Q-CHEM™
A Quantum Leap Into the Future of Chemistry

Using Q-Chem for molecular simulations at NERSC

Evgeny Epifanovsky

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What is Q-Chem?

Established in 1993, first release in 1997.

Software

Q-Chem 3.0 (2006)
4.0 (2012)
4.1 (2013) 4.2 (2014)
4.3 (2015) 4.4 (2016)
5.0 (2017)
5.1 (2018)

Development platform

Supported infrastructure for state-of-the-art quantum chemistry

Open source for developers

> 200 contributors (Q-Chem 5)

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List of features

By electronic structure method

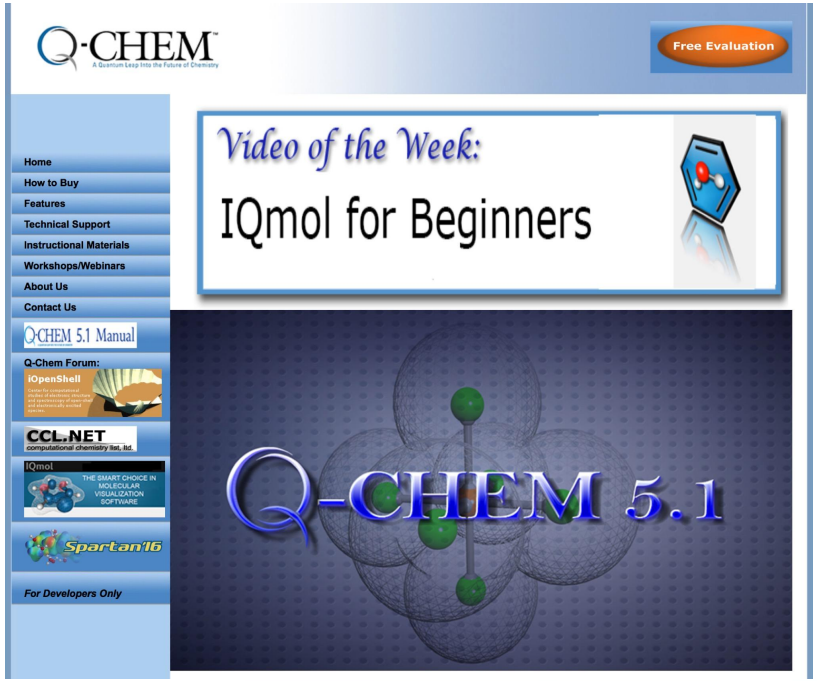
- Hartree-Fock and density functional theory (200+ density functionals)
- Post-Hartree-Fock methods: MP2, coupled cluster theory
- Excited state methods: TD-DFT, CIS, ADC, EOM
- Implicit and explicit solvation models
- Built-in QM/MM capabilities

List of features

By calculation type

- Single point energy
- Molecular structure optimization
- Transition state search and intrinsic reaction path
- Vibrational frequency analysis
- Spectroscopic properties of molecules

