DFTB Manual

Amsterdam Modeling Suite 2026.1

www.scm.com

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CHAPTER

ONE

GENERAL

1.1 Introduction

The DFTB engine implements density functional based tight-binding methods, which can be viewed as computationally efficient approximations to density functional theory (DFT). As such it is a good engine for inexpensive calculations that still include quantum effects. DFTB is a computational engine that runs through the AMS driver. It can be used directly from the command line, from Python, and through our graphical interface.

1.2 What's new in DFTB?

1.2.1 New in DFTB2025.1

- *Dispersion correction* (page 11) uses updated libraries for D3 (s-dftd3 1.2.1 https://github.com/dftd3/simple-dftd3) and D4 (dftd4 3.7.0 https://github.com/dftd4/dftd4)
- *QM/FQ* (page 13) ground-state gradients and geometry optimizations are now available with DFTB.
- For EffectiveMass the position of the HOMO and LUMO is determined along the high-symmetry path. To get the pre-2025 behavior, set useBandStructureInfoFromPath=No.

Changed default:

- Before AMS2025 the band structure (if requested) was not calculated if only 1 k-point was used. In AMS2025 this exception has been removed. If you do not need it, use BandStructure%Enabled=No.

1.2.2 New in DFTB2024.1

- Default DOS is now divided by DeltaE, which scales the overall DOS and PDOS so that they have the standard unit (1/(energy*volume)).

1.2.3 New in DFTB2023.1

- Improved SCC convergence with the *MultiStepper* (page 23).

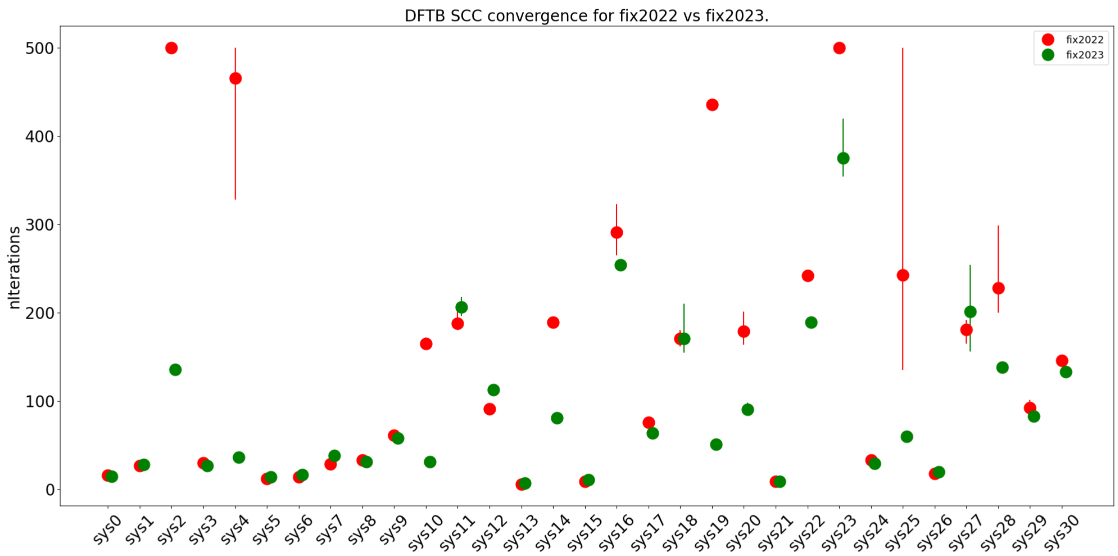

Fig. 1.1: Comparison of the number of SCC cycles needed. For easy systems there is not much difference, for more difficult systems, however, the fix2023 (green) is an improvement over the fix2022 (red). As there can be some randomness in the number of iterations the calculations are repeated five times (using a different number of cores), the dot is the average number of cycles used, and the vertical lines show the spread in the number of iterations (if any). The maximum number of iterations was set to 500.

1.2.4 New in DFTB2022.1

- Visualization of orbitals in AMSview now also works for calculations with (most) DFTB.org parameter sets.
- *Fragment orbital analysis* (page 54)
- *Charge transport (transfer integrals)* (page 63)

1.2.5 New in DFTB2021.1

- The D4 *dispersion correction* (page 11) has been added. It can be used with the Slater-Koster based model Hamiltonians and the DFTB.org parameter sets.

1.2.6 New in DFTB2020

- Calculations with the *GFN1-xTB model* (page 9) and many k-points are significantly faster.
- The default model has been changed from SCC-DFTB to GFN1-xTB, as the latter supports all elements.
- Various new applications in the AMS driver.

1.2.7 New in DFTB2019.3

- The internals of the DFTB engine have been restructured, making it faster, more scalable and more accurate for periodic systems, while at the same time enabling previously locked combinations of features:
  - The default for the accuracy of *k-space integration* (page 33) has been changed: DFTB used to sample only the Γ-point by default. As of this release the default k-points depend on the system size, using the same logic as in BAND. See the page on k-space integration in the BAND manual.
  - Calculations with *k-space integration* (page 33) are generally faster and scale much better on parallel machines.
  - The *GFN1-xTB model* (page 9) can now be used together with *k-space integration* (page 33).
  - *Unrestricted calculations* (page 9) can now also be performed in conjunction with *k-space integration* (page 33).
  - The orbital dependent (l-dependent) *SCC cycle* (page 9) is now compatible with *k-space integration* (page 33).
  - The stress tensor is now calculated analytically, making its calculation faster and the result more accurate.
- An *implicit solvation model* (page 11) (GBSA: Generalized Born (GB) model augmented with the solvent accessible surface area (SA) term) has been added to DFTB, allowing simulations of molecules in solution.
- Various new applications in the AMS driver.

1.2.8 New in DFTB2019.1

- Grimme's GFN1-xTB has been added as a new *model Hamiltonian* (page 9). It supports molecular as well as periodic calculations for systems including elements up to Radon. Visualization of the results (e.g. molecular orbitals) in AMSview is also supported.
- Various new applications in the AMS driver.
- More robust and easier to set up *k-space integration* (page 33).
- More robust SCC convergence:
  - *Adaptive mixing* (page 9): The charge mixing parameter is automatically decreased if the energy increases during the SCC cycle.
  - The default electronic temperature has been increased to 300K, making SCC convergence more robust for systems with small HOMO-LUMO gaps.

1.2.9 New in DFTB2018

New features

- Elastic tensor and related properties (e.g. Bulk modulus) (via AMS driver)
- Linear transit and PES scan (via AMS driver)
- Geometry optimization under pressure (via AMS driver)
- …

AMS: a new driver program

Important: In the 2018 release of the Amsterdam Modeling Suite we introduced a new driver program call **AMS**. We recommend you first read the General section of the AMS Manual

If you use DFTB exclusively via the Graphical User Interface (GUI), this change should not create any issues. If, on the other hand, you create input files *by hand* (or you use DFTB via PLAMS), then you should be aware that **shell scripts for DFTB2017 and previous versions are not compatible with DFTB2019 and have to be adjusted to the new setup.**

The example below shows how a shell script for DFTB2017 is converted to DFTB2019.

