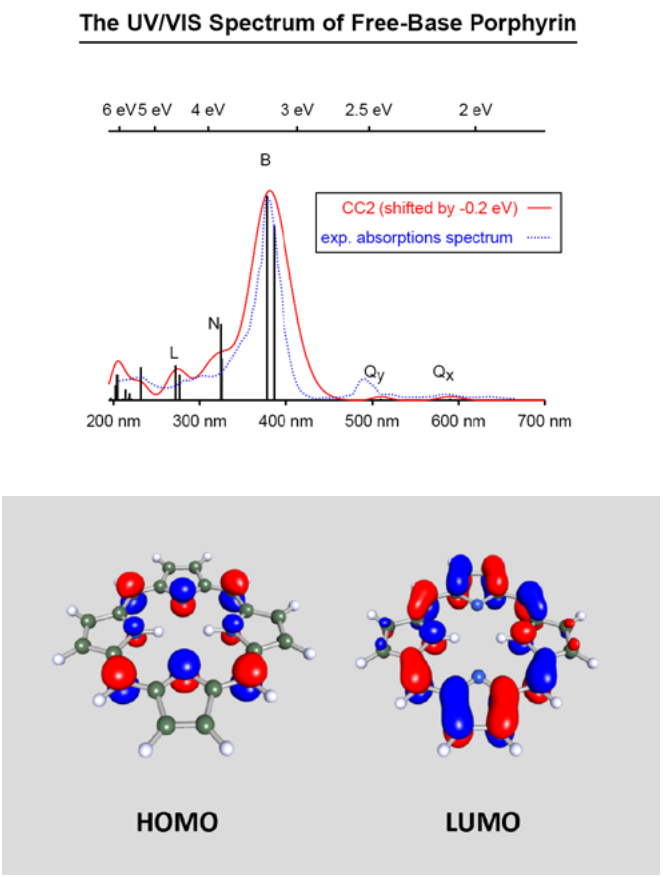
Timings per SCF iteration: **86 Seconds**

Calculated on an off-the-shelf Linux system using 8 cores of an Intel Xeon E5-2643 @ 3.3 GHz

EXCITED STATES

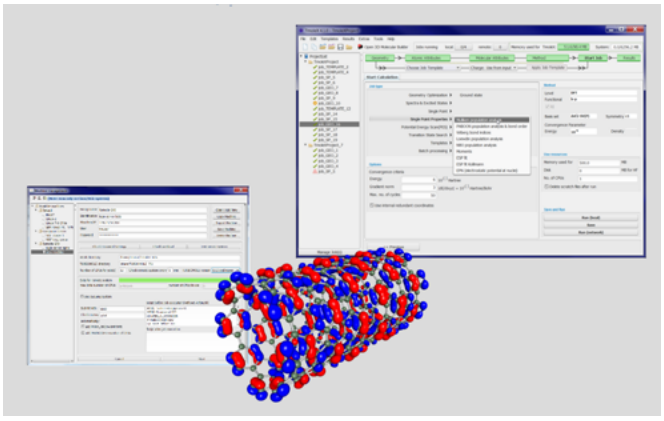
One of the key features of TURBOMOLE is the efficient description of excited states.

Structure optimizations with analytical gradients can be performed at the TDDFT and CC2 level of theory. UV/Vis and CD spectra are ready for calculation with these methods.



TMOLEX – FREE GRAPHICAL USER INTERFACE

- Build or import structures
- Pre-optimize
- Set up and fine-tune
- Run on local or remote computer
- Visualize and analyze your results
- Export results



Key Benefits

- State-of-the-art methods and latest developments
- High quality user support
- Optimized for Linux, Windows, Mac, IBM, Cray, ...
- Serial and parallel versions
- Front-ends available for experts and casual users

1. **TURBOMOLE, a development of University of Karlsruhe and Forschungszentrum Karlsruhe GmbH, 1989-2007, TURBOMOLE GmbH, since 2007**
2. **www.turbomole.org**

TURBOMOLE

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Dassault Systèmes, the **3D**EXPERIENCE Company, is a catalyst for human progress. We provide business and people with collaborative virtual environments to imagine sustainable innovations. By creating 'virtual experience twins' of the real world with our **3D**EXPERIENCE platform and applications, our customers push the boundaries of innovation, learning and production.

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Americas
Dassault Systèmes
175 Wyman Street
Waltham, Massachusetts
02451-1223
USA

Europe/Middle East/Africa
Dassault Systèmes
10, rue Marcel Dassault
CS 40501
78946 Vélizy-Villacoublay Cedex
France

Asia-Pacific
Dassault Systèmes K.K.
ThinkPark Tower
2-1-1 Osaki, Shinagawa-ku,
Tokyo 141-6020
Japan