

# 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)

# List of features

## By electronic structure method

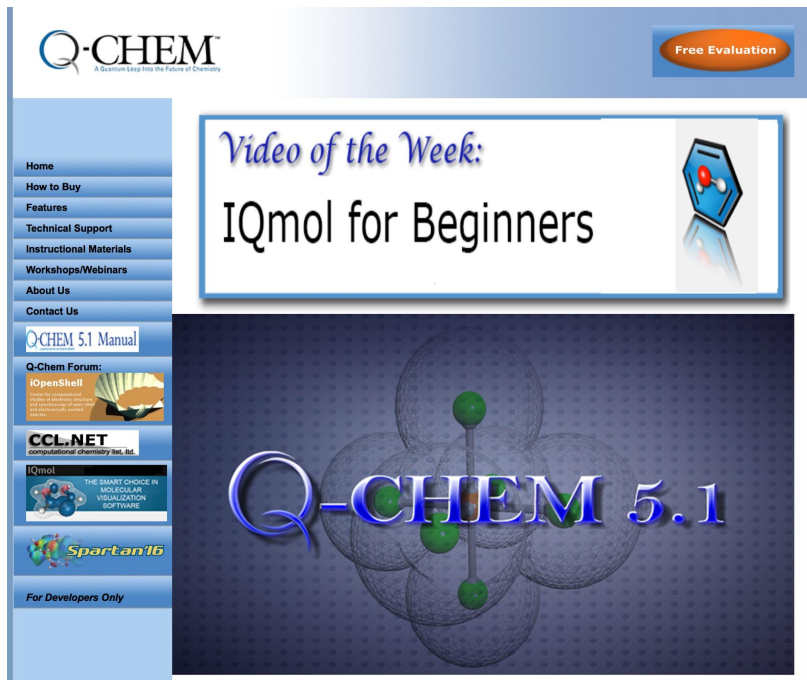
- Hartree-Fock and density functional theory (200+ density functionals)
- Post-Hartree-Fock methods: MP2, coupled cluster theory
- Excited state methods: TD-DFT, CIS, ADC, EOM
- Implicit and explicit solvation models
- Built-in QM/MM capabilities

# 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

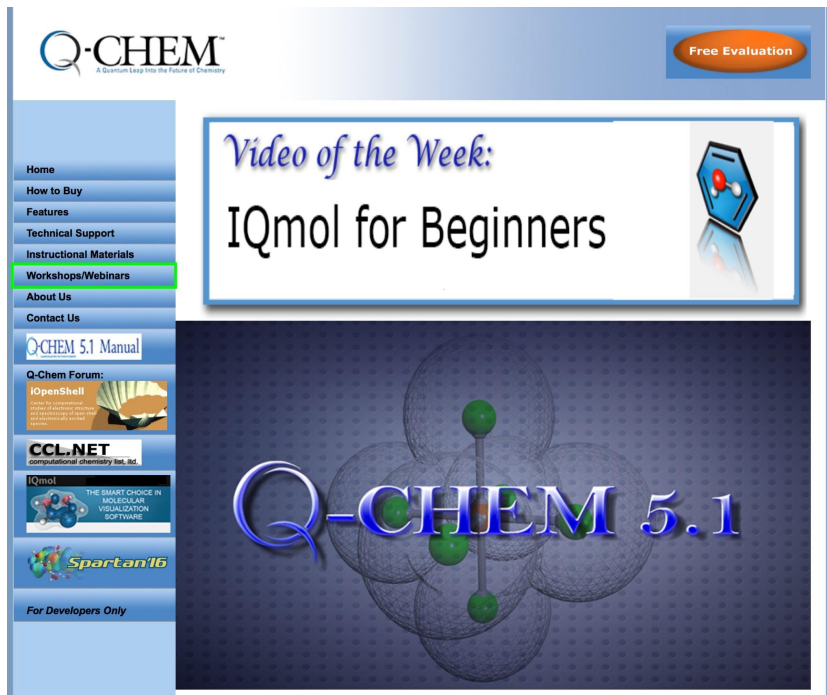
# Resources: Q-Chem Website



[www.q-chem.com](http://www.q-chem.com)

