Density Functional Theory

Gain access to a vast built-in library of more than 200 density functionals. Q-Chem's innovative algorithms provide accurate results faster than ever!

Solvation, QM/MM, and Embedding

Account for solvent effects using Q-Chem's implicit solvent models, including SMD, C-PCM, and COSMO, and explicit solvent modeling. Run simulations with density embedding methods, or use QM/MM interfaces to Amber, CHARMM, and GROMACS.

Excited States & Properties

Utilize state-of-the-art tools for modeling excited states from CIS and TDDFT and open-shell species to the EOM-CC and ADC methods.

Post-HF Methods

Take advantage of Q-Chem's cutting-edge correlated methods, including coupled-cluster and algebraic diagrammatic approaches, CASSCF, selected CI, RAS-CI, spin-flip, and variational 2-RDM.

Spectroscopy Modeling

Simulate IR, UV-Vis, vibronic, photoelectron, VCD, NMR, and non-linear spectroscopies in gas and condensed phase. Q-Chem also offers an extensive set of tools for X-ray spectroscopy (XPS, XAS, XES, Auger, XECD, and more).

Ready-To-Launch Cloud Capabilities

Q-Cloud provides fast and easy cloud computing through Amazon EC2, providing flexibility, scalability, and efficient performance for effective workflows.

Learning & Teaching Resources

Q-Chem provides free teaching resources, including lab assignments, video tutorials, webinars, workshops, and guest lectures.
https://www.q-chem.com/learn/

Webinar Series

Tune in for the Q-Chem webinar series to hear from expert developers about the exciting work they're doing in Q-Chem!
https://www.q-chem.com/webinars/

Q-Chem Talk Forum

Talk with other users, get help, and review an archive of questions and answers.
https://talk.q-chem.com/

Q-Chem Manual

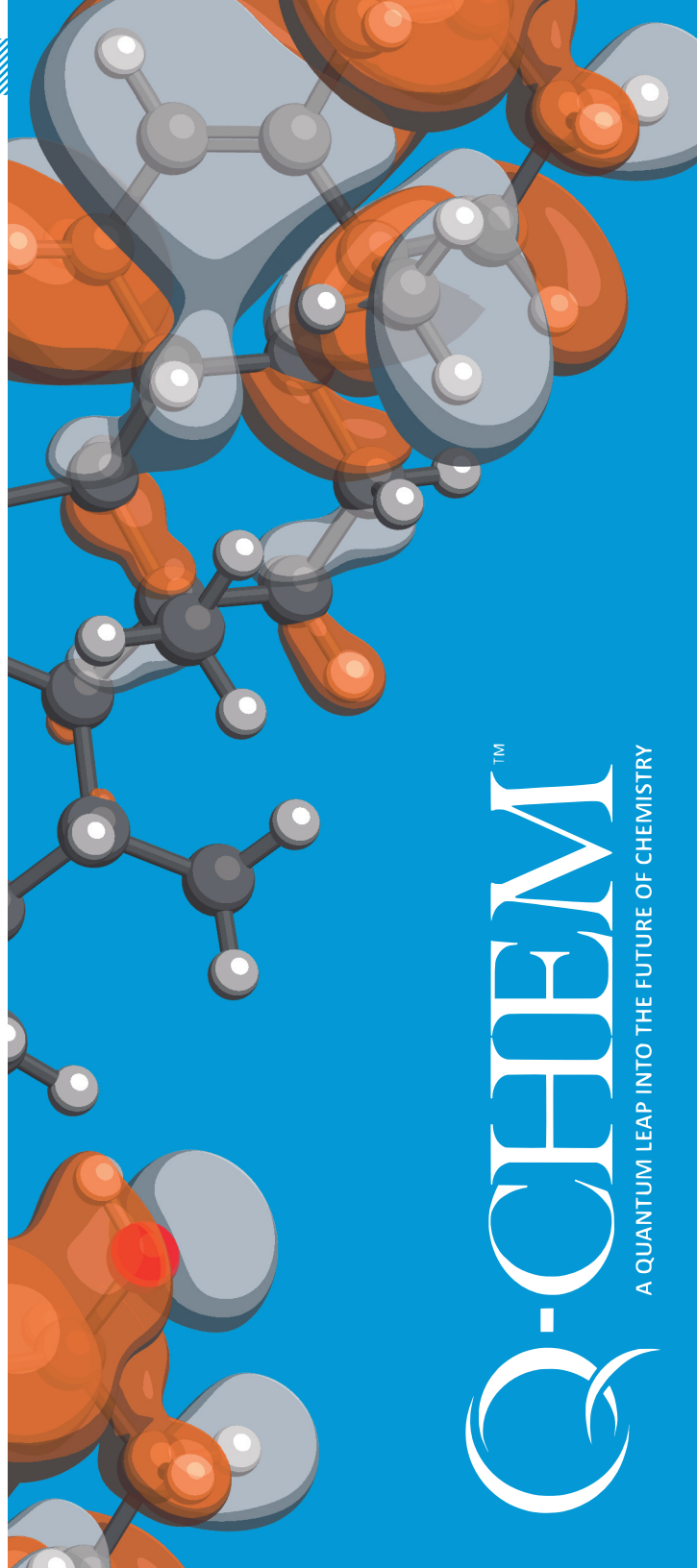
Read the Q-Chem manual to learn more about features and the underlying theory.
https://manual.q-chem.com/

