



Scientific Computing & Modelling

DFTB Manual

**ADF Program System
Release 2012**

Scientific Computing & Modelling NV
Vrije Universiteit, Theoretical Chemistry
De Boelelaan 1083; 1081 HV Amsterdam; The Netherlands
WWW: www.scm.com
E-mail: support@scm.com

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Introduction

Our implementation of the DFTB method can perform single point calculations, geometry optimizations, transition state searches, frequency calculations, and molecular dynamics. Molecules as well as periodic systems can be handled ensuring a smooth link with our full DFT codes ADF and BAND. It can be used as a stand-alone command line program, or from the graphical interface.

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. Many elements can be handled with the Dresden parameter set included in the distribution, while many other parameter sets (from DFTB.org) can be [enabled](#), free of charge for non-profit users. Alternatively, sets of parameters in the SKF format can be downloaded and used from third party sources.

Release 2012

The 2012 release of our DFTB program features major updates:

Method improvements

- Self-consistent charges at the second order (SCC) and third-order (DFTB3)
- Dispersion corrections
- Speed-ups and reduced memory consumption
- Code is now parallelized
- Fully integrated in our GUI, seamless link with our full DFT programs ADF and BAND

Functionality

- Evaluation of periodic (1D, 2D, 3D) and non-periodic systems
- Optimization of lattice parameters
- Molecular dynamics with Velocity Verlet; Berendsen and scale thermostats
- Phonons
- Analysis: density of states, band structure

DFTB-GUI

Note that the graphical user interface DFTB-GUI enables all users to set up complicated calculations with a few mouse clicks, and provides graphical representations of calculated data fields, see the [DFTB-GUI tutorials](#).

Input

The input for DFTB slightly differs from the one found in ADF, and from the input for previous version of DFTB. For this reason, old DFTB input files will not be usable by the current version. Nevertheless, although layout and keywords are organized differently, general nomenclature and structure are unchanged. We refer to the ADF User Guide for more information on this topic. In the following sections, a list of the relevant Keys and the contained sub-keys will be presented.

After the run, results of the computation are written to standard output. Binary information about the evaluation are also written to a keyed-file dftb.rkf.

Specification of the System

The input of the initial structure can be given with the key System. This key is generally mandatory, but for molecular dynamics restarts, it can be omitted. In that case, the molecular configuration of the last recorded iteration will be used.

```
System
  {Atoms
    Atom Coords
  End}
  {Charge NetQ}
  {Lattice
    Vectors
  End}

  {LatticeStrain
    eps1 value
    eps2 value
    eps3 value
    eps4 value
    eps5 value
    eps6 value
  }
  {FractionalCoords}
End
```

The System key accepts a set of sub-keys to specify various details of the chemical system under evaluation

Atoms

Specifies the geometry of the molecular system as a list of rows, one row per atom.

Atom

The name of an *atom type*. It must be the standard one- or two-characters 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 are by default interpreted in Angstrom.

Charge

The net charge of the molecule can be controlled with the optional sub-key CHARGE. If this sub-key is omitted the net total charge of the molecule is by default zero.

NetQ

The net total charge of the molecule.

Lattice

Information about the periodicity of the system is given through this sub-key. Its presence is optional, and it implies a periodic system. The subsequent computation will therefore evaluate the system accordingly. A list of up to three vectors (one per row) for the cell must be specified.

Vector

Three floating point values defining the periodicity vector along a given direction. One, two, or three vectors can be specified (each on a different row) to express linear, planar or bulk periodicity, respectively. If one vector is specified, periodicity must develop along the x axis. If two vectors are specified, periodicity must develop along the xy plane. The unit is the same of the Atoms section.

LatticeStrain

Allows the application of a strain tensor to the lattice. The values of eps1 to eps6 represent the unique elements of the strain tensor, as follows

```
eps1 eps6 eps5
eps6 eps2 eps4
eps5 eps4 eps3
```

FractionalCoords

This optional keyword modifies how the ATOMS coordinates are interpreted. When the keyword is present, coordinates will be interpreted as fractions of the periodicity lattice vectors, instead of absolute geometric positions in 3D space. Necessarily, the presence of this sub-key requires LATTICE to be specified.

Specification of the computational Task

The Task section is mandatory and allows to specify the computational task to perform. It accepts only one mandatory sub-key, runType.

```
Task
  runType type
End
```

type

The type of evaluation to perform.

It can be:

- SinglePoint or SP
- GeometryOptimization or GO
- TransitionState or TS
- Frequencies or F
- MolecularDynamics or MD
- Phonons

Changing the default Units

The Units key is optional. It allows to specify different units for Length and Time, in place of the default ones.

```
Units
  {length    angstrom|bohr}
  {time      femtosec|au}
End
```

Setting DFTB Calculation details

```
DFTB
ResourcesDir  relativepath
{RadialExtrapolation  none|linear|improved|original|bezier}
{SCC
  {iterations NIter}
  {thirdOrder}
  {converge charge=QDiff}
End}
{UseSymmetry  yes|no}
{Repulsion
  forcePolynomial
End}
{Occupation  hund|fermi {temperature=FermiTemp}}
End
```

This mandatory key allows to specify and control different aspects of the DFTB evaluation engine.

ResourcesDir

Allows to specify the path (relative to \$ADFRESOURCES/DFTB) of the directory containing DFTB parameter files. Different parameters may be suitable for different DFTB evaluations. It is important to choose the appropriate parameter set for the type of calculation and molecular system under study.

RadialExtrapolation

Advanced control option. Overrides the extrapolation method for Slater-Koster grid values between the end of the tabulated grid and the cutoff distance (value for which atoms are considered too far to interact). Depending on the structure of your Slater Koster tables, a different radial extrapolation method may be needed in order to guarantee correct behavior, in particular for large and periodic systems. Five different extrapolation strategies are available:

none

Performs no extrapolation, the value being forced to zero at distances greater than the grid last position.

linear

performs a linear interpolation between the last point of the grid and the value of zero, at cutoff distance.

improved (default)

Perform a 9th grade polynomial interpolation between 6 points of the grid and three zeros. This interpolation may prove unstable for particular Slater Koster data

`original`

same as improved, but reproducing behavior of previous reference programs. Should not be used in general.

`bezier`

Uses a bezier curve passing through the last grid point and the cutoff point, guaranteeing continuity and smoothness. This is the suggested method in case of unexpected behavior.

SCC

The SCC key is optional. Its presence enables the Self Consistent Charge iterative procedure in DFTB. If the key is not present, DFTB will perform a non-Self Consistent Charge evaluation. SCC is not available for periodic evaluations. Additional optional keys can be used to control the SCC procedure

`iterations NIter`

Allows to specify the maximum number of SCC iterations. Default is 100 iterations, which is a very high number. Most computations will converge in less iterations. Lack of convergence within this limit may be due to use of hund Occupation. fermi occupation may improve convergence. See the Occupation key below.

`thirdOrder`

When this optional keyword is specified, a third order correction will be applied to the SCC evaluation.

`converge charge=QDiff`

Specifies the tolerance for convergence on the variation of the atomic charges. The default is 1.0e-8.

`UseSymmetry yes|no`

Enables or disables the use of symmetry during the evaluation. The key is optional, and in its absence the default is yes.

Repulsion

This key allows to specify some details about the Repulsion contribute evaluation. It accepts only one sub-key "forcePolynomial", which forces the use of polynomials as defined in the Slater Koster parameter files, in place of the Spline description.

Occupation

This optional key allows to specify the fill strategy to use for the orbitals. It can be either "hund", to fill the orbitals according to the hund rule, or "fermi", to perform electronic charge distribution over the orbitals. If "fermi" is specified, a further "temperature" option must be present, specifying the fermi temperature in kelvin. If this key is absent, the default is fermi occupation with a temperature of 5 kelvin.

Geometry optimization

```
Geometry
{Optim      Cartesian|Delocal|Primitive|Internal}
{Iterations Niter}
{Converge   {E=TolE} {Grad=TolG} {Rad=TolR}}
{Step       {TrustRadius=MaxRadius}}
{OptimizeLattice}
End
```

Geometry allows to specify information about the geometry optimization strategy. The keyword must be specified only for those Task runTypes requiring a geometry optimization (GeometryOptimization and TransitionState).

Optim

```
Cartesian|Delocal|Primitive|Internal
```

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, there may be an underlying cause to consider, instead of simply increasing the allowed number of cycles.

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-5.

```
TolG
```

Applies to gradients, in hartree/angstrom. Default: 1e-3.

```
TolR
```

The maximum Cartesian step allowed for a converged geometry, in angstrom. Default: 0.001 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).

OptimizeLattice

Enables optimization of the Lattice parameters, in addition to the molecular geometry. This can only be applied to periodic systems.

Restart

```
Restart
  {RestartFile}
  {RestartMulliken}
  {RestartOrbitals}
End
```

Molecular Dynamics

```
MD
  Steps      NSteps
  TimeStep   TStep
  {Restart   file=path}
  {Checkpoint frequency=ChkFreq}
  {Trajectory samplingFreq=SFreq}
  {Preserve   [TotalMomentum AngularMomentum CenterOfMass All None]}
  {InitialVelocities zero|inline|random {temperature=InitTemp}}
  {InlineVelocities
    velocityVector
  }
  End}
  {Thermostat type=ThermoType {thermostat options}}
End
```

The DFTB program supports molecular dynamics (with Velocity Verlet) with and without thermostats. This key, used with Task runType is set to MD, allows to specify the information needed by the molecular dynamics evaluation. This implementation of MD supports periodic systems.

Steps NSteps

Specifies the number of steps to be taken in the MD simulations. It accepts a simple integer number NSteps.

TimeStep TStep

Specifies the time for each step. By default, the unit is femtoseconds. Through the Units key, it can be changed to atomic units of time.

Restart file=path

Triggers a restart procedure, recovering the latest known information from the specified file (either a final .rkf file, or a checkpoint .chk file). When this keyword is present, System, Velocity, previous average values and energy transfers will be recovered from the file, ignoring any redundant specification made in the input file. This is the only situation where the System keyword can be omitted.

Checkpoint frequency=ChkFreq

Sets the frequency (in steps) for checkpoint the current status to a file. This allows to restart from an intermediate configuration in case of a crash of the program or the system. The keyword is optional; if not specified, by default is equal to the number of steps divided by 4. Only the most recent checkpoint is preserved. In case of crash, the checkpoint may be found in the execution temporary directory, instead of the working path. Checkpoint files can be inspected with the GUI for the latest configuration.

Trajectory samplingFreq=SFreq

Sets the frequency for printing to stdout and storing the molecular configuration on the .rkf file. This keyword is optional, and the default is the number of steps divided by 1000 (minimum one).

Preserve [TotalMomentum AngularMomentum CenterOfMass All None]

Constrains the molecular dynamics simulation to preserve different whole-system parameters. Note that this option has poor meaning for periodic systems. The keys can be given as a sequence out of the allowed list, with words separated by spaces

TotalMomentum

removes the overall velocity of the system from the atomic velocities.

AngularMomentum

removes the overall angular velocity of the system from the atomic velocities.

CenterOfMass

keeps the molecular system centered on the current center of mass.

All

Specifying "All" is equivalent of specifying all of the above keywords

None

None of the above options will be enabled. This is the default setup if the Preserve keyword is not specified.

InitialVelocities zero|inline|random {temperature=InitTemp}

Specifies the initial velocities to assign to the atoms. Three methods to assign velocities are available

zero

All atom's velocities are set to zero

inline

Atom's velocities are set to the values specified in the key InlineVelocities (see below)

random temperature=InitTemp

Atom's velocities are set to random values according to the specified temperature InitTemp, in kelvin. The temperature keyword is mandatory for this choice.

InlineVelocities

This optional key is read when InitialVelocities inline option is used. It allows to specify the velocities for each atom. Each row must contain three floating point values (corresponding to the x,y,z component of the velocity vector) and a number of rows equal to the number of atoms must be present, given in the same order as the System Atoms specification.

Available Thermostats

The key Thermostat allows to specify the use of a thermostat during the simulation. Depending on the selected thermostat type, different additional options may be needed to characterize the specific thermostat behavior. At the moment, the following choices for the type parameter are available

None

No thermostat applied. This is the default if no Thermostat key is present.

Scale

Applies a scaling of the velocities in agreement to the specified temperature. The following options are required for this thermostat

`frequency=NSteps`

This parameter is optional. If specified, the thermostat will be applied every NSteps, using that step's ensemble temperature and the specified thermostat temperature to compute the scaling factor. If not specified, the thermostat will be applied at every step, using the mean temperature of the ensemble and the specified thermostat temperature to compute the scaling factor.

`temperature=Temp`

Specifies the temperature of the thermostat, in kelvin. This parameter is mandatory.

Berendsen

Applies the Berendsen thermostat. The following options are required for this thermostat

`tau`

Specifies the initial tau parameter for the Berendsen thermostat, in femtoseconds (can be changed via Units key).

`apply=local|global`

Defines the scope of application of the scaling correction, either per-atom-velocity (option local) or on the molecular system as a whole (option global)

`temperature=Temp`

Specifies the temperature of the thermostat, in kelvin. This parameter is mandatory.

Additional Periodicity Data

```
Periodic
  {KSpace NK}
  {BZStruct {enabled=yes|no} {automatic=yes|no} {interpol=intVal}}
  {Phonon reorderatoms=yes|no interpol=N rcelx=N stepsize=N}
  {BZPath
```

```

        KMesh NMesh
        {Path
        End}
    End}
    {SuperCell
    End}
    {LatticeStepSize}
    {stressTensor}
    {Screening}
End

```

KSpace

This parameter controls the number of k-points used in the calculation. For very small unit cells (one atom wide) a value of 5 is advised. For medium sized unit cells 3 is adequate. For very large ones (10 atoms wide) kspace=1 suffices. (Default is 5)

BZStruct

This controls the path taken through the Brillouin zone (for plotting purposes). It has no effect on the calculated energy. Specifying *intVal* the band structure is interpolated along the path (so extra k-points are generated). You can also specify a path by hand, setting automatic to *no*. The points in the path should be entered in the BZPath key.

enabled

By default this feature is enabled.

automatic

Whether or not to use the automatic path generation.

interpol

Level of interpolation to use along the path

Phonon

This enables a phonon run. One should start from a completely optimized system. Next one should choose a super cell. The phonon spectrum converges with super cell size. How big it should be depends on the system.

reorderatoms

Technical option: put atoms of the same type after each other.

stepsize

Step size to be taken to obtain the force constants (second derivative) from the analytical gradients.

BZPath

Allows the user to specify manually a path through the BZ. The points are in terms of reciprocal lattice vectors.

KMesh

The amount of points on each line segment

Path

Each path consists of a number of points, which are assumed to be connected.

SuperCell

Used for the phonon run. The super lattice is expressed in the lattice vectors. Most people will find a diagonal matrix easiest to understand.

Examples

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

```
$ADFBIN/dftb << eor

Task
  RunType GO
End

System
  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
End

DFTB
  ResourcesDir Dresden
  SCC
    iterations 200
    converge charge=1.0e-8
  End
End

Geometry
  iterations 100
End

eor
```

Parameter files

The set of DFTB parameter files available in the ADF package were designed by J. Frenzel, A.F. Oliveira, N. Jardillier, T. Heine, and G. Seifert, mainly at the Technische Universität in Dresden, Germany, see also some [additional information about the generation of these parameter files](#). These parameter files are kept in the directory `$ADFHOME/atomicdata/DFTB/Dresden`.

You can also use a different set of parameter files. Note that different sets of parameter files are often not compatible. Note also that often parameter files were designed for a specific purpose, which may be different than your application, and therefore may give not the desired accuracy.

The DFTB implementation shipped by SCM provides the most up-to-date parameter sets available on the DFTB.org website. Additional licensing requirements may however be needed to access the content of the files. Please contact our licensing department to evaluate the available options.

The following sets are currently shipped

- mio-0-1 and mio-1-1 (H, C, N, O, S, P): for organic molecules
- pbc-0-3 (Si, F, O, N, C, H, Fe): for solid and surfaces
- matsci-0-3 (Al, Si, Cu, Na, Ti, Ba): for various compounds in material science

In addition, the following extension sets are provided to the mio set (either version 0-1 or 1-1):

- hyb-0-1 (Ag, Ga, As, Si) + mio-0-1: for organic and inorganic hybrid systems
- chalc-0-1 (As, S) + mio-0-1: for Chalcogenide glasses
- miomod-hh-0-1 + mio-1-1: contains a modified parameter set for H2
- miomod-nh-0-1 + mio-1-1: contains a modified parameter set for N-H to improve N-H binding energies
- tiorg-0-1 (Ti-(C, H, N, O, S, Ti)) + mio-0-1 : for Ti bulk, TiO2 bulk, TiO2 surfaces, and TiO2 with organic molecules
- trans3d-0-1 (Sc, Ti, Fe, Co, Ni) + mio-0-1: Transition metal elements for biological systems
- znorg-0-1 (Zn-(C, H, N, O, S, Zn)) + mio-0-1: for Zn bulk, ZnO bulk, ZnO surfaces, and ZnO with organic molecules

We recommend to visit the DFTB.org web site for more detailed information about each set. Please note that our implementation of DFTB does not support parameter sets files containing f-functions, such as the "rare" set.

Installing additional DFTB.org parameter files

To install new parameter sets released by the DFTB.org website in the future, we recommend the following procedure

1. Unpack the tar.gz file containing the parameters (for example, `newset-0-1.tar.gz`) with the command `tar -C $ADFRESOURCES/DFTB/DFTB.org -xzvf newset-0-1.tar.gz`.
2. Make sure the files have the name in the format `X-Y.skf`, with X and Y element symbols (for example, `C-C.skf`, `C-H.skf`, `Al-H.skf`). If this is not the case, rename the files to follow this naming.
3. Take note of the new directory name created in `$ADFRESOURCES/DFTB/DFTB.org` while unpacking (for example, `newset-0-1`)

The new parameter set can be now specified with the key `ResourcesDir`

```
| ResourcesDir DFTB.org/newset-0-1
```

Third Order parameter files

The parameter files for third order evaluation are available under a separate license agreement. Contact our licensing department for more information. Third order parametrization uses the values classified as "DFTB3 fit" in the reference paper (Gaus, Cui, Elstner). The values for the parameters are as follows: Zeta = 4.2; Hubbard derivatives for atoms: C = -0.23; H = -0.16; N = -0.13; O = -0.19; P = -0.14.

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

Dresden

The DFTB parameter files in \$ADFHOME/atomicdata/DFTB/Dresden are distributed with the ADF package. For more detailed information, see also the README file in the directory \$ADFHOME/atomicdata/DFTB/Dresden.

General reference for the construction of all integral tables in \$ADFHOME/atomicdata/DFTB/Dresden: J. Frenzel, A. F. Oliveira N. Jardillier, T. Heine, and G. Seifert, *Semi-relativistic, self-consistent charge Slater-Koster tables for density-functional based tight-binding (DFTB) for materials science simulations*, TU-Dresden 2004-2009.

For construction and application of integral tables for Al-O-H:

J. Frenzel, A.F. Oliveira, H.A. Duarte, T. Heine, and G. Seifert, *Structural and electronic properties of bulk gibbsite and gibbsite, surfaces*, *Zeitschrift für Anorganische und Allgemeine Chemie* **631**, 1267 (2005)

For construction and application of integral tables for Al-Si-O-H:

L. Guimarães, A.N. Enyashin, J. Frenzel, T. Heine, H.A. Duarte, and G. Seifert, *Imogolite Nanotubes: Stability, electronic and mechanical properties*, *Nano* **1**, 362 (2007)

For construction and application of integral tables for Al-O-P-C-H:

R. Luschtinetz, A.F. Oliveira, J. Frenzel, J. Joswig, G. Seifert, and H.A. Duarte, *Adsorption of phosphonic and ethylphosphonic acid on aluminum oxide surfaces*, *Surface Science* **602**, 1347 (2008)

For construction and application of integral tables for Ti-O-P-C-H:

R. Luschtinetz, J. Frenzel, T. Milek, and G. Seifert, *Adsorption of phosphonic acid at the TiO₂ anatase (101) and rutile (110) surface*, *Journal of Physical Chemistry C* **113**, 5730 (2009)

DFTB.org

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)

T. Niehaus, M. Elstner, T. Frauenheim, S. Suhai, *Application of an approximate density functional method to sulfur containing compounds*. [Journal of Molecular Structure \(THEOCHEM\)](#) **541**, 185 (2001)

M. Elstner, Q. Cui, P. Munih, E. Kaxiras, T. Frauenheim, M. Karplus, *Parametrization of the Self-consistent charge density functional tight-binding (SCC-DFTB) for Zink: Tests and applications*. [Journal of Computational Chemistry](#) **24**, 565 (2003)

Additional specific references for each parameter set can be found in the output of the DFTB program.

ThirdOrder

M. Gaus, Q. Cui and M. Elstner, *"DFTB3: Extension of the Self-Consistent-Charge Density- Functional Tight-Binding Method (SCC-DFTB)"*, [J. Chem. Theory Comput.](#) **7**, 931–948 (2011)

Keywords

DFTB 6

GEOMETRY 8

MD 9

RESOURCE DIR 15

Restart 9

SYSTEM 4

TASK 5

UNITS 6