DFTB2017 shell script (obsolete):

```
#!/bin/sh

# This is a shell script for DFTB2017 which will not work for DFTB2019

$AMSBIN/dftb << EOF

Task
   RunType GO
End

System
   Atoms
      H 0.0 0.0 0.0
      H 0.9 0.0 0.0
   End
End

DFTB
   ResourcesDir Dresden
End

Geometry
   iterations 100
End

EOF
```

DFTB2019 shell script:

```
#!/bin/sh

# This is a shell script for DFTB2019

# The executable '$AMSBIN/dftb' is no longer present.
# You should use '$AMSBIN/ams' instead.

$AMSBIN/ams << EOF
   # Input options for the AMS driver:

   System
      Atoms
         H 0.0 0.0 0.0
         H 0.9 0.0 0.0
```

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```
      End
   End

   Task GeometryOptimization

   GeometryOptimization
      MaxIterations 100
   End

   # The input options for DFTB, which are described in this manual,
   # should be specified in the 'Engine DFTB' block:

   Engine DFTB
      ResourcesDir Dresden
   EndEngine
EOF
```

CHAPTER

TWO

AMS DRIVER'S TASKS AND PROPERTIES

DFTB is an engine used by the AMS driver. While DFTB's specific options and properties are described in this manual, the definition of the system, the selection of the task and certain (PES-related) properties are documented in the AMS driver's manual.

On this page you will find useful links to the relevant sections of the AMS driver's Manual.

2.1 Geometry, System definition

The definition of the system, i.e. the atom types and atomic coordinates (and optionally, the system's net charge, the lattice vectors, the input bond orders, external homogeneous electric field, external point charges, atomic masses for isotopes) are part of the AMS driver input. See the System definition section of the AMS manual.

2.2 Tasks: exploring the PES

The job of the AMS driver is to handle all changes in the simulated system's geometry, e.g. during a geometry optimization or molecular dynamics calculation, using energy and forces calculated by the engine.

These are the tasks available in the AMS driver:

- Single Point
- Geometry Optimization
- Transition State Search
- IRC (Intrinsic Reaction Coordinate)
- PESScan (Potential Energy Surface Scan, including linear transit)
- NEB (Nudged Elastic Band)
- Vibrational Analysis
- Molecular Dynamics
- GCMC (Grand Canonical Monte Carlo)

2.3 Properties in the AMS driver

The following properties can be requested to the DFTB engine in the AMS driver's input:

- Bond orders
- Atomic charges
- Dipole Moment
- Dipole Gradients
- Elastic tensor
- Nuclear Gradients / Forces
- Hessian
- Infrared (IR) spectra / Normal Modes
- Thermodynamic properties
- PES point character
- Phonons
- Stress tensor
- Elastic tensor
- VCD (Vibrational Circular Dichroism)

CHAPTER

THREE

MODEL HAMILTONIANS

As of the 2020 release, the DFTB engine supports two different classes of model Hamiltonians, Grimme's extended tight-binding, and the classic Slater-Koster based DFTB. All of these model Hamiltonians are obtained by applying tight-binding approximations to the DFT total energy expression.

3.1 Slater-Koster based DFTB

The efficiency of Slater-Koster based DFTB stems from its use of an optimized minimum valence orbital basis that reduces the linear algebra operations, and a two-center approximation for the Kohn-Sham potential that allows pre-calculation and storage of integrals using the Slater-Koster technique. This makes DFTB orders of magnitude faster than DFT, but requires parameter files (containing the integrals) for all pair-wise combinations of atoms in a molecule. Many elements can be handled with the parameter sets included in the distribution. Alternatively, sets of parameters in the SKF format can be downloaded and used from third-party sources.

There are three flavors of Slater-Koster based DFTB available in our implementation:

- The "plain" DFTB Hamiltonian as introduced by Porezag and Seifert without a self-consistency cycle.
- The second order self-consistent charge extension SCC-DFTB (also called DFTB2), which accounts for density fluctuations and improves results on polar bonds. Note that the self-consistent calculations are about an order of magnitude slower than calculations with the "plain" DFTB Hamiltonian.
- The third order extension known as DFTB3, which improves the description of hydrogen-bonded complexes and proton affinities. Note that DFTB3 calculations are only marginally slower than SCC-DFTB based calculations.

Note that since these methods have been respectively parametrized, it is important to specify a matching parameter set when applying one of these models.

3.2 Extended tight-binding (xTB)

The extended tight-binding (xTB) model Hamiltonian was introduced by Grimme and coworkers. It makes similar approximations as Slater-Koster based DFTB, but instead of using precalculated integrals, xTB employs a (small) basis of Slater-type orbitals and uses an extended Hückel-like approximation for the Hamiltonian.

The DFTB engine supports the GFN1-xTB parameterization of xTB, which is optimized for geometries, frequencies, and non-covalent interactions and covers all elements of the periodic table up to radon.

3.3 Model Hamiltonian

The following keys allow you to select a model Hamiltonian and control different aspects of how the stationary Schrodinger equation is solved.

```
Model [DFTB | SCC-DFTB | DFTB3 | GFN1-xTB | NonSCC-GFN1-xTB]
```

Model

Type
Multiple Choice

Default value
GFN1-xTB

Options
[DFTB, SCC-DFTB, DFTB3, GFN1-xTB, NonSCC-GFN1-xTB]

Description
Selects the Hamiltonian used in the DFTB calculation:

- DFTB/DFTB0/DFTB1 for classic DFTB without a self-consistent charge cycle

- SCC-DFTB/DFTB2 with a self-consistency loop for the Mulliken charges

- DFTB3 for additional third-order contributions.

- GFN1-xTB for Grimme's extended tight-binding model in the GFN1 version.

- NonSCC-GFN1-xTB for a less accurate but faster version of GFN1-xTB without a self-consistency cycle

The choice has to be supported by the selected parameter set.

Different parameters may be suitable for different model Hamiltonians. It is important to choose the appropriate parameter set for the type of calculation and molecular system under study, see *parameter sets* (page 68).

```
ResourcesDir string
```

ResourcesDir

Type
String

Description
The directory containing the parameter files. The path can be absolute or relative. Relative paths starting with ./ are considered relative to the directory in which the calculation is started, otherwise they are considered relative to $AMSRESOURCES/DFTB. This key is required for the Slater-Koster based DFTB models, but optional for xTB.

Examples:

ResourcesDir Dresden
Uses the resource directory $AMSRESOURCES/DFTB/Dresden.

ResourcesDir /home/myusername/myparamsdir
Uses the specified path /home/myusername/myparamsdir as the resource directory.

NOTE: Each resource directory must contain a file called *metainfo.yaml*, which specifies the capabilities of the parameter set. For details see *metainfo.yaml* (page 67).

3.4 Dispersion correction

The selected model Hamiltonian can be extended with dispersion correction:

```
DispersionCorrection [None | Auto | UFF | ULG | D2 | D3-BJ | D4]
```

DispersionCorrection

Type
Multiple Choice

Default value
None

Options
[None, Auto, UFF, ULG, D2, D3-BJ, D4]

GUI name
Dispersion

Description
This key is used to specify an empirical dispersion model. Please refer to the DFTB documentation for details on the different methods.

By default no dispersion correction will be applied. Setting this to auto applies the dispersion correction recommended in the DFTB parameter set's metainfo file. Note that the D3-BJ dispersion correction is enabled by default when using the GFN1-xTB model Hamiltonian, but can be disabled manually by setting this keyword to None.

The newest and most accurate dispersion correction is D4. We recommend both the D3-BJ and D4 dispersion corrections as good defaults, depending on their availability for the specific combination of the model Hamiltonian and parameterization. Note that the D4 dispersion correction is computationally more expensive than D3-BJ for bulk periodic systems (it scales as O(N^3) with the number of atoms and is not parallelized), so you may first want to evaluate whether the increased accuracy justifies the increased computational cost.

3.5 Solvation (GBSA)

Solvation effects can be included via the implicit GBSA solvation model. We gratefully acknowledge Grimme's group in Bonn for their contribution of the GBSA solvation method code.

To enable the GBSA method, specify the desired solvent:

```
Solvation
   Solvent [None | Acetone | Acetonitrile | CHCl3 | CS2 | DMSO | Ether | H2O |␣
↪Methanol |
            THF | Toluene]
End
```

Solvation

Type
Block

Description
Generalized Born solvation model with Solvent Accessible Surface Area (GBSA).

Solvent

Type
Multiple Choice

Default value
None

Options
[None, Acetone, Acetonitrile, CHCl3, CS2, DMSO, Ether, H2O, Methanol, THF, Toluene]

Description
Solvent used in the GBSA implicit solvation model.

More options can be specified in the `Solvation` block:

```
Solvation
   UseGSASA Yes/No
   GSolvState [Gas1BarSolvent | Gas1MSolvent1M | Gas1BarSolvent1M]
   Temperature float
   SurfaceGrid [230 | 974 | 2030 | 5810]
End
```

Solvation

UseGSASA

Type
Bool

Default value
Yes

GUI name
Solvation Free Energy

Description
Include shift term and G(SASA) terms in the energy and gradient.

GSolvState

Type
Multiple Choice

Default value
Gas1MSolvent1M

Options
[Gas1BarSolvent, Gas1MSolvent1M, Gas1BarSolvent1M]

Description
Reference state for solvation free energy shift.

Temperature

Type
Float

Default value
298.15

Unit
Kelvin

Description
The temperature used when calculating the solvation free energy shift. Only used for 'Gas1BarSolvent' and 'Gas1BarSolvent1M' GSolvState options.

SurfaceGrid

Type
Multiple Choice

Default value
230

Options
[230, 974, 2030, 5810]

Description
Number of angular grid points for the construction of the solvent accessible surface area. Usually the default number of grid point suffices, but in case of suspicious behaviors you can increase the number of points.

3.6 QM/FQ Embedding

Environmental effects can be included in the calculation by means of the Fluctuating Charge (FQ) model. The theory behind the model is presented in the corresponding ADF manual page . The method can be used for both ground-state and TD-DFTB calculations, as well as in ground-state geometry optimizations.

To enable the FQ model one must include the QMFQ block keyword containing the method options, parameters, and coordinates of the environment atoms. More details on the input structure can also be found in the ADF manual page .

