SMASH

Author

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Homepage

The homepage contains the sources, user/programmer manuals and more. The project is located at SourceForge and GitHub as well.

http://smash-qc.sourceforge.net/
https://sourceforge.net/projects/smash-qc/
https://github.com/cmsi/smash

Source

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

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https://sourceforge.net/projects/smash-qc/
https://github.com/cmsi/smash

Reference

Ishimura, K., Scalable molecular analysis solver for high-performance computing systems (SMASH) (2016).

Description & Use

SMASH is capable of Hartree-Fock, DFT and MP2 computations with built in as well as custom basis sets. Both single point and geometry optimization procedures are available.

Quick start

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

```
job runtype=[energy/gradient/optimize] method=[HF/B3LYP/B3LYP5/MP2]
basis=[STO-3G/6-31G/6-31G(d)cc-pvdz/cc-pvtz/cc-pvqz/d95v/lanl2dz]
charge=[charge] multi=[multiplicity] scftype=[RHF/UHF]
geom
[atom symbol] [x] [y] [z]
...
```

Use in command line / shell:

```
smash < [input file] > [output file]
```
(in Windows command line)

or

```
./smash < [input file] > [output file]
```
(in Android shell).

The result will appear in the same location.

Program status

The current package contains SMASH binaries of version 2.2.0 compiled for the particular Android hardware platforms and adapted for running in terminal environment.

License

SMASH

The original source code is published under Apache License 2.0 in the homepage. This distribution is published as freeware at Mobile Chemistry Portal and Google Play Store with kind permission of Kazuya Ishimura.

MinGW

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

BLAS

SMASH 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

SMASH 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 Růžičková (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.
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