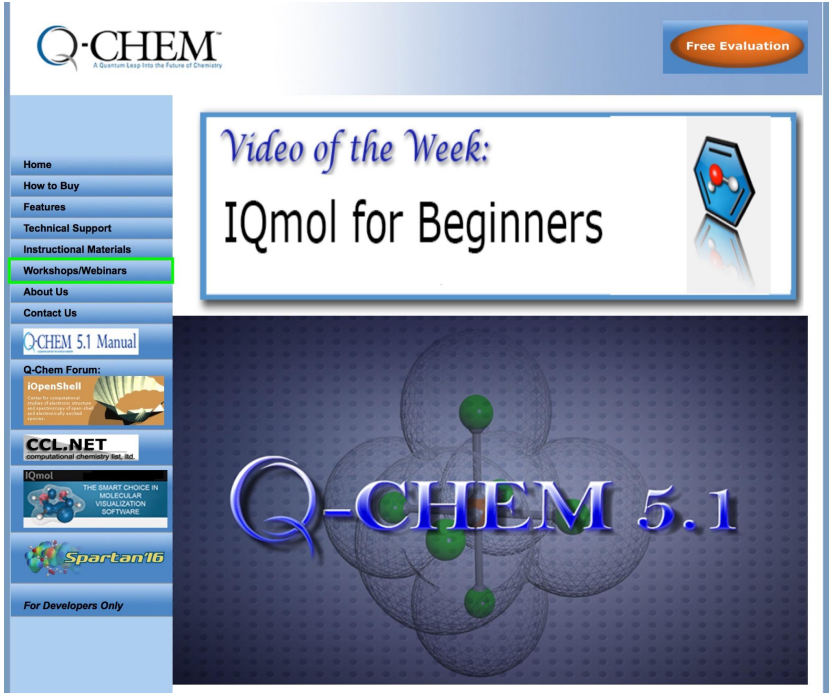
Resources: Q-Chem Website



www.q-chem.com

- Technical Information
- Customer Support
- Instructional Material
- Webinars

Resources: Q-Chem Website



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- Technical Information
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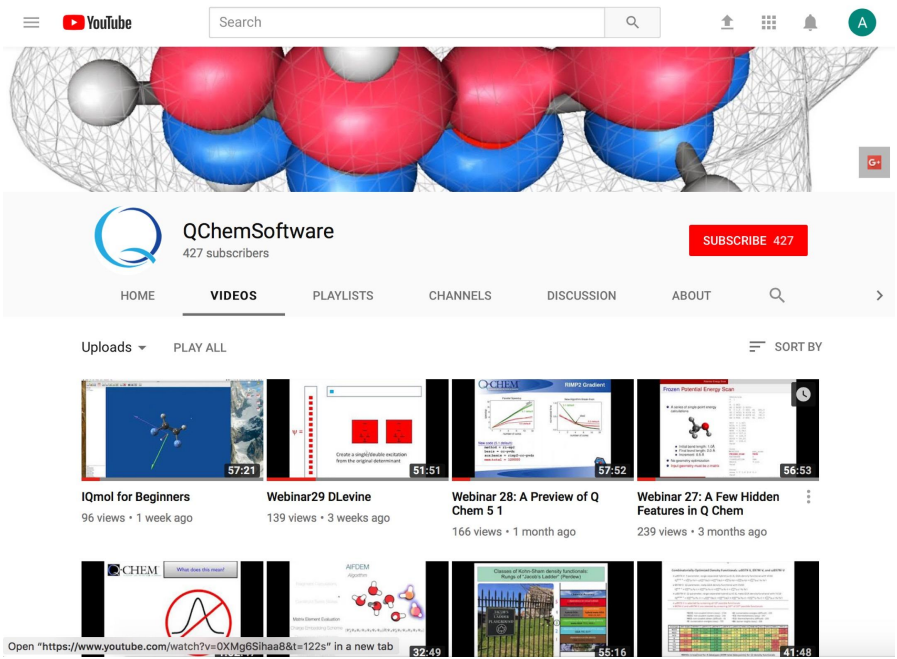
- Instructional Material
- Webinars

Resources: Webinars

www.q-chem.com/qchem-website/ws_sch4.html

- 60 minute presentations by Q-Chem contributors, users, and scientists
- Include question and answer session from viewers
- Wide variety of subjects, from basics to advanced material
- Over 30 webinars recorded and hosted on Youtube