```
QMFQ
   AtomType
      Alpha float
      Area float
      Charge float
      Chi float
      Dfermi float
      Efermi float
      Eta float
      R0 float
      Sfermi float
      Sigma0 float
      Symbol string
      Tau float
      wFQFMuFile string
   End
   Coords # Non-standard block. See details.
      ...
   End
   FDERESP Yes/No
   Forcefield [FQ | FQFMU | wFQ | wFQ_RQ | wFQFmu | wFQFmu_RQRMU]
   Frozen Yes/No
   Kernel [OHNO | COUL | GAUS]
   LifeFrequency float
   LifeState integer
   MolCharge float
   NonEle [LJ | None]
   QMSCREEN [ERF | EXP | GAUS | NONE]
```

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```
   QMSCREENFACTOR float
   ReadDynamicMatrix string
End
```

QMFQ

Type
Block

Description
Block input key for QM/(w)FQ(FMu).

AtomType

Type
Block

Recurring
True

Description
Definition of atomic types in MM environment

Alpha

Type
Float

Description
Polarizability of FQFMU atom

Area

Type
Float

Description
Effective charge-transfer area time between same-type wFQ atoms

Charge

Type
Float

Description
MM fixed charge (non-polarizable only)

Chi

Type
Float

Description
Electronegativity of FQ atom

Dfermi

Type
Float

Description
wFQ d parameter for Fermi damping

Efermi

Type
Float

Description
Fermi Energy of wFQ carbon-based structure

`Eta`

Type
Float

Description
Chemical Hardness of FQ atom

`R0`

Type
Float

Description
wFQ R0 parameter for Fermi damping

`Sfermi`

Type
Float

Description
wFQ s parameter for Fermi damping

`Sigma0`

Type
Float

Description
Static conductivity time of wFQ atom

`Symbol`

Type
String

Description
Symbol associated with atom type

`Tau`

Type
Float

Description
Scattering time of wFQ atom

`wFQFMuFile`

Type
String

Description
The absolute path to the wFQFMu interband polarizability file

`Coords`

Type
Non-standard block

Description
Coordinates and fragment information (FQ only)

`FDERESP`

Type
Bool

Default value
No

Description
In response calculations (TD), the polarization contribution of the FDE part is introduced at the FQ level [See F. Egidi et al. J. Chem. Phys. 2021, 154, 164107].

`Forcefield`

Type
Multiple Choice

Default value
FQ

Options
[FQ, FQFMU, wFQ, wFQ_RQ, wFQFmu, wFQFmu_RQRMU]

Description
Version of the FQ family of polarizable forcefields

`Frozen`

Type
Bool

Default value
No

Description
Expert option. Do not introduce polarization effect in response calculations.

`Kernel`

Type
Multiple Choice

Default value
OHNO

Options
[OHNO, COUL, GAUS]

Description
Expert option. KERNEL can be used to choose the functional form of the charge-charge interaction kernel between MM atoms. Recommended is to use the default OHNO. The COUL screening is the standard Coulomb interaction 1/r. The OHNO choice introduce the Ohno functional (see [K. Ohno, Theoret. Chim. Acta 2, 219 (1964)]), which depends on a parameter n that is set equal to 2. Finally, the GAUS screening models each FQ charge by means of a spherical Gaussian-type distribution, and the interaction kernel is obtained accordingly. For QM/FQFMU only GAUS SCREEN is implemented.

`LifeFrequency`

Type
Float

Default value
0.0

Description
Input frequency for calculating TDDFT/wFQ(Fmu) lifetimes

`LifeState`

Type
Integer

Default value
0

Description
Target excited state for state-specific TDDFT/wFQ(Fmu) lifetimes

`MolCharge`

Type
Float

Default value
0.0

Description
Total charge of each fragment (FQ only)

`NonEle`

Type
Multiple Choice

Default value
LJ

Options
[LJ, None]

Description
Whether to include non-electrostatic contributions to the energy. Default is the Lennard-Jones (LJ) model.

`QMSCREEN`

Type
Multiple Choice

Default value
GAUS

Options
[ERF, EXP, GAUS, NONE]

Description
Expert option. QMSCREEN can be used to choose the functional form of the charge-charge interaction kernel between MM atoms and the QM density. The screening types available are ERF (error function), EXP (exponential), GAUS (Gaussian), or NONE. The default is GAUS.

`QMSCREENFACTOR`

Type
Float

Default value
0.2

Description
Expert option. Sets the QM/MM interaction kernel screening length. Recommended is to use the default value 0.2 with the GAUS QM/MM screening function.

ReadDynamicMatrix

Type
String

Description
The absolute path to the decomposed wFQ(FMu) matrix file

3.7 SCC details and spin-polarization

With SCC DFTB the parametrized Hamiltonian depends on partial atomic charges that need to be determined self-consistently. These charges are usually atomic charges, but they may be shell and/or spin resolved. The self-consistency requirement

$\vec{q}^{\text{in}} = \vec{q}^{\text{in}}$

is numerically expressed as

$\frac{1}{\sqrt{N_{\text{atoms}}}}|\vec{q}^{\text{in}} - \vec{q}^{\text{in}}| < \epsilon$

The vector norm is by default the so-called L-infinity norm, being the maximum absolute value of the vector elements. The underlying algorithm, however, will minimize the L-2 norm. Based on the history of past input and output charge vectors, a next one is guessed

$\vec{q}^{\text{guess}} = \sum_i c_{i-1}^N(\vec{q}_i^{\text{in}} + \sigma(\vec{q}_i^{\text{out}} - \vec{q}_i^{\text{in}}))$

How many past vectors (N) are used and the value of the coefficients depends on the algorithm, as does the mix factor σ. The default method is the *MultiStepper* (page 23), which is explained separately. The older *DIIS* (page 32) method is simpler to tweak in case the SCC does not converge.

```
SCC
   AlwaysClaimConvergence Yes/No
   Converge
      Charge float
      Norm [L2 | L-Infinity]
   End
   HXDamping Yes/No
   InheritMixFromPreviousResult Yes/No
   Iterations integer
   Method [DIIS | MultiStepper]
   MinimumAdaptiveMixingFactor float
   OrbitalDependent Yes/No
   SpinOrbit Yes/No
   Unrestricted Yes/No
End
```

SCC

Type
Block

Description
This optional section configures various details of the self-consistent charge cycle. If the model Hamiltonian does not need a self-consistent solution (e.g. plain DFTB0), none of this information is used and the entire section will be ignored.

`AlwaysClaimConvergence`

Type
Bool

Default value
No

Description
Even if the SCC does not converge, claim convergence.

`Converge`

Type
Block

Description
Controls the convergence criteria of the SCC cycle.

`Charge`

Type
Float

Default value
1e-08

GUI name
Charge convergence

Description
The maximum change in atomic charges between subsequent SCC iterations. If the charges change less, the SCC cycle is considered converged.

`Norm`

Type
Multiple Choice

Default value
L-Infinity

Options
[L2, L-Infinity]

Description
The LInfinity norm is the more stringent choice. The L2 norm is directly what is optimized by the DIIS procedure, it is scaled by the extra constant factor 2/sqrt(nAtoms).

`HXDamping`

Type
Bool

Description
This option activates the DFTB3 style damping for H-X bonds. Note that this is always enabled if the DFTB%Model key is set to DFTB3. Not used with xTB.

