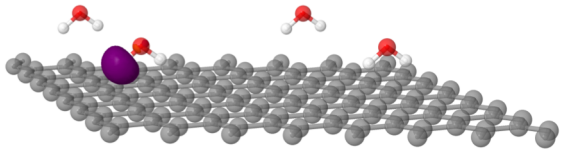
QCPBC: A New Module for Fast, Accurate Materials Modeling



Features

- Energies
- Band structures
- Geometry optimization
- Solvation
- Fully analytic frequency and phonon calculations

Methods

- Fast DFT including hybrid functionals
- TDDFT
- CC
- MP2
- EDA
- Open-MP and MPI parallel
- Solvation models

A One-Stop-Shop For Computational Chemistry

Q-Chem 7.0 includes modules for molecular, material, and biomolecular modeling with no additional licensing.

Learning & Teaching Resources

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

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

Learn more about features and the underlying theory.
https://manual.q-chem.com/

Contact Us

info@q-chem.com
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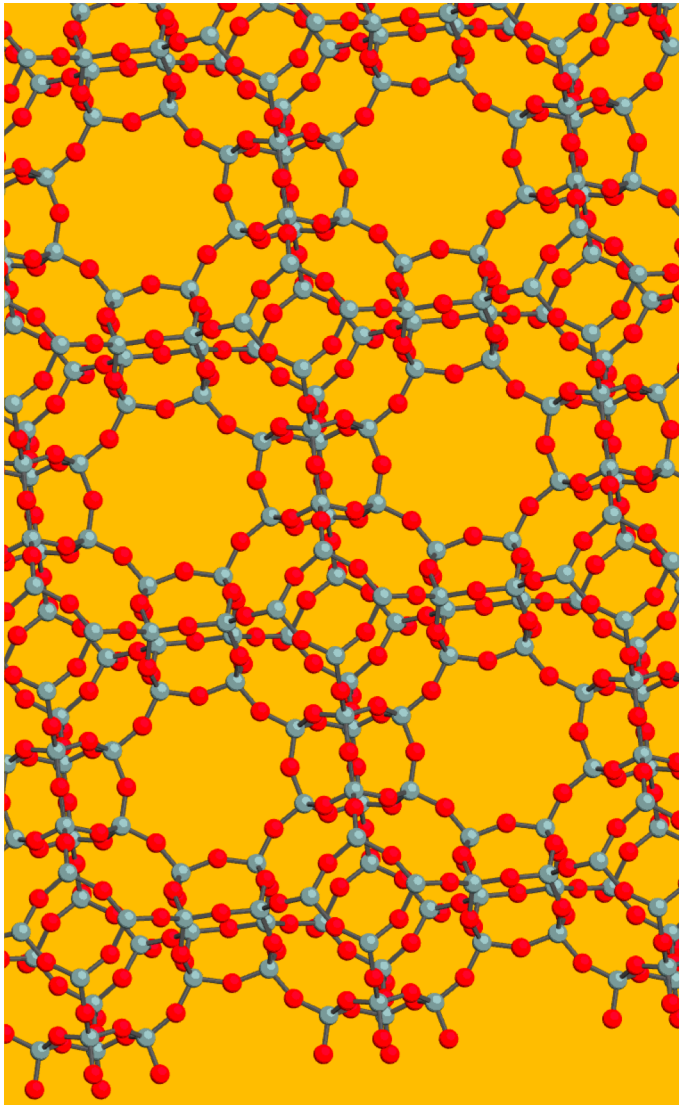
https://www.q-chem.com

Q-CHEM™
A QUANTUM LEAP INTO THE FUTURE OF CHEMISTRY



QCPBC
Materials Modeling

Part of the Q-CHEM Suite

Extending Q-Chem to Materials

QC-PBC is an effective and parallel periodic code that uses a GTO basis and periodic boundary conditions.

Highlights include: fast hybrid DFT; CC and MP2; analytic derivatives; excited states; solvation; and EDA.

Fast Density Functional Theory

- Parallel implementation
- Fastest integral libraries
- GPW
- Density fitting

Post-HF Methods

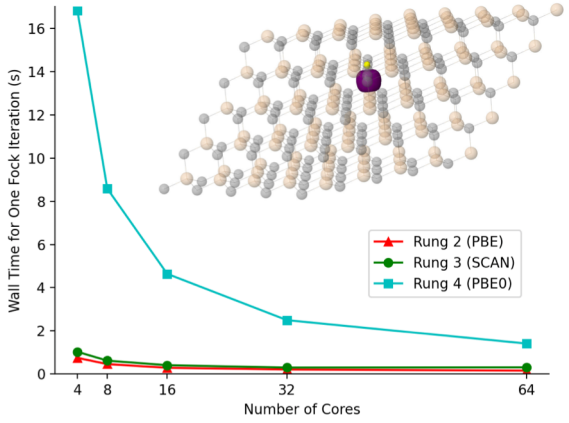
- MP2, LT-MP2, and MP3
- BW-s2
- dRPA
- CCSD, CCSD(T), and CCSDT (gamma-point only)

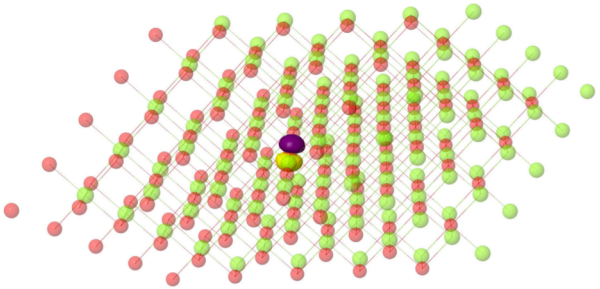
Excited-State Methods

- CIS
- TDDFT

Analytic Frequency & Phonon Calculations

Parallel performance for Fock build (SiC with TZ basis set)





Intrinsic bond orbitals (IBOs) for MgO.

Solvation Methods

- LPCM
- NLPCM
- CANDLE
- Finite-temperature grand-canonical DFT for solid-liquid interfaces

Other Features

- Energy decomposition analysis (EDA)
- Scalar and relativistic effects via X2c1e
- Mulliken population analysis
- Localization methods, including Intrinsic Bonding Orbitals (IBO) and Pipek Mezey (PM)
- Python interfaces enable interfacing to workflows and machine learning packages like PyTorch

Try QCPBC

Request a one-month free trial today!
https://q-chem.com/try/