Resources: Webinars

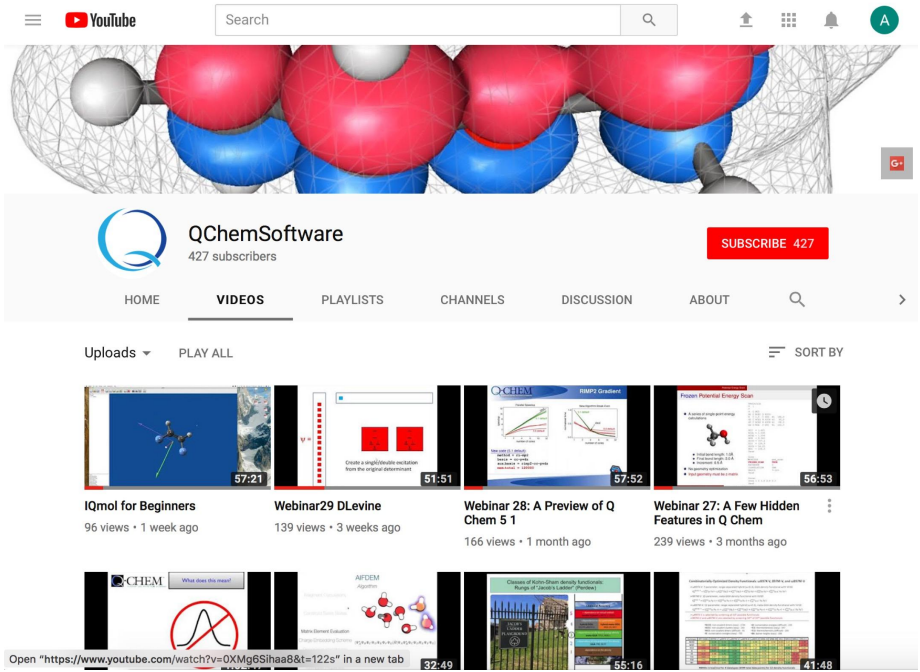


https://www.youtube.com/user/QChemSoftware/

Most Popular Webinars:

- The Q-Chem/CHARMM interface for QM/MM Studies
- Exploring Reaction Paths Using the Freezing String Method
- The Electronic Couplings in Electron Transfer and Excitation Energy Transfer
- Using the IQMol Interface to Q-Chem
- Exploring Reaction Pathways using QM/MM Free Energy Simulations: Applications to Biochem. Reactions

Resources: Webinars

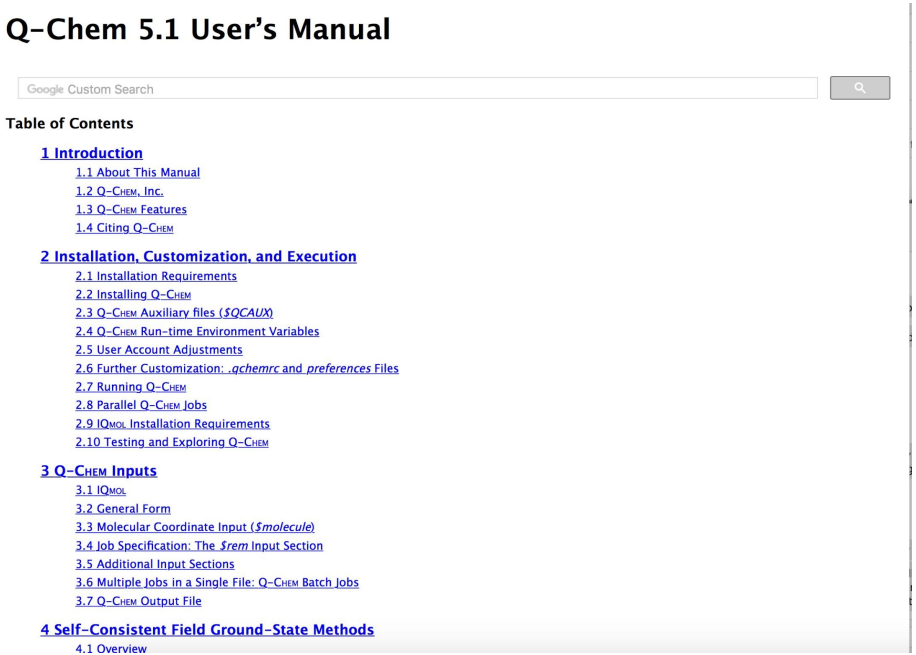


https://www.youtube.com/user/QChemSoftware/

Most Recent Webinars:

- IQMol For Beginners
- New Multi-Reference Methods in Q-Chem 5.1
- A Preview of Q-Chem 5.1
- A Few Hidden Features in Q-Chem
- A Preview of Q-Chem 5.0

Resources: Q-Chem Manual



Q-Chem 5.1 User's Manual

Google Custom Search

Table of Contents

http://www.q-chem.com/qchem-website/manual/qchem51_manual/index.html
(google "qchem 5.1 manual")

- Exhaustive compendium of all Q-Chem features
- Contains fairly thorough theoretical background as well as calculation setup information
- Appendix of all input file variables
- Most methods have example inputs

Resources: Sample jobs

```
> module load qchem/5.1
> cd $QC/samples
> ls
adc          exciton          qc510new
aimd         freq             qcref
ccman        gen_scfman       qmmm
ccman2       gpu              rdm
cdft         gvb              ri
cis          intracule        sapt
couplings    mgc              scf
dft          mom              solvent
ecp          mp2              spin_flip
eda          pes              tddft
efp          polarizability   wfa
```

- Large collection of sample inputs used for our own internal testing
- Every (working) feature should have a corresponding sample
- Most have useful comments
- Search this directory for an example of any feature of interest

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Sample Input File

```
$comment
Single point DFT energy calculation of ethane with the B3LYP functional and
an added Grimme D3 dispersion corrections
$end

$rem
jobtype = sp
method = b3lyp
basis = 6-31g*
dft_d = d3
$end

$molecule
0 1
C       0.000000   -0.000323    1.755803
H      -0.887097    0.510784    1.390695
H       0.887097    0.510784    1.390695
H       0.000000   -1.024959    1.393014
H       0.000000    0.001084    2.842908
C       0.000000    0.000323   -1.755803
H       0.000000   -0.001084   -2.842908
H      -0.887097   -0.510784   -1.390695
H       0.887097   -0.510784   -1.390695
H       0.000000    1.024959   -1.393014
$end
```

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H     -0.887097   -0.510784   -1.390695
H      0.887097   -0.510784   -1.390695
H      0.000000    1.024959   -1.393014
$end
```

- All input file sections begin with $*section_name* and end with $end
- Ordering of sections does not matter
- There are more sections. See manual.

Sample Input File

```
$comment
Single point DFT energy calculation of ethane with the B3LYP functional and
an added Grimme D3 dispersion corrections
$end

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H      -0.887097   -0.510784   -1.390695
H       0.887097   -0.510784   -1.390695
H       0.000000    1.024959   -1.393014
$end
```

Comment Section

“Rem” section. Job parameter keywords

Molecule description section

Sample Input File

```
$comment
Single point DFT energy calculation of ethane with the B3LYP functional and
an added Grimme D3 dispersion corrections
$end

$rem
jobtype = sp
method = b3lyp
basis = 6-31g*
dft_d = d3
$end

$molecule
0 1
C       0.000000   -0.000323    1.755803
H      -0.887097    0.510784    1.390695
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H       0.000000   -0.001084   -2.842908
H      -0.887097   -0.510784   -1.390695
H       0.887097   -0.510784   -1.390695
H       0.000000    1.024959   -1.393014
$end
```

Rem Section:

- Type of Job. SP= single point
- Method is DFT with the B3LYP Functional
- Basis set specification with standard basis names (These three keywords required for all jobs)
- Specifies additional dispersion correction

Note that keywords are not case sensitive.

Sample Input File

```
$comment
Single point DFT energy calculation of ethane with the B3LYP functional and
an added Grimme D3 dispersion corrections
$end

