DeFT

Author

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Homepage

Currently does not exist.

Source

Source code is available in CCL archives.
http://www.ccl.net/cca/software/SOURCES/FORTRAN/DeFT/index.shtml

Reference

Gallant, R. T., St-Amant, A., Chemical physics letters, 256(6) (1996) 569-574.
(and similar papers)

Description & Use

DeFT performs DFT calculations.

Quick start

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

```
Description
cartesian angstroms
[atom] [x] [y] [z]
...
end
runtype start
potential local
grid coarse
charge 0
multiplicity 1
end
```

`a-basis` (exact a-basis name from basis file)
`...` (for each next atom, the order must be the same as in the xyz block above)
`...`
`o-basis` (exact o-basis name from basis file)
`...` (for each next atom, the order must be the same as in the xyz block above)
`...`

Use in command line / shell:

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

or

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

It should be emphasized that the input file must be copied as old_restart in the same folder as well as the basisfile named basis must be also present there. On the other hand, any other earlier calculation intermediate files must not be present. The result will appear in the same location.

Program status

The current package contains DeFT binaries of primary version compiled for x86 based Windows operating system.

License

DeFT

The distribution is published as freeware at Mobile Chemistry Portal and Google Play Store with kind permission of Alain St-Amant.

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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