`InheritMixFromPreviousResult`

Type
Bool

Default value
No

Description
For some run types, such as GeometryOptimization, a previous result is available. By using the charges from the previous geometry a better initial guess for the SCC procedure may be obtained.

Also the last mix factor from the previous result can be loaded, possibly speeding up the SCC.

`Iterations`

Type
Integer

Default value
500

Description
Allows to specify the maximum number of SCC iterations. The default should suffice for most standard calculations.

Convergence issues may arise due to the use of the Aufbau occupations for systems with small HOMO-LUMO gaps. In this case the use of a Fermi broadening strategy may improve convergence.

Choosing a smaller mixing parameter (see DFTB%SCC%Mixing) may also help with convergence issues: it often provides a more stable but slower way to converge the SCC cycle.

`Method`

Type
Multiple Choice

Default value
MultiStepper

Options
[DIIS, MultiStepper]

Description
The DIIS option is the old method. The MultiStepper is much more flexible and is controlled by the SCFMultiSolver block

`MinimumAdaptiveMixingFactor`

Type
Float

Default value
0.003

Description
In case of AdaptiveMixing the lower bound for the MixingFactor.

`OrbitalDependent`

Type
Bool

Description
Activates or disables orbital resolved calculations. If this key is absent the recommended settings from the parameter file's metainfo.

SpinOrbit

Type
Bool

Default value
No

Description
test

Unrestricted

Type
Bool

Default value
No

Description
Enables spin unrestricted calculations.

Only collinear spin polarization is supported, see Theor Chem Acc (2016) 135: 232, for details.

Must be supported by the chosen parameter set. Not yet compatible with DFTB3, k-space sampling periodic calculations or the xTB models.

```
Occupation
   KT float
   NumBoltz integer
   Strategy [Auto | Aufbau | Fermi]
   Temperature float
End
```

Occupation

Type
Block

Description
Configures the details of how the molecular orbitals are occupied with electrons.

KT

Type
Float

Unit
Hartree

Description
(KT) Boltzmann constant times temperature, used for electronic temperature with strategy is auto.

The default value is the default value for Temperature*3.166815423e-6.

This key and Temperature are mutually exclusive.

NumBoltz

Type
Integer

Default value
10

Description
The electronic temperature is done with a Riemann Stieltjes numerical integration, between zero and one occupation. This defines the number of points to be used.

Strategy

Type
Multiple Choice

Default value
Auto

Options
[Auto, Aufbau, Fermi]

GUI name
Occupation

Description
This optional key allows to specify the fill strategy to use for the molecular orbitals.

Can either be 'Aufbau' for simply filling the energetically lowest orbitals, or 'Fermi' for a smeared out Fermi-Dirac occupation. By default the occupation strategy is determined automatically, based on the other settings (such as the number of unpaired electrons).

Temperature

Type
Float

Default value
300.0

Unit
Kelvin

GUI name
Fermi temperature

Description
The Fermi temperature used for the Fermi-Dirac distribution. Ignored in case of aufbau occupations.

```
UnpairedElectrons integer
```

UnpairedElectrons

Type
Integer

Default value
0

GUI name
Spin polarization

Description
This specifies the number of unpaired electrons (not the multiplicity!).

This number will then be used in the orbital-filling strategy. Has to be compatible with the total number of electrons, meaning it must be an even number if the total number of electrons is even and odd if the total number is odd. Must be an integer value.

Note that this does not activate spin polarization, it only affects the filling of the orbitals.

3.7.1 MultiStepper

The MultiStepper introduces the concept of alternating between different steppers (methods). Methods are not switched at every SCF cycle, but rather after a sequence of them, called a stint. At the end of a stint it is considered whether it makes sense to try another stepper.

The key component is the Stepper. This wraps the type of the Stepper, say DIIS or SimpleMixing. Another important component is the MixAdapter. A step is controlled by a mix factor σ, also often called greed. The next guess charge vector is a linear combination of previous input and output charges

$\vec{q}^{\text{guess}} = \sum_i c^N_{i-1}(\vec{q}^{\text{in}}_i + \sigma(\vec{q}^{\text{out}}_i - \vec{q}^{\text{in}}_i))$

The larger the mix factor the more aggressive the algorithm. Choosing it too small may simply stall the progress and choosing it too large can cause the error to grow. That is why using a MixAdapter is useful. It tries to predict a reasonable mix value, based on the progress of the error and also based on the number of previous iterations N that can be used without running into numerical problems.

A whole SCFMultiStepper block can be loaded from a file as a preset, and many reside in `$AMSHOME/data/presets/multi_stepper`. Normal users are not recommended to try to improve the standard preset. Which preset is loaded is controlled by the `SCF%MultiStepperPresetPath` key, and this may be an absolute path to your own preset.

The log file (ams.log) shows the active stepper and mix factor.

```
<Nov22-2022> <15:24:28>  cyc=  0 err=0.00E+00 cpu=  75s ela=  76s
<Nov22-2022> <15:25:26>  cyc=  1 err=4.26E+00 meth=1 nvec= 1 mix=0.0750 cpu=  57s␣
↪ela=  58s fit=7.06E-02
<Nov22-2022> <15:26:26>  cyc=  2 err=8.33E+00 meth=1 nvec= 2 mix=0.1455 cpu=  59s␣
↪ela=  60s fit=6.49E-02
<Nov22-2022> <15:27:23>  cyc=  3 err=7.85E+00 meth=1 nvec= 3 mix=0.1499 cpu=  56s␣
↪ela=  57s fit=6.42E-02
<Nov22-2022> <15:28:24>  cyc=  4 err=7.09E+00 meth=1 nvec= 4 mix=0.1544 cpu=  60s␣
↪ela=  61s fit=6.37E-02
<Nov22-2022> <15:29:21>  cyc=  5 err=9.49E+00 meth=2 nvec= 1 mix=0.0060 cpu=  57s␣
↪ela=  57s fit=7.91E-02
<Nov22-2022> <15:30:20>  cyc=  6 err=2.63E+00 meth=2 nvec= 2 mix=0.0062 cpu=  59s␣
↪ela=  59s fit=7.88E-02
<Nov22-2022> <15:31:18>  cyc=  7 err=3.82E+00 meth=2 nvec= 3 mix=0.0060 cpu=  57s␣
↪ela=  58s fit=7.84E-02
<Nov22-2022> <15:32:16>  cyc=  8 err=3.53E+00 meth=2 nvec= 4 mix=0.0062 cpu=  58s␣
↪ela=  58s fit=7.81E-02
```

From cycle 5 (cyc=5) on the second stepper is tried (meth=2), in this case because the error has grown too much since the start. Furthermore it restarts from the first density, not shown in the log file, using only one older density (nvec=1). Note that the second stepper starts with using a much more conservative mix factor (mix=0.006).

```
SCC
   SCFMultiStepper
      AlwaysChangeStepper Yes/No
      ErrorGrowthAbortFactor float
      FractionalStepFactor float
```

(continues on next page)

(continued from previous page)

```
      MinStintCyclesForAbort integer
      Stepper header
         AbortSlope float
         DIISStepper
            EDIISAlpha float
            MaxCoefficient float
            MaxVectors integer
            MinVectors integer
            Mix float
         End
         ErrorGrowthAbortFactor float
         ExpectedSlope float
         FractionalStepFactor float
         MaxInitialError float
         MaxIterationNumber integer
         MaxStintNumber integer
         MinInitialError float
         MinIterationNumber integer
         MinStintCyclesForAbort integer
         MinStintNumber integer
         MixAdapter
            ErrorGrowthPanicFactor float
            GrowthFactor float
            MaxMix float
            MinMix float
            NTrialMixFactors integer
            TrialMode [CurrentMixCentered | FullRange]
            Type [Error | Energy | UnpredictedStep | Trial]
         End
         MixStepper
            Mix float
         End
         MultiSecantStepper
            MaxCoefficient float
            MaxVectors integer
            Mix float
            Variant [MSB1 | MSB2 | MSR1 | MSR1s]
         End
         StintLength integer
      End
      StintLength integer
      UsePreviousStintForErrorGrowthAbort Yes/No
   End
   MultiStepperPresetPath string
End
```

SCC

SCFMultiStepper

Type
Block

Description
To solve the self-consistent problem multiple steppers can be tried during stints using the ones that give the best progress.