$rem
jobtype = sp
method = b3lyp
basis = 6-31g*
dft_d = d3
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$molecule
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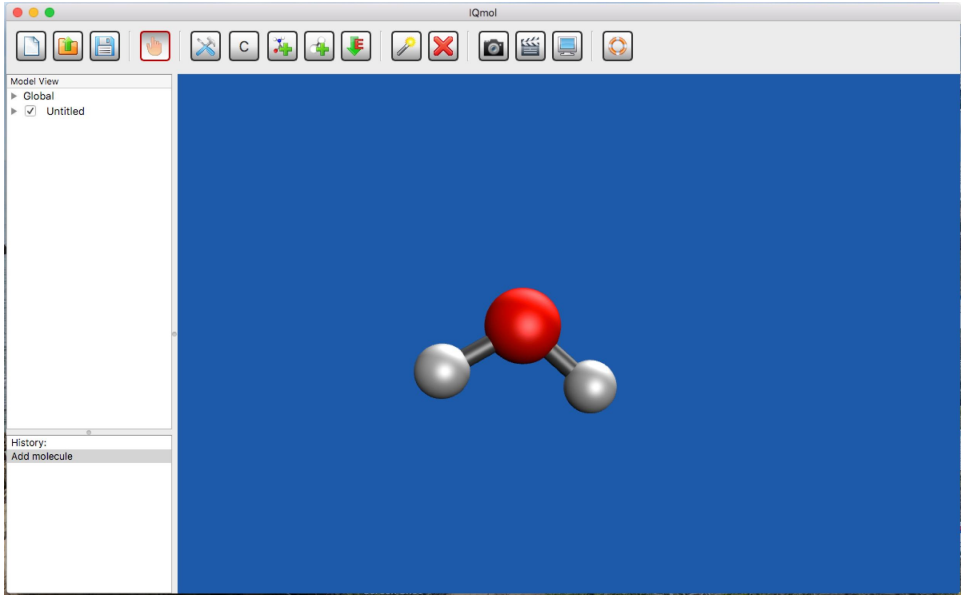
H      -0.887097   -0.510784   -1.390695
H       0.887097   -0.510784   -1.390695
H       0.000000    1.024959   -1.393014
$end
```

Molecule Section:

- Charge and Multiplicity
- Geometry in cartesian or Z-Matrix (units of Angstrom)

IQmol



GUI Application for Setting up Q-Chem jobs and viewing results:

- Build molecules, generate input files
- Read outputs, parse results
- Visualize properties, render MOs, animate normal modes
- Add $rem keyword GUI = 2 to standard input files, save and open generated .fchk file.

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How to run Q-Chem at NERSC

Cori

```
#!/bin/bash -l
#SBATCH -N 1
#SBATCH -t 00:30:00
#SBATCH -q debug
#SBATCH -L SCRATCH
#SBATCH -C haswell

module load qchem/5.1
qchem -nt 32 B3LYP_water.in
```

Edison

```
#!/bin/bash -l
#SBATCH -N 1
#SBATCH -t 00:30:00
#SBATCH -q debug


module load qchem/5.1
qchem -nt 24 B3LYP_water.in
```

Using scratch on NERSC Cori

Choosing the right memory and scratch settings is very important for good performance.

/tmp RAM drive
for small to medium DFT/HF jobs

```
#!/bin/bash -l
#SBATCH -N 1
#SBATCH -t 00:30:00
#SBATCH -q debug
#SBATCH -C haswell

module load qchem/5.1
export QCSCRATCH=/tmp
qchem -nt 32 B3LYP_water.in
```

BurstBuffer scratch
for large coupled cluster, EOM, ADC jobs

```
#!/bin/bash -l
#SBATCH -N 1
#SBATCH -t 00:30:00
#SBATCH -q debug
#SBATCH -C haswell
#DW jobdw capacity=500GB access_mode=striped type=scratch

module load qchem/5.1
export QCSCRATCH=$DW_JOB_STRIPED
qchem -nt 32 CC_job.in
```

Thanks to: Zhengji Zhao (NERSC)
Adrian Morrison (Q-Chem)

Questions?

Running Q-Chem at NERSC: contact help desk

Questions about this talk: epif@q-chem.com

```
**************************************************************
*                                                            *
*  Thank you very much for using Q-Chem.  Have a nice day.   *
*                                                            *
**************************************************************
```