"*Harvard Clean Energy Project - Powered by Q-Chem . . . the result of nearly 40 million DFT calculations with Q-Chem.*"

- Johannes Hachmann
Postdoctoral Fellow
Harvard University

The Q-Chem Commitment

Founded in 1993, Q-Chem is striving to bring its customers state-of-the-art methods and algorithms for performing quantum chemistry calculations. Cutting-edge innovation, performance, and robustness are Q-Chem's distinguishing features. Q-Chem is an open-teamware project and the latest release includes contributions from more than 100 developers in 9 countries.

How to Obtain Q-Chem 4

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Free 60 day trial.

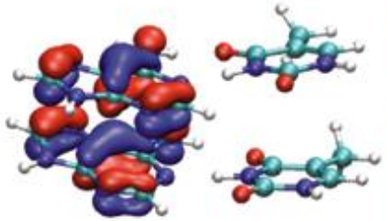
Q-CHEM™

NEW MAJOR RELEASE:
Q-Chem 4.0!

Post Hartree-Fock Features:

Coupled-Cluster, Equation-of-Motion, and Adiabatic Diagrammatic Construction

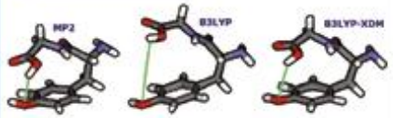
- Significantly enhanced coupled-cluster codes rewritten for better performance on multicore systems
- Energy, gradient, and properties for CCSD, EOM-EE/SF/IP/EA-CCSD
- New EOM methods (2SF, DIP) and triples corrections for chemical accuracy



New Approaches for Strong Correlation:

- Perfect quadruples and perfect hextuples methods for strong correlation problems
- Coupled Cluster Valence Bond (CCVB) and related methods for multiple bond breaking

Exchange-Correlation Functionals



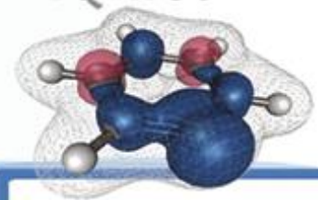
More than 20 new functionals, including:

- **Dispersion corrections:**
  - Becke-Johnson XDM model
  - DF-04, VV09, VV10 van der Waals
  - DFT-D3 long-range corrections
- **General purpose functionals:**
  - M11 and M11-L hybrid meta GGAs
  - Becke-05 nondynamic correlation model
  - MCY2 hyper-GGA functional of Yang et al
- **Double hybrid density functionals:**
  - XYG3 and XYG3-OS double hybrids
  - ωB97X-2 double hybrid

Q-CHEM™

A Quantum Leap Into the Future of Chemistry

IQmol



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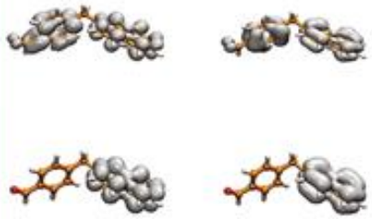
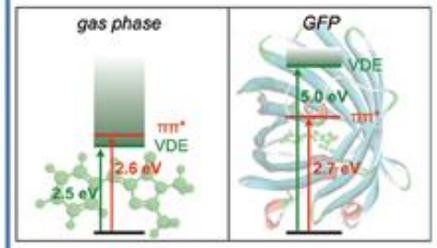
Q-Chem 4: Getting the most mileage from your computational resources. Enhanced performance and parallel execution from laptops to supercomputers. Best choice for shared memory multicore machines.

DFT and TDDFT

- A large set of innovative functionals and algorithms for ground, excited, and ionized states
- Analytic nuclear gradients and hessians for TDDFT
- Constrained DFT for charge-transfer systems
- Diabatization schemes, overlap analysis, and electronic couplings calculations
- Non-collinear SF-DFT (improved accuracy for multi-configurational species)



Q-CHEM
A QUANTUM LEAP INTO THE FUTURE OF CHEMISTRY

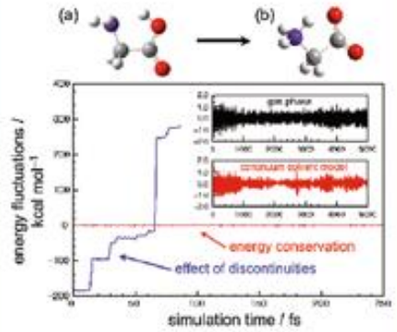


Wave Function-Based Methods for Electronically Excited and Open-Shell Species

- EOM-CC methods (gradients and properties calculations, multicore parallel, interface with Effective Fragment Potential method) for excited (EE), ionized/electron-attached (IP/EA), and diradical states (SF, DIP)
- ADC family of methods including ADC(2X)
- RI-SOS-CIS(D): N^4 excited state method
- Restricted active space double SF method for polyradicals and multiple bond breaking

Condensed Phase, Solvation, and QM/MM

- A variety of popular solvent models including SM8, COSMO, C-PCM, SS(V)PE, IEF-PCM, and more
- Smooth potential energy surfaces for QM/PCM and QM/MM/PCM geometry optimizations and ab initio molecular dynamics with implicit solvent models
- QM/MM functionality including correlated methods and excited states; Yin-Yang atoms
- Effective fragment potential method interfaced with DFT and wave-function based methods for the ground and excited states. Unique feature: Built-in library of standard effective fragments



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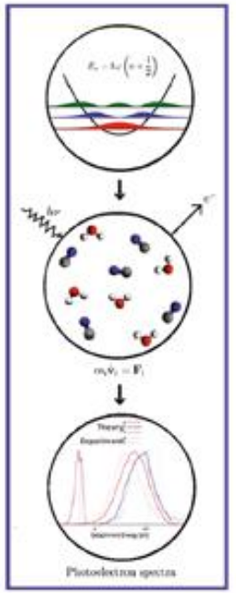

Optimizations, Vibrations, and Dynamics

- Freezing and Growing String methods for efficient automatic reaction path finding
- Quantum mechanical treatment of nuclear motions with path integral methods
- Calculation of local vibrational modes with partial Hessian vibrational analysis
- Ab initio dynamics with extrapolated z-vector techniques for MP2 and/or dual-basis methods
- Quasiclassical ab initio molecular dynamics