

UQUANTCHEM

Author

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Homepage

The project homepage contains the sources, binaries (Windows, Mac OS X), manuals and lots of other usefull stuff. The project is located at GitHub as well.

<http://www.uquantchem.com/uquantchem.html>

<https://github.com/petrossou/uquantchem>

Source

Source code is available in the project homepage and at GitHub.

<http://www.uquantchem.com/uquantchem.html>

<https://github.com/petrossou/uquantchem>

Reference

Souvatzis, P., Computer Physics Communications 185(1) (2014) 415-421.

Description & Use

UQUANTCHEM offers wide computational methodology possibilities from ab initio through DFT, perturbation theory up to molecular dynamics. Both single point and geometry optimization procedures are available.

Quick start

Structure of a typical input file includes e.g.:

```
CORRLEVEL [method]
TOL [tolerance]
Ne [number of electrons]
NATOMS [number of atoms]
ATOM [proton number] [x] [y] [z]
...
```

The inputfile must be saved as INPUTFILE to the same location where the UQUANTCHEM executable resides. Additionally, the basis specification must be stored in BASISFILE which is also there.

Use in command line / shell:

```
uquantchem > [output file]  
(in Windows command line)
```

or

```
./uquantchem > [output file]  
(in Android shell).
```

The result will appear in the same location.

Program status

The current package contains UQUANTCHEM binaries of version V.35 compiled for x86 based Windows operating system.

License

UQUANTCHEM

The original source code is published under GPL v.3 in the homepage. This distribution is published as freeware at Mobile Chemistry Portal and Google Play Store with kind permission of Petros Souvatzis.

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MinGW

The Windows version contains few essential dynamic link libraries which are part of MinGW runtime.
<http://www.mingw.org/>

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BLAS

UQUANTCHEM binaries for Android offered by us were statically linked to BLAS library (freely-available software package, available in the homepage). The Windows package contains the corresponding dynamic library.

<http://www.netlib.org/blas/>

LAPACK

UQUANTCHEM binaries for Android offered by us were statically linked to LAPACK library (released under modified BSD license, check the homepage for details). The Windows package contains the corresponding dynamic library.

<http://www.netlib.org/lapack/>

X11-Basic

GUI of the Windows version was built using X11-Basic (by Markus Hoffmann) framework (GPL v.3). For correct functionality, SDL library (available under GNU LGPL license) is included in package.

<http://x11-basic.sourceforge.net/>

<https://www.libsdl.org/>

Advanced Installer

The MSI installer for Windows was created using the Advanced Installer (Freeware edition).

<https://www.advancedinstaller.com/>

<https://www.advancedinstaller.com/top-freeware-features.html>

Contact

Compilation of the source code for Android/Windows as well as the Android/Windows app development was done by Alan Liška (alan.liska@jh-inst.cas.cz) and Veronika Růžicková (sucha.ver@gmail.com), J. Heyrovský Institute of Physical Chemistry of the CAS, v.v.i., Dolejškova 3/2155, 182 23 Praha 8, Czech Republic.

Website: <http://www.jh-inst.cas.cz/~liska/MobileChemistry.htm>