

Feature overview of Q-Chem 5.x package

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October 31, 2018

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Q-Chem 5.x: Features and availability

Availability and setup on Numerikserver

- Available as **unlimited cluster license on Numerikserver**
for Kaupp's working group (*no installation on ZECM (a.k.a. tubIT HPC)*)
- Access to **Q-Chem** 5.0 package:
`module load qchem/5.0` or `module load qchem/5.0-mpi`
- different types of parallelization: **OpenMP**, **Open MPI** and *hybrid*
(**OpenMP+Open MPI**)
- **Open MPI** and *hybrid* only partly implemented (missing for EDA, ADC
and perturbation methods, see **Q-Chem** manual)
- *Running in parallel:*
 1. *SMP execution:* `-nt <no_threads>`
 2. **Open MPI** execution: `-np <no_processes>`
 3. *hybrid execution:* `-np <no_processes> -nt <no_threads>`

Features: Fragment-based methods

- **Available energy partitioning schemes:**

1. *Intermolecular first generation EDA (energy decomposition analysis: ALMO-EDA (absolutely localized MO)*
2. *Adiabatic ALMO-EDA*: extension to calculation of mol. properties
3. *Second generation EDA (EDA2)*: including extension to intramol. single-bond interactions (spin-projection)
4. *Symmetry-adapted perturbation (SAPT), explicit polarization (XPol) and XPol+SAPT (XSAPT)*
5. *TD-DFT and BSSE corrected SCF* molecular interaction energies

Features: Density functional methods and Valence Bond

- **DFT functionals:**

1. *Hybrid HF-GGA* (incl. SOGGA11-X), *meta GGA*, *hybrid meta GGA* and *hyper-GGA*
2. *Double hybrid functionals* (including B2PLYP-D and XYGJ-OS)
3. *Long-range corrected functionals*: Baer-Neuhauser-Livshits (BNL), CAM-B3LYP, LRC- ω PBE(h)PBE etc.
4. *Dispersion correction*: Grimme's D2/D3, VV09, vdw-DF-04, Becke and Johnson's XDM
5. Coupled Cluster Valence Bond (CCVB): multiple bond breaking
6. For further features see:
<http://www.q-chem.com/qchem-website/features4.htm>

Literature and references

Finding further information

- Further references **Q-Chem** 5.x:

Q-Chem 5.x documentation: **Q-Chem** 5.x manual and
<http://www.q-chem.com/qchem-website/technical-info.html>