Contact Us

info@q-chem.com
sales@q-chem.com
support@q-chem.com

6601 Owens Drive, Ste 240
Pleasanton, CA 94588

https://www.q-chem.com



Q-Chem Open Teamware Project

Since 1993, Q-Chem Inc. has provided scientists worldwide with high-quality quantum chemistry software, enabling quick and accurate solutions to computational chemistry problems.

Our open-teamware approach allows researchers from all across the globe to contribute their code to Q-Chem. These developers benefit from Q-Chem's stable, rigorously tested code base, while customers benefit from access to cutting-edge, peer-reviewed methods and professional support.

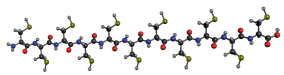
Black-Box "Robust SCF" Procedure

Q-Chem's sophisticated new multi-stage "Robust SCF" procedure (new in version 6.3) provides more robust SCF and DFT convergence, including automatic detection and correction of incipient SCF divergence and algorithm switching in cases where DIIS fails. This approach will be valuable in big-data applications and will assist with difficult-to-converge cases.

Improved SCF & DFT Performance

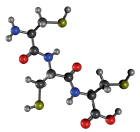
Q-Chem 6.3 improves the performance of medium and large DFT energy and force calculations substantially within the already-fast density fitting approximation. Benchmark timings show 20-30% speedup relative to the Q-Chem 6.2 release.

DFT w/ Density Fitting: ~20% Speedup



Cysteine-11
20.9% speedup
B3LYP/def2-TZVP(2485)/
rijk-def2-TZVP(6680)

Pure DFT Frequency: ~20–30% Speedup



Cysteine-3
34.8% speedup
B97-D3/def2-SVP(363)

Benchmark results showing speedup relative to Q-Chem 6.2. Calculations were run using Q-Chem 6.3 on AMD EPYC (Milan) 7713P processors on 32 cores.

Coupled-Cluster & Equation-of-Motion

Methods for open-shell systems include complex-valued RI-EOM-CCSD, spin-orbit coupling in EOM-DEA/DIP, and EOM-DIP/DEA-CCSD gradients.

Many-body methods for improved accuracy now include CC2 with size-consistent Brillouin-Wigner partitioning, and EOM-CCSDT for EE, SF, IP, EA, DIP, and DEA.

New Tools for Environmental Effects

Heterogeneous PCM allows assignment of different dielectric constants to different regions of the molecule, providing realistic simulation of anisotropic solvation.

GMBE-DM reduces the cost of SCF calculations by an order of magnitude in appropriate systems, and it can be used with high-quality basis sets.

Frequency calculations with SMD are now tractable for large molecules, thanks to semi-numerical gradients.

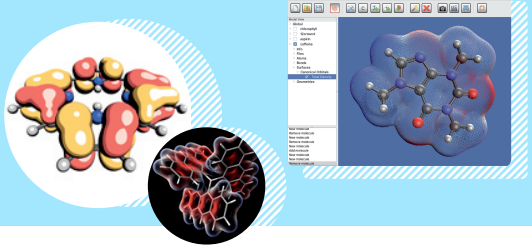
And Much More...

- New analysis tools, including the Broken Bond Orbitals approach and TDDFT charge-transfer metrics
- MPI parallelization for finite difference and MBE
- New tools for modeling Auger decay spectroscopy
- New methods and improvements in the NEO suite
- New PV mechanochemical pressure model

Try Q-Chem

IQmol

IQmol is Q-Chem's free, open-source molecular editor and visualization package. Use our server to run short Q-Chem jobs!
https://www.iqmol.org



Q-Cloud

No hardware? No problem! Use Q-Cloud to easily run calculations on AWS servers in the cloud.

Free Demo

Request a free Q-Chem demo license, no strings attached!
https://www.q-chem.com/try