- Technical Information
- Customer Support
- Instructional Material
- Webinars

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# Resources: Webinars

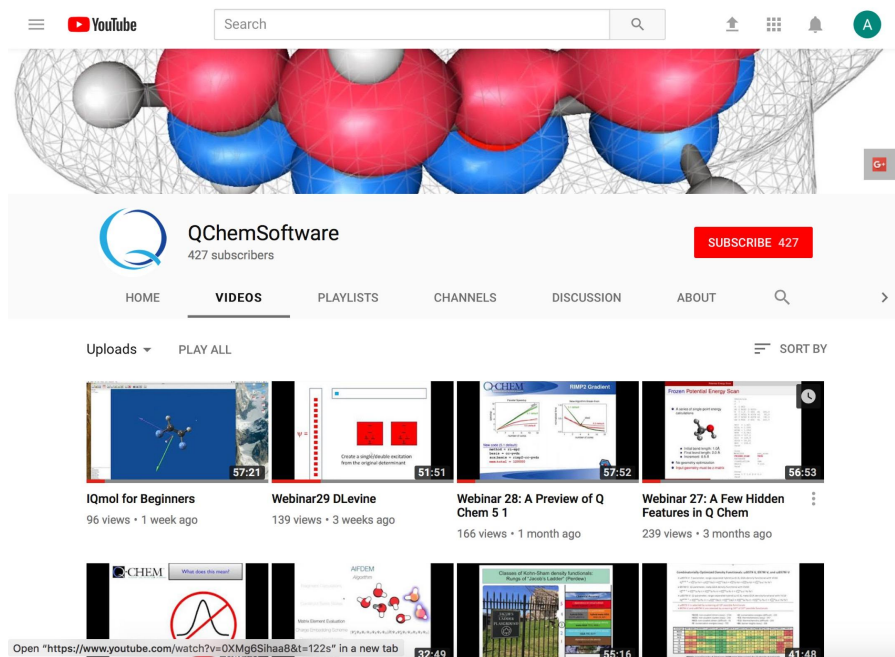


The screenshot shows the Q-Chem website interface. On the left is a navigation menu with links: Home, How to Buy, Features, Technical Support, Instructional Materials, Workshops/Webinars, About Us, and Contact Us. Below the menu are buttons for 'Free Evaluation', 'Find us on Facebook', 'Q-Chem Forum', 'OpenShell', 'Q-CHEM 5.1 Manual', and 'IQmol'. The main content area is titled 'Current workshops:' and states 'No workshops are scheduled at this time.' Below this is a link for 'Webinar Series - Exploring Chemistry with Q-Chem'. The 'Upcoming Webinars:' section lists several presentations by Dr. Andrew Gilbert, Dr. Daniel Levine, Prof. John Herbert, Prof. Yihan Shao, Prof. Martin Head-Gordon, and Prof. Adrian Morrison. A 'YouTube Video Presentations of Previous Webinars' section lists presentations by Prof. Peter Gill, Prof. Martin Head-Gordon, and Prof. Troy Van Voorhis.

[www.q-chem.com/  
qchem-website/ws\\_sch4.html](http://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



YouTube channel page for QChemSoftware (427 subscribers). The page displays a grid of video thumbnails and titles:

- IQMol for Beginners** (96 views • 1 week ago)
- Webinar29 DLevine** (139 views • 3 weeks ago)
- Webinar 28: A Preview of Q Chem 5.1** (166 views • 1 month ago)
- Webinar 27: A Few Hidden Features in Q Chem** (239 views • 3 months ago)
- Webinar 26: A Preview of Q Chem 5.0** (166 views • 1 month ago)
- Webinar 25: A Preview of Q Chem 5.0** (166 views • 1 month ago)
- Webinar 24: A Preview of Q Chem 5.0** (166 views • 1 month ago)
- Webinar 23: A Preview of Q Chem 5.0** (166 views • 1 month ago)
- Webinar 22: A Preview of Q Chem 5.0** (166 views • 1 month ago)
- Webinar 21: A Preview of Q Chem 5.0** (166 views • 1 month ago)
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- Webinar 19: A Preview of Q Chem 5.0** (166 views • 1 month ago)
- Webinar 18: A Preview of Q Chem 5.0** (166 views • 1 month ago)
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- Webinar 16: A Preview of Q Chem 5.0** (166 views • 1 month ago)
- Webinar 15: A Preview of Q Chem 5.0** (166 views • 1 month ago)
- Webinar 14: A Preview of Q Chem 5.0** (166 views • 1 month ago)
- Webinar 13: A Preview of Q Chem 5.0** (166 views • 1 month ago)
- Webinar 12: A Preview of Q Chem 5.0** (166 views • 1 month ago)
- Webinar 11: A Preview of Q Chem 5.0** (166 views • 1 month ago)
- Webinar 10: A Preview of Q Chem 5.0** (166 views • 1 month ago)
- Webinar 9: A Preview of Q Chem 5.0** (166 views • 1 month ago)
- Webinar 8: A Preview of Q Chem 5.0** (166 views • 1 month ago)
- Webinar 7: A Preview of Q Chem 5.0** (166 views • 1 month ago)
- Webinar 6: A Preview of Q Chem 5.0** (166 views • 1 month ago)
- Webinar 5: A Preview of Q Chem 5.0** (166 views • 1 month ago)
- Webinar 4: A Preview of Q Chem 5.0** (166 views • 1 month ago)
- Webinar 3: A Preview of Q Chem 5.0** (166 views • 1 month ago)
- Webinar 2: A Preview of Q Chem 5.0** (166 views • 1 month ago)
- Webinar 1: A Preview of Q Chem 5.0** (166 views • 1 month ago)

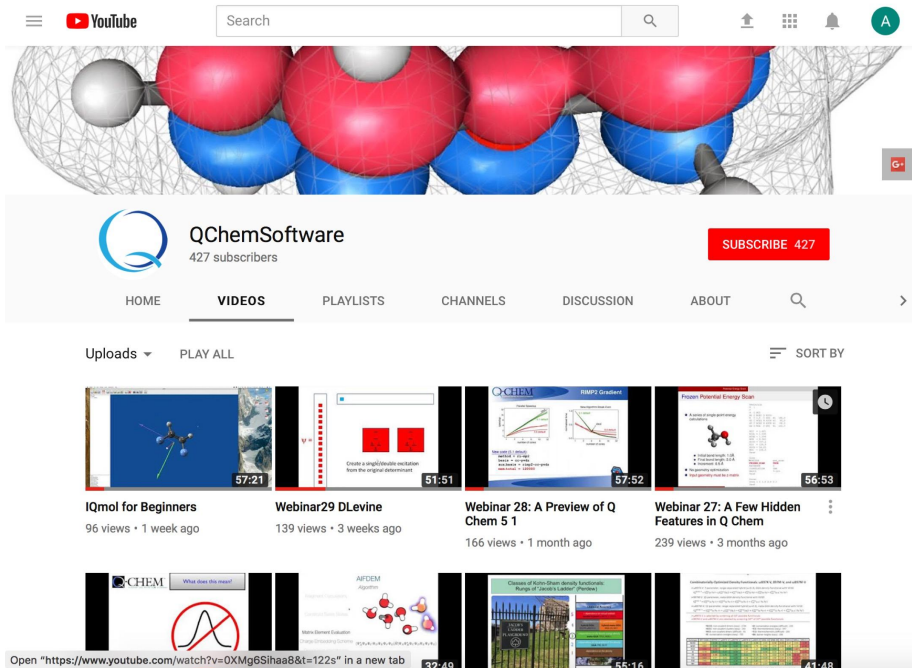
<https://www.youtube.com/user/QChemSoftware/>