AlwaysChangeStepper

Type
Bool

Default value
No

Description
When the progress is fine there is no reason to change the stepper. In practice this is always set to true, because also the Stepper%ExpectedSlope can be used to achieve similar behavior.

`ErrorGrowthAbortFactor`

Type
Float

Default value
1000.0

Description
Abort stint when the error grows too much, compared to the error at the start of the stint.

`FractionalStepFactor`

Type
Float

Default value
-1.0

Description
Multiply the step by this factor. If smaller than zero this is not used.

`MinStintCyclesForAbort`

Type
Integer

Default value
0

Description
Look at ErrorGrowthAbortFactor only when a number of steps has been completed since the start of the stint. A value of 0 means always.

`Stepper`

Type
Block

Recurring
True

Description
??

`AbortSlope`

Type
Float

Default value
100.0

Description
If the slope (at the end of a stint) is larger than this: abort the stepper

`DIISStepper`

Type
Block

Description
DIIS stepper

`EDIISAlpha`

Type
Float

Default value
0.01

Description
The extra energy vector is weighed by this factor. .

`MaxCoefficient`

Type
Float

Default value
20.0

Description
The largest allowed value of the expansion coefficients. If exceed the number of vectors is reduces until the criterion is met.

`MaxVectors`

Type
Integer

Default value
10

Description
Maximum number of previous densities to be used (size of the history).

`MinVectors`

Type
Integer

Default value
-1

Description
Try to prevent to make nVectors shrink below this value, by allowing for significantly larger coefficients.

`Mix`

Type
Float

Default value
0.2

Description
Also known as greed. It determines the amount of output density to be used. May be changed by the MixAdapter.

`ErrorGrowthAbortFactor`

Type
Float

Default value
-1.0

Description
Abort stint when the error grows too much, compared to the error at the start of the stint. Overrides global ErrorGrowthAbortFactor when set to a value > 0

`ExpectedSlope`

Type
Float

Default value
-100.0

Description
If the slope of the total SCF is better than this keep on going.

`FractionalStepFactor`

Type
Float

Default value
-1.0

Description
Multiply the step by this factor. If smaller than zero this is not used.

`MaxInitialError`

Type
Float

Description
Only use the stepper when error is smaller than this.

`MaxIterationNumber`

Type
Integer

Default value
-1

Description
Stepper will only be active for iterations smaller than this number. (Negative value means: Ignore this option)

`MaxStintNumber`

Type
Integer

Default value
-1

Description
Stepper will only be active for stints smaller than this number. (Negative value means: Ignore this option)

`MinInitialError`

Type
Float

Description
Only use the stepper when error is larger than this.

`MinIterationNumber`

Type
Integer

Default value
-1

Description
Stepper will only be active for iterations larger than this number.

`MinStintCyclesForAbort`

Type
Integer

Default value
0

Description
Look at ErrorGrowthAbortFactor only when a number of steps has been completed since the start of the stint. A value of 0 means always. Overrides global value.

`MinStintNumber`

Type
Integer

Default value
-1

Description
Stepper will only be active for stints larger than this number.

`MixAdapter`

Type
Block

Description
Generic mix adapter

`ErrorGrowthPanicFactor`

Type
Float

Default value
10.0

Description
When the error increases more than this factor, this mix is reduced a lot.

`GrowthFactor`

Type
Float

Default value
1.1

Description
When the mix is considered too low it is multiplied by this factor. Otherwise it is divided by it.

`MaxMix`

Type
Float

Default value
0.3

Description
Do not grow the mix above this value.

`MinMix`

Type
Float

Default value
0.1

Description
Do not shrink the mix below this value.

`NTrialMixFactors`

Type
Integer

Default value
3

Description
Only used with Type=Trial. Must be an odd number.

`TrialMode`

Type
Multiple Choice

Default value
CurrentMixCentered

Options
[CurrentMixCentered, FullRange]

Description
How are the NTrialMixFactors chosen?

`Type`

Type
Multiple Choice

Default value
Error

Options
[Error, Energy, UnpredictedStep, Trial]

Description
Adapt the mix factor based on the observed progress (slope).

`MixStepper`

Type
Block

Description
Simple mixing stepper, only using the previous (in/out) density.

`Mix`

Type
Float

Default value
0.1

Description
???.

`MultiSecantStepper`

Type
Block

Description
Multi secant stepper.

`MaxCoefficient`

Type
Float

Default value
20.0

Description
???.

`MaxVectors`

Type
Integer

Default value
10

Description
???.

`Mix`

Type
Float

Default value
0.2

Description
???.

`Variant`

Type
Multiple Choice

Default value
MSB2

Options
[MSB1, MSB2, MSR1, MSR1s]

Description
There are several version of the Multi secant method.

`StintLength`

Type
Integer

Description
Override global StintLength.

`StintLength`

Type
Integer

Default value
10

Description
A stepper is active during a number of SCF cycles, called a stint.

`UsePreviousStintForErrorGrowthAbort`

Type
Bool

Default value
No

Description
The error is normally checked against the first error of the stint. With this option that will be the one from the previous stint, if performed with the same stepper.

`MultiStepperPresetPath`

Type
String

Default value
DFTB/default2023.inc

Description
Name of file containing a SCFMultiStepper key block. This will be used if no Explicit SCF-MultiStepper block is in the input, and Method=MultiStepper.

If the path is not absolute, it is relative to $AMSHOME/data/presets/multi_stepper'

3.7.2 DIIS

When selecting the SCC method DIIS, these are the relevant options. Compared to the MultiStepper it is more straightforward to tweak.

```
SCC
   AdaptiveMixing Yes/No
   DIIS
      Enabled Yes/No
      MaxSamples integer
      MaximumCoefficient float
      MinSamples integer
      MixingFactor float
   End
End
```

SCC

AdaptiveMixing

Type
Bool

Default value
Yes

Description
Change the mixing parameter based on the monitored energy. A significant increase of energy will strongly reduce the mixing. Then it will slowly grow back to the SCC%Mixing value.

DIIS

Type
Block

Description
Parameters influencing the DIIS self-consistency method

Enabled

Type
Bool

Default value
Yes

Description
If not enabled simple mixing without DIIS acceleration will be used.

MaxSamples

Type
Integer

Default value
20

Description
Specifies the maximum number of samples considered during the direct inversion of iteration of subspace (DIIS) extrapolation of the atomic charges during the SCC iterations. A smaller number of samples potentially leads to a more aggressive convergence acceleration, while a larger number often guarantees a more stable iteration. Due to often occurring linear

dependencies within the set of sample vectors, the maximum number of samples is reached only in very rare cases.

MaximumCoefficient

Type
Float

Default value
10.0

Description
When the diis expansion coefficients exceed this threshold, the solution is rejected. The vector space is too crowded. The oldest vector is discarded, and the expansion is re-evaluated.

MinSamples

Type
Integer

Default value
-1

Description
When bigger than one, this affects the shrinking of the DIIS space on linear dependence. It will not reduce to a smaller space than MinSamples unless there is extreme dependency.

MixingFactor

Type
Float

Default value
0.15

Description
The parameter used to mix the DIIS linear combination of previously sampled atomic charge vectors with an analogous linear combination of charge vectors resulting from population analysis combination. It can assume real values between 0 and 1.

3.8 k-space integration

As of the 2019 release, the k-space integration is unified between BAND and DFTB and uses the same keys as input, and the same defaults. See the page on k-space integration in the BAND manual for details and recommendations.

```
KSpace
   Analytical Yes/No
   Quality [Auto | GammaOnly | Basic | Normal | Good | VeryGood | Excellent]
   Regular
      NumberOfPoints integer_list
   End
   Symmetric
      KInteg integer
   End
   Type [Regular | Symmetric]
End
```

KSpace

Type
Block

Description
Options for the k-space integration (i.e. the grid used to sample the Brillouin zone)

`Analytical`

Type
Bool

Default value
Yes

Description
For analytical integration the BZ is split into simplices, whereover the bands are interpolated, ater which the integrals can be performed analytically.

Alternatively, the set of eigenvalues in the discrete set of k-points are just handled as distinct molecular orbitals.

