SIESTA

Authors

Emilio Artacho, José M. Cela, Julian Gale, Alberto García, Javier Junquera, Richard M. Martin, Pablo Ordejón, Nick R. Papior, Daniel Sánchez-Portal, José M. Soler

Homepage

The homepage contains sources, basis and pseudopotential files, documentation and other useful resources.
https://departments.icmab.es/leem/siesta/

Source

The original source code is available in the homepage, this and other modified versions are available in our website.
https://launchpad.net/siesta
www.jh-inst.cas.cz/~liska/Siesta.htm

Reference

Artacho, E., Anglada, E., Diéguez, O., Gale, J. D., García, A., Junquera, J., Martin, R.M., Ordejón, P., Pruneda, J.M. Sánchez-Portal, D., Soler, J. M. (2008). The SIESTA method; developments and applicability. *Journal of Physics: Condensed Matter*, *20*(6), 064208.

Description & Use

Siesta is both program and method capable of highly accurate quantum chemical condensed matter modelling.

Quick start

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

```
SystemName          [title]
SystemLabel         /mnt/sdcard/siesta/work/example
NumberOfAtoms       [number of atoms in the structure]
NumberOfSpecies     [number of elements employed]

%block ChemicalSpeciesLabel
 [element number]  [atomic number]  /mnt/sdcard/ps/O (path, e.g. for O)
...
%endblock ChemicalSpeciesLabel

AtomicCoordinatesFormat  Ang
%block AtomicCoordinatesAndAtomicSpecies
 [x] [y] [z] [element number]
...
%endblock AtomicCoordinatesAndAtomicSpecies
```

Use in command line / shell (input file and corresponding basis / pseudopotential files must be present in the same location):

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

or

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

The result will appear in the same directory.

Program status

The current package contains SIESTA binaries of version 4.1 compiled for x86 based Windows operating system.

License

SIESTA

The distribution is published for free (under GPL v.3) at Mobile Chemistry Portal and Google Play Store with kind permission of Alberto García. Both the slightly modified source codes for generic Android binaries as well as for the binaries adapted to running in a standard Android filesystem (with defined hardlinks to each used file) are available for download in our website (please check the corresponding download links at www.jh-inst.cas.cz/~liska/Siesta.htm). The inluded basis and pseudopotential files were taken from the SIESTA websites

(https://departments.icmab.es/leem/siesta/Databases/Pseudopotentials/periodictable-intro.html, https://departments.icmab.es/leem/siesta/Databases/BasisSets/) and NNIN Virtual Vault for Pseudopotentials website (http://nninc.cnf.cornell.edu/periodic_table.html).

MinGW

The Windows version contains few essential dynamic link libraries and unix2dos binary which are part of MinGW runtime.
http://www.mingw.org/

BLAS

SIESTA binaries offered by us use internal BLAS library (reference BLAS is freely-available software package, available in the homepage). The Windows package contains the corresponding dynamic library.
http://www.netlib.org/blas/

LAPACK

SIESTA binaries offered by us use internal LAPACK library (official LAPACK is 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.
Website: http://www.jh-inst.cas.cz/~liska/MobileChemistry.htm