



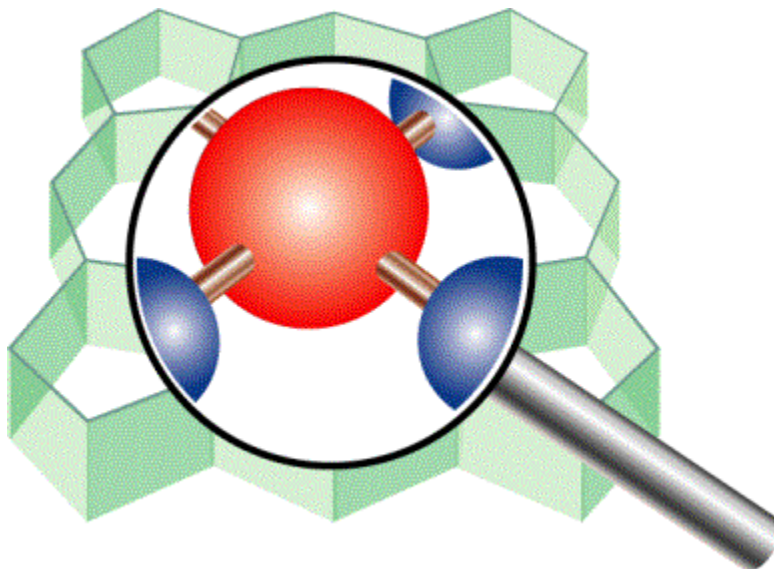
Scientific Computing & Modelling

DFTB Manual

**ADF Program System
Release 2008.01**

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Manual for the Density Functional Tight Binding (DFTB) program.
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Introduction

The DFTB program is orders of magnitude faster than DFT, but requires parameter files to be installed for all pair-wise combinations of atoms in a molecule. Unfortunately, parameters are not available for some elements, but calculations for many common molecules should be possible.

The ADF package contains an implementation of the DFTB method. It can be used as a stand-alone program, or as a pre-optimizer with the ADF-GUI.

To use DFTB you need parameter files. These are not included with the ADF package, you will need to download them yourself.

Parameter files

To use DFTB, you need to request parameter files at the DFTB.org web site, and put these files in the directory `$ADFHOME/atomicdata/DFTB`.

The DFTB naming scheme for parameter files, which are kept in `$ADFHOME/atomicdata/DFTB` is the same as the scheme used in the DFTB+ code. That is, the (mixed-case) name of each atom, separated by a hyphen, and including the extension 'skf' (Eg. C-Co.skf)

Input

The input for DFTB is similar to ADF, but not exactly the same. At this point, it is possible to perform single point, geometry optimization, transition state search, and frequency calculations. Results are written to standard output and to a keyed-file DFTB.kf.

Atomic coordinates

The input of (initial) atomic positions as Cartesian coordinates can be given with the key ATOMS.

```
| ATOMS  
| Atom Coords  
| ...  
| End
```

Atom

The name of an *atom type*. It must be the standard one- or two-character symbol for the chemical element: H, He, Li, and so on.

Coords

This specifies the coordinates of the atom. The x, y, z values of the Cartesian coordinates must be given in Angstrom.

Net Charge

The net charge of the molecule can be controlled with the key CHARGE.

```
| CHARGE NetQ
```

NetQ

The net total charge of the molecule. If the key CHARGE is omitted the net total charge of the molecule is zero.

SCF

The SCF procedure is regulated with a key that sets the convergence criterion.

```
| SCF  
| Converge SCFenv  
| End
```

SCFenv

The criterion to stop the SCF updates. The default is 1e-10.

Runtype

With the block key GEOMETRY you define the runtype and strategy parameters.

```

GEOMETRY
{RunType RunTypeData}
{Optim Cartesian|Delocal}
{Iterations Niter}
{Converge {E=TolE} {Grad=TolG} {Rad=TolR}}
{Step {TrustRadius=MaxRadius}}
End

```

RunType

RunTypeData

Can be:

- SinglePoint or SP
- GeometryOptimization or GO
- TransitionState or TS
- Frequencies or F

If omitted the run type is GeometryOptimization.

If the key GEOMETRY is not used at all the run type is SinglePoint.

Optim

Cartesian|Delocal

Optimization in delocalized coordinates (Delocal) can only be used in geometry optimizations or transition state searches.

Iterations

Niter

The maximum number of geometry iterations allowed to locate the desired structure. The default is 50.

This is a fairly large number. If the geometry has not converged (at least to a reasonable extent) within that many iterations you should sit down and consider the underlying cause rather than simply increase the allowed number of cycles and try again.

Converge

Convergence is monitored for two items: the energy and the Cartesian gradients. Convergence criteria can be specified separately for each of these items:

TolE

The criterion for changes in the energy, in Hartrees. Default: 1e-3.

TolG

Applies to gradients, in Hartree/angstrom. Default: 1e-2.

TolR

The maximum Cartesian step allowed for a converged geometry. Default: 0.01 Angstrom.

Step

Controls that changes in geometry from one cycle to another are not too large:

MaxRadius

By default, the trust radius is set to 0.2. Using the key, the user can override this, setting a constant value. A conservative value is 0.2. A large system (eg 100 atoms) typically needs a larger trust radius (eg 0.8).

Examples

Examples of DFTB calculations can be found in the \$ADFBIN/examples/dftb directory. Here is a run script for one such example:

```
$ADFBIN/dftb << eor

Geometry
RunType GO
Optim Delocal
Converge Grad=0.0001
End

Atoms
C      0.000000 0.000000 0.000000
C      1.402231 0.000000 0.000000
C      2.091015 1.220378 0.000000
C      1.373539 2.425321 0.004387
C      -0.034554 2.451759 0.016301
C      -0.711248 1.213529 0.005497
O      -0.709522 3.637718 0.019949
C      -2.141910 1.166077 -0.004384
O      -2.727881 2.161939 -0.690916
C      -0.730162 4.530447 1.037168
C      -0.066705 4.031914 2.307663
H      -0.531323 -0.967191 -0.007490
H      1.959047 -0.952181 -0.004252
H      3.194073 1.231720 -0.005862
H      1.933090 3.376356 -0.002746
O      -2.795018 0.309504 0.548870
H      -2.174822 2.832497 -1.125018
O      -1.263773 5.613383 0.944221
H      -0.337334 4.693941 3.161150
H      1.041646 4.053111 2.214199
H      -0.405932 3.005321 2.572927
End

eor
```

References

DFTB: general description

M. Elstner, D. Porezag, G. Jungnickel, J. Elsner, M. Haugk, T. Frauenheim, S. Suhai, G. Seifert, *Self-consistent charge density functional tight-binding method for simulation of complex material properties*. [Physical Review B **58**, 7260 \(1998\)](#)

Th. Frauenheim, G. Seifert, M. Elstner, Z. Hajnal, G. Jungnickel, D. Porezag, S. Suhai, R. Scholz, *A self-consistent charge density-functional based tight-binding method for predictive materials simulations in physics, chemistry and biology*. [Physica Status Solidi \(b\) **217**, 41 \(2000\)](#)

M. Elstner, Th. Frauenheim, E. Kaxiras, G. Seifert, S. Suhai, *A self-consistent charge density-functional based tight-binding scheme for large biomolecules*. [Physica Status Solidi \(b\) **217**, 357 \(2000\)](#)

C. Koehler, G. Seifert, U. Gerstmann, M. Elstner, H. Overhof, and T. Frauenheim, *Approximate density-functional calculations of spin densities in large molecular systems and complex solids*. [Physical Chemistry Chemical Physics **3**, 5109 \(2001\)](#)

T. Frauenheim, G. Seifert, M. Elstner, T. Niehaus, C. Kohler, M. Armkrecht, M. Sternberg, Z. Hajnal, A. di Carlo, S. Suhai, *Atomistic Simulations of complex materials: ground and excited state properties*. [Journal of Physics: Condensed Matter **14**, 3015 \(2002\)](#)

DFTB: elements

For construction of integral tables for O, N, C, H:

M. Elstner, D. Porezag, G. Jungnickel, J. Elsner, M. Haugk, T. Frauenheim, S. Suhai, G. Seifert, *Self-consistent charge density functional tight-binding method for simulation of complex material properties*. [Physical Review B **58**, 7260 \(1998\)](#)

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