Using analytical=no can improve SCF convergence in combination with smearing/temperature.

`Quality`

Type
Multiple Choice

Default value
Auto

Options
[Auto, GammaOnly, Basic, Normal, Good, VeryGood, Excellent]

GUI name
K-space

Description
Select the quality of the K-space grid used to sample the Brillouin Zone. If 'Auto', the quality defined in the 'NumericalQuality' will be used. If 'GammaOnly', only one point (the gamma point) will be used.

The actual number of K points generated depends on this option and on the size of the unit cell. The larger the real space cell, the fewer K points will be generated.

The CPU-time and accuracy strongly depend on this option.

`Regular`

Type
Block

Description
Options for the regular k-space integration grid.

`NumberOfPoints`

Type
Integer List

Description
Use a regular grid with the specified number of k-points along each reciprocal lattice vector.

For 1D periodic systems you should specify only one number, for 2D systems two numbers, and for 3D systems three numbers.

`Symmetric`

Type
Block

Description
Options for the symmetric k-space integration grid.

`KInteg`

Type
Integer

GUI name
Accuracy

Description
Specify the accuracy for the Symmetric method.

1: absolutely minimal (only the G-point is used)

2: linear tetrahedron method, coarsest spacing

3: quadratic tetrahedron method, coarsest spacing

4,6,… (even): linear tetrahedron method

5,7…. (odd): quadratic method

The tetrahedron method is usually by far inferior.

`Type`

Type
Multiple Choice

Default value
Regular

Options
[Regular, Symmetric]

GUI name
K-space grid type

Description
The type of k-space integration grid used to sample the Brillouin zone (BZ) used.

'Regular': simple regular grid.

'Symmetric': symmetric grid for the irreducible wedge of the first BZ (useful when high-symmetry points in the BZ are needed to capture the correct physics of the system, graphene being a notable example).

3.9 xTB specific keywords

A few keywords only apply to the xTB model Hamiltonian.

```
XTBConfig
   SlaterRadialThreshold float
   useXBTerm Yes/No
End
```

XTBConfig

Type
Block

Description
This block allows for minor tweaking.

SlaterRadialThreshold

Type
Float

Default value
1e-05

Description
Threshold determining the range of the basis functions. Using a larger threshold will speed up the calculation, but will also make the results less accurate.

useXBTerm

Type
Bool

Default value
No

Description
Whether to use the Halogen bonding (XB) term. This is not advised as it has a non-continuous PES.

Note: The GFN1-xTB implementation in AMS currently does not implement the electronic entropy term from the article by Grimme et al. It therefore gives slightly different energies (but not gradients!) for systems with partially occupied molecular orbitals.

3.10 Technical options

```
Technical
   AnalyticalStressTensor Yes/No
   EwaldSummation
      CellRangeFactor float
      Enabled Yes/No
      Tolerance float
   End
   MatricesViaFullMaxSize integer
```

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```
   Parallel
      nCoresPerGroup integer
      nGroups integer
      nNodesPerGroup integer
   End
   ReuseKSpaceConfig Yes/No
   Screening
      dMadel float
      rMadel float
   End
   UseGeneralizedDiagonalization Yes/No
End
```

Technical

Type
Block

Description
This optional section is about technical aspects of the program that should not concern the normal user.

AnalyticalStressTensor

Type
Bool

Default value
Yes

Description
Whether to compute the stress tensor analytically. Note: This can only be used together with Ewald summation as it will give (slightly) wrong results with Madelung screening.

EwaldSummation

Type
Block

Description
Configures the details of the Ewald summation of the Coulomb interaction.

CellRangeFactor

Type
Float

Default value
2.0

Description
Smaller values will make the Ewald summation less accurate but faster.

Enabled

Type
Bool

Default value
Yes

Description
Whether to use Ewald summation for the long-range part of the Coulomb interaction. Otherwise screening is used.

Tolerance

Type
Float

Default value
1e-10

Description
Larger values will make the Ewald summation less accurate but faster.

MatricesViaFullMaxSize

Type
Integer

Default value
2047

Description
Matrices smaller than this size are constructed via a full matrix. This is faster, but uses more memory in the construction.

Parallel

Type
Block

Description
Calculation of the orbitals in several k-points is trivially parallel.

nCoresPerGroup

Type
Integer

Description
Number of cores in each working group.

nGroups

Type
Integer

Description
Total number of processor groups. This is the number of tasks that will be executed in parallel.

nNodesPerGroup

Type
Integer

GUI name
Cores per task

Description
Number of nodes in each group. This option should only be used on homogeneous compute clusters, where all used compute nodes have the same number of processor cores.

ReuseKSpaceConfig

Type
Bool

Default value
Yes

Description
Keep the number of k-points constant during a lattice optimization. Otherwise the PES might display jumps, because the number of points depends on the lattice vector sizes. If this option is on it will always use the number of k-points that was used from a previous result.

`Screening`

Type
Block

Description
For SCC-DFTB in periodic systems the Coulomb interaction can (instead of using Ewald summation) be screened with a Fermi-Dirac like function defined as S(r)=1/(exp((r-r_madel)/d_madel)+1). This section allows to change some details of the screening procedure. Note that Coulomb screening is only used if the Ewald summation is disabled.

`dMadel`

Type
Float

Unit
Bohr

Description
Sets the smoothness of the screening function. The default is 1/10 of [rMadel].

`rMadel`

Type
Float

Unit
Bohr

Description
Sets the range of the screening function. The default is 2x the norm of the longest lattice vector.

`UseGeneralizedDiagonalization`

Type
Bool

Default value
Yes

Description
Whether or not to use generalized diagonalization. Does not affect the results, but might be faster or slower.

```
StoreMatrices Yes/No
```

`StoreMatrices`

Type
Bool

Default value
No

Description
Determines whether the Hamiltonian and overlap matrices are stored in the binary result file.

CHAPTER

FOUR

SPECTROSCOPY AND PROPERTIES

4.1 Electronic structure of periodic systems