## 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



The screenshot shows the YouTube channel for QChemSoftware, which has 427 subscribers. The channel is categorized under 'Science & Technology'. The video tab is selected, showing a list of uploads. The first video is 'IQMol For Beginners' (96 views, 1 week ago). The second is 'Webinar29 DLevine' (139 views, 3 weeks ago). The third is 'Webinar 28: A Preview of Q Chem 5.1' (166 views, 1 month ago). The fourth is 'Webinar 27: A Few Hidden Features in Q Chem' (239 views, 3 months ago). Below these, there are more video thumbnails, including one with a red 'X' over it and another titled 'What does this mean?'. At the bottom, there is a link to open a specific video in a new tab: 'Open "https://www.youtube.com/watch?v=QXMG6Sihaa8&t=122s" in a new tab'.

<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**

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  - [1.4 Citing Q-CHEM](#)
- [2 Installation, Customization, and Execution](#)**
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  - [2.2 Installing Q-CHEM](#)
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  - [3.7 Q-CHEM Output File](#)
- [4 Self-Consistent Field Ground-State Methods](#)**
  - [4.1 Overview](#)

[http://www.q-chem.com/qchem-website/manual/qchem51\\_manual/index.html](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

# 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
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\$end

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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

Comment Section

\$rem

jobtype = sp

method = b3lyp

basis = 6-31g\*

dft\_d = d3

\$end

“Rem” section. Job  
parameter keywords

\$molecule

0 1

C	0.000000	-0.000323	1.755803
---	----------	-----------	----------

H	-0.887097	0.510784	1.390695
---	-----------	----------	----------

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---	----------	----------	-----------

\$end

Molecule description  
section

# Sample Input File

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an added Grimme D3 dispersion corrections

\$end

\$rem

jobtype = sp

method = b3lyp

basis = 6-31g\*

dft\_d = d3

\$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

\$molecule

0 1

C 0.000000 -0.000323 1.755803

H -0.887097 0.510784 1.390695

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H -0.887097 -0.510784 -1.390695

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\$end

Note that keywords are not case sensitive.

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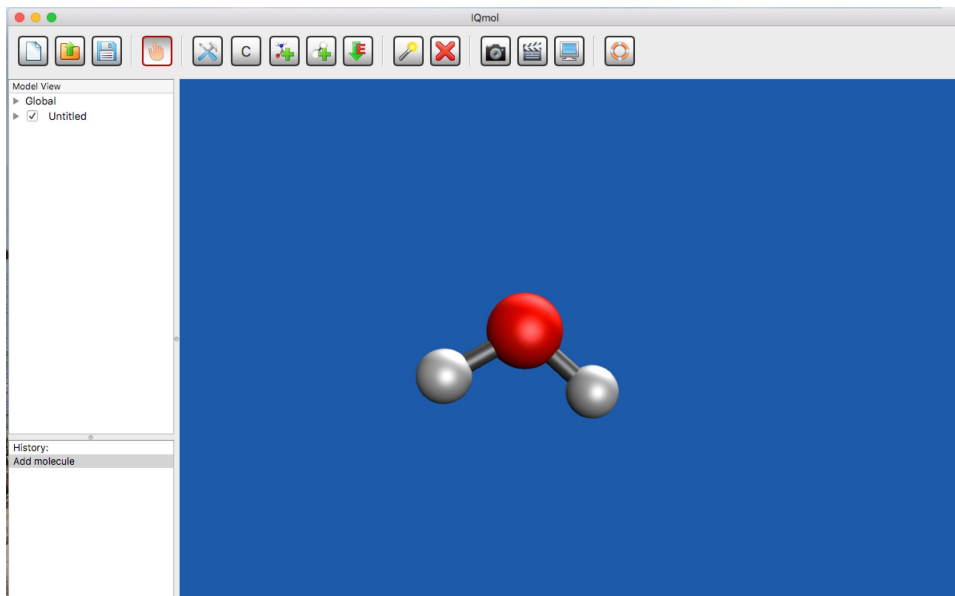
\$end

## 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.

# 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](mailto:epif@q-chem.com)

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