```
Periodic
   EffectiveMass
      Enabled Yes/No
      KPointCoord float_list
      NumAbove integer
      NumBelow integer
      StepSize float
      UseBandStructureInfoFromPath Yes/No
   End
   BandStructure
      Automatic Yes/No
      DeltaK float
      Enabled Yes/No
      FatBands Yes/No
      KPathFinderConvention [Setyawan-Curtarolo | Hinuma]
      UseSymmetry Yes/No
   End
   BZPath
      Path # Non-standard block. See details.
         ...
      End
   End
   DOS
      EMax float
      EMin float
      Enabled Yes/No
      NSteps integer
   End
End
```

Periodic

Type
Block

Description
Block that sets various details of the calculation only relevant for periodic systems.

EffectiveMass

Type
Block

Description
In a semi-conductor, the mobility of electrons and holes is related to the curvature of the bands at the top of the valence band and the bottom of the conduction band.

With the effective mass option, this curvature is obtained by numerical differentiation.

The estimation is done with the specified step size, and twice the specified step size, and both results are printed to give a hint on the accuracy. By far the most convenient way to use this key is without specifying any options.

`Enabled`

Type
Bool

Default value
No

GUI name
Effective mass

Description
In a semi-conductor, the mobility of electrons and holes is related to the curvature of the bands at the top of the valence band and the bottom of the conduction band.

With the effective mass option, this curvature is obtained by numerical differentiation.

The estimation is done with the specified step size, and twice the specified step size, and both results are printed to give a hint on the accuracy. By far the most convenient way to use this key is without specifying any options.

`KPointCoord`

Type
Float List

Unit
1/Bohr

Recurring
True

GUI name
At K-point

Description
Coordinate of the k-points for which you would like to compute the effective mass.

`NumAbove`

Type
Integer

Default value
1

GUI name
Include N bands above

Description
Number of bands to take into account above the Fermi level.

`NumBelow`

Type
Integer

Default value
1

GUI name
Include N bands below

Description
Number of bands to take into account below the Fermi level.

`StepSize`

Type
Float

Default value
0.001

Description
Size of the step taken in reciprocal space to perform the numerical differentiation

`UseBandStructureInfoFromPath`

Type
Bool

Default value
Yes

Description
The (automatic) location of the HOMO and LUMO can be determined via band interpolation, or from the path as used by the BandStructure feature. The latter works better when they are located on the path. See also comments in the BandStructure block. To reproduce results from before ams2025 set to no.

`BandStructure`

Type
Block

Description
Options for band structure plotting. This has no effect on the calculated energy. [Warning: The band structure is only computed in case of k-space sampling, i.e. it is not computed for Gamma-only calculations (see: Periodic%KSpace).]

`Automatic`

Type
Bool

Default value
Yes

GUI name
Automatic generate path

Description
Generate and use the standard path through the Brillouin zone.

If not, use the user defined path (set via Custom path in the GUI, or with the Periodic%BZPath keyword in the run script).

DeltaK

Type
Float

Default value
0.1

Unit
1/Bohr

GUI name
Interpolation delta-K

Description
Step size in reciprocal space for band structure interpolation. Using a smaller number will produce smoother band curves at an increased computational time.

Enabled

Type
Bool

Default value
Yes

GUI name
Calculate band structure

Description
Whether or not to calculate the band structure.

FatBands

Type
Bool

Default value
Yes

GUI name
Calculate fatbands

Description
Control the computation of the fat bands (only when the bandstructure is calculated).

The fat bands are the periodic equivalent of the Mulliken population analysis. The definition of the fat bands can be found in the Band Documentation.

KPathFinderConvention

Type
Multiple Choice

Default value
Setyawan-Curtarolo

Options
[Setyawan-Curtarolo, Hinuma]

Description
This option determines how the path through the Brillouin zone is generated when using the automatic k-point mode.

Available options:

- `Setyawan-Curtarolo` (default for 1D and 2D lattices): Uses our built-in KPath program to find a path through high-symmetry points based on the method by Setyawan and Curtarolo (https://doi.org/10.1016/j.commatsci.2010.05.010). For 2D lattices, the path is derived from the intersection of the 3D Brillouin zone with a plane. For 1D lattices, the path is simply Gamma-Z.
- `Hinuma`: Uses the external SeeKPath utility to generate the k-path (https://github.com/giovannipizzi/seekpath and https://doi.org/10.1016/j.commatsci.2016.10.015).

UseSymmetry

Type
Bool

Default value
Yes

Description
If set, only the irreducible wedge of the Wigner-Seitz cell is sampled. If not, the whole (inversion-unique) Wigner-Seitz cell is sampled. Only available for Setyawan and Curtarolo convention (see `KPathFinderConvention`).

BZPath

Type
Block

Description
If [BandStructure%Automatic] is disabled, DFTB will compute the band structure for the user-defined path in the [BZPath] block. You should define the vertices of your path in fractional coordinates (with respect to the reciprocal lattice vectors) in the [Path] sub-block. If you want to make a jump in your path, you need to specify a new [Path] sub-block.

Path

Type
Non-standard block

Recurring
True

Description
A section of a k space path.

DOS

Type
Block

Description
The subkeys of [DOS] allow to customize the calculation of the density of states.

EMax

Type
Float

Default value
0.75

Unit
Hartree

Description
Upper end of the energy interval in which the density of states is calculated.

EMin

Type
Float

Default value
-0.75

Unit
Hartree

Description
Lower end of the energy interval in which the density of states is calculated.

Enabled

Type
Bool

Default value
Yes

GUI name
Calculate DOS

Description
Whether or not to calculate the DOS. Note that the DOS will always be calculated when also the band structure is calculated.

NSteps

Type
Integer

Default value
300

Description
The number of energy intervals between [EMin] and [EMax] for which the density of states is calculated.

4.2 Excited states with time-dependent DFTB

DFTB allows for excited state calculations on molecular systems by means of single orbital transitions as well as time-dependent DFTB as published by Niehaus et al. in *Phys. Rev. B* **63**, 085108 (2001). Singlet-singlet as well as singlet-triplet excitations can be calculated. DFTB also supports the calculation of excited state gradients, which allows geometry optimizations and vibrational frequency calculations for excited states.

The TD-DFTB implementation uses the PRIMME library (PReconditioned Iterative MultiMethod Eigensolver) by Andreas Stathopoulos and James R. McCombs, PRIMME: PReconditioned Iterative MultiMethod Eigensolver (https://www.cs.wm.edu/~andreas/publications/primmeTOMS.pdf): Methods and software description ACM Transaction on Mathematical Software Vol. 37, No. 2, (2010), 21:1–21:30 (https://doi.org/10.1145/1731022.1731031).

DFTB excited state calculations are controlled by the following keywords:

```
Properties
   Excitations
      SingleOrbTrans
         Enabled Yes/No
         Filter
            OSMin float
            dEMax float
            dEMin float
         End
         PrintLowest integer
      End
      TDDFTB
         Calc [None | Singlet | Triplet]
         DavidsonConfig
            ATCharges [Precalc | OnTheFly]
            SafetyMargin integer
            Tolerance float
         End
         Diagonalization [Auto | Davidson | Exact]
         Lowest integer
         Print string
         ScaleKernel float
         UpTo float
      End
      TDDFTBGradients
         Eigenfollow Yes/No
         Excitation integer_list
      End
   End
End
```

Properties

Type
Block

Description
DFTB can calculate various properties of the simulated system. This block configures which properties will be calculated.

Excitations

Type
Block

Description
Contains all options related to the calculation of excited states, either as simple single orbitals transitions or from a TD-DFTB calculation.

SingleOrbTrans

Type
Block

Description
The simplest approximation to the true excitations are the single orbital transitions (sometimes called Kohn-Sham transitions), that is transitions where a single electron is excited from an occupied Kohn-Sham orbital into a virtual orbital. The calculation of these transitions is configured in this section. Note that the SingleOrbTrans section is optional even

though the single orbital transitions are also needed for TD-DFTB calculations. If the section is not present all single orbital transitions will still be calculated and used in a subsequent TD-DFTB calculation, but no output will be produced.

Enabled

Type
Bool

Default value
No

GUI name
Single orbital transisitions: Calculate

Description
Calculate the single orbital transitions.

Filter

Type
Block

Description
This section allows to remove single orbital transitions based on certain criteria. All filters are disabled by default.

OSMin

Type
Float

GUI name
Minimum oscillator strength

Description
Removes single orbital transitions with an oscillator strength smaller than this threshold.

A typical value to start (if used at all) would be 1.0e-3.

dEMax

Type
Float

Unit
Hartree

Description
Removes single orbital transitions with an orbital energy difference larger than this threshold.

dEMin

Type
Float

Unit
Hartree

Description
Removes single orbital transitions with an orbital energy difference smaller than this threshold.

PrintLowest

Type
Integer

Default value
10

Description
The number of single orbital transitions that are printed to the screen and written to disk.

If not a TD-DFTB calculation, the default is to print the 10 lowest single orbital transitions.

In case of a TD-DFTB calculation it is assumed that the single orbital transitions are only used as an input for TD-DFTB and nothing will be printed unless PrintLowest is specified explicitly.

`TDDFTB`

Type
Block

Description
Calculations with time-dependent DFTB can be configured in the TDDFTB section and should in general give better results than the raw single orbital transitions. TD-DFTB calculates the excitations in the basis of the single orbital transitions, whose calculation is configured in the SingleOrbTrans section. Using a filter in SingleOrbTrans can therefore be used to reduce the size of the basis for TD-DFTB. One possible application of this is to accelerate the calculation of electronic absorption spectra by removing single orbital transitions with small oscillator strengths from the basis. Note that the entire TDDFTB section is optional. If no TDDFTB section is found, the behavior depends on the existence of the SingleOrbTrans section: If no SingleOrbTrans section is found (the Excitations section is completely empty then) a TD-DFTB calculation with default parameters will be performed. If only the SingleOrbTrans section is present no TD-DFTB calculation will be done.

`Calc`

Type
Multiple Choice

Default value
None

Options
[None, Singlet, Triplet]

GUI name
Type of excitations

Description
Specifies the multiplicity of the excitations to be calculated.

`DavidsonConfig`

Type
Block

Description
This section contains a number of keywords that can be used to override various internals of the Davidson eigensolver. The default values should generally be fine.

`ATCharges`

Type
Multiple Choice

Default value
Precalc

Options
[Precalc, OnTheFly]

GUI name
Transition charges

Description
Select whether the atomic transition charges are precalculated in advance or reevaluated during the iterations of the Davidson solver.

Precalculating the charges will improve the performance, but requires additional storage.

The default is to precalculate the atomic transition charges, but the precalculation may be disabled if not not enough memory is available.

`SafetyMargin`

Type
Integer

Default value
4

Description
The number of eigenvectors the Davidson method will calculate in addition to the ones requested by the user. With the Davidson eigensolver it is generally a good idea to calculate a few more eigenvectors than needed, as depending on the initial guess for the eigenvectors it can happen that the found ones are not exactly the lowest ones. This problem is especially prominent if one wants to calculate only a small number of excitations for a symmetric molecule, where the initial guesses for the eigenvectors might have the wrong symmetry. Note that the additionally calculated excitations will neither be written to the result file nor be visible in the output.

`Tolerance`

Type
Float

Default value
1e-09

Description
Convergence criterion for the norm of the residual.

`Diagonalization`

Type
Multiple Choice

Default value
Auto

Options
[Auto, Davidson, Exact]

GUI name
Method

Description
Select the method used to solve the TD-DFTB eigenvalue equation.

The most straightforward procedure is a direct diagonalization of the matrix from which the excitation energies and oscillator strengths are obtained. Since the matrix grows quickly with system size (number of used single orbital transitions squared), this option is possible only for small molecules.

The alternative is the iterative Davidson method, which finds a few of the lowest excitations within an error tolerance without ever storing the full matrix.

The default is to make this decision automatically based on the system size and the requested number of excitations.

Lowest

Type
Integer

Default value
10

GUI name
Number of excitations

Description
Specifies the number of excitations that are calculated.

Note that in case of the exact diagonalization all excitations are calculated, but only the lowest ones are printed to screen and written to the output file.

Also note that if limited both by number and by energy, (lowest and upto), DFTB will always use whatever results in the smaller number of calculated excitations.

Print

Type
String

Description
Specifies whether to print details on the contribution of the individual single orbital transitions to the calculated excitations.

ScaleKernel

Type
Float

Default value
1.0

Unit
None

Description
Set the scaling parameter of the response kernel.

A scaling approach can be used to identify plasmons in molecules. While single-particle excitations are only slightly affected by scaling of the response kernel, plasmonic excitations are sensitive to variations in the scaling parameter. Default no scaling is used (scaling parameter = 1.0)

UpTo

Type
Float

Unit
Hartree

GUI name
Excitations up to

Description
Set the maximum excitation energy.

Attempts to calculate all excitations up to a given energy by calculating a number of excitations equal to the number of single orbital transitions in this window. This is only approximately correct, so one should always add some safety margin.

Note that if limited both by number and by energy, (lowest and upto), DFTB will always use whatever results in the smaller number of calculated excitations.

`TDDFTBGradients`

Type
Block

Description
This block configures the calculation of analytical gradients for the TD-DFTB excitation energies, which allows the optimization of excited state geometries and the calculation of vibrational frequencies in excited states (see J. Comput. Chem., 28: 2589-2601). If the gradients are calculated, they will automatically be used for geometry optimizations or vibrational frequency calculations, if the corresponding Task is selected and only 1 excitation is selected. Vibrationally resolved UV/Vis spectroscopy (Franck-Condon Factors) can be calculated in combination with the FCF program or using the Vibrational Analysis Tools in AMS. See the ADF documentation on Vibrationally resolved electronic spectra or the AMS documentation for the Vibrational Analysis Tools.

`Eigenfollow`

Type
Bool

Default value
No

GUI name
Follow initial excitation

Description
If this option is set, DFTB uses the transition density in atomic orbital basis to follow the initially selected excited state during a geometry optimization. This is useful if excited state potential energy surfaces cross each other and you want to follow the surface you started on.

`Excitation`

Type
Integer List

GUI name
Excitation number

Description
Select which excited states to calculate the gradients for.

Gradients can only be calculated for an excited states that has been calculated using TD-DFTB. Make sure that enough excitations are calculated.

4.3 Excited state gradients

Excited state gradients can be calculated with TD-DFTB, see the section *Excited states with time-dependent DFTB* (page 46).

4.4 Frequencies, phonons, VCD

Frequencies, phonons, and VCD can be computed via numerical differentiation by the AMS driver. Several thermodynamic properties, such as zero-point energy, internal energy, entropy, free energy, and specific heat, are computed by default when calculating phonons.

- AMS manual: Vibrational Analysis
  - AMS manual: Infrared (IR) spectra / Normal Modes
  - AMS manual: Phonons
  - AMS manual: Thermodynamic properties
  - AMS manual: VCD (Vibrational Circular Dichroism)

4.5 Vibrationally resolved electronic spectra

- AMS manual: Vibrationally resolved electronic spectra.
  - AMS manual: AH-FC Adiabatic Hessian Franck-Condon.
  - AMS manual: VG-FC Vertical Gradient Franck-Condon.

4.6 Stress tensor, Elasticity

The stress tensor and elastic tensor (and related elastic properties such as bulk modulus, shear modulus, and Young modulus) can be computed via numerical differentiation by AMS.

- AMS manual: Stress tensor
- AMS manual: Elastic tensor

4.7 Charges, Bond Orders, Dipole Moment, Polarizability

Charges, Mayer bond orders, Dipole Moment, and Polarizability can be requested to the DFTB engine in the AMS driver's input:

- AMS manual: Atomic charges
- AMS manual: Bond orders
- AMS manual: Dipole Moment
- AMS manual: Dipole Gradients

4.8 Fragment orbital analysis

The fragment orbital analysis is not available for periodic systems calculated with multiple K-points.

A Mulliken population analysis based on the elementary atomic basis functions can be calculated using

```
Properties
   Fragments
   End
End
```

For an atomic Mulliken population one should not specify any subkey `File` in Properties%Fragments.

A Mulliken population analysis based on orbitals coming from larger fragments, that may consist of more than 1 atom, can be calculated if one includes the binary dftb.rkf result files of the calculated fragments in the input, for example, like:

```
Properties
   Fragments
      File frag1.results/dftb.rkf
      File frag2.results/dftb.rkf
   End
End
```

Note that the nuclear coordinates of the atoms in the fragments should be at exactly the same position as in the whole system. In addition, each atom of the whole system should be present exactly once in one of the fragment dftb.rkf files.

```
Properties
   Fragments
      Analysis Yes/No
      EMax float
      Emin float
      File string
      TIDegeneracyThreshold float
      TransferIntegrals Yes/No
   End
End
```

Properties

Fragments

Type
Block

Description
Fragment files

Analysis

Type
Bool

Default value
Yes

GUI name
Fragment analysis

Description
Mulliken population analysis in terms of fragment orbitals.

`EMax`

Type
Float

Default value
0.25

Unit
Hartree

Description
Upper end of the energy interval for which the orbitals are analyzed.

`Emin`

Type
Float

Default value
-0.75

Unit
Hartree

Description
Lower end of the energy interval for which the orbitals are analyzed.

`File`

Type
String

Recurring
True

Description
Path (either absolute or relative) of fragment file

`TIDegeneracyThreshold`

Type
Float

Default value
0.1

Unit
eV

Description
If the orbital energy of the fragment MO is within this threshold with fragment HOMO or LUMO energy, then this fragment MO is included in the calculation of the transfer integrals. Relevant in case there is (near) degeneracy.

`TransferIntegrals`

Type
Bool

Default value
No

GUI name
Charge transfer integrals

Description
Calculate the charge transfer integrals, spatial overlap integrals and site energies.

Charge transfer integrals can be used in models that calculate transport properties.

4.9 NBO analysis

An input for the GENNBO program of Prof. Weinhold's Natural Bond Orbital (NBO) package, by E. Glendening et al., can be generated using the key Properties%NBOInput. Not available for periodic systems.

```
Properties
   NBOInput Yes/No
End
```

Properties

NBOInput

Type
Bool

Default value
No

Description
Whether or not an input file for the NBO program is written to disk as nboInput.FILE47. The input file follows the FILE47 format as described in the NBO6 manual available on nbo6.chem.wisc.edu. By default, only the calculation of the natural bond orbitals and the natural localized molecular orbitals is enabled, but the nboInput.FILE47 file can be edited by hand to enable other analysis models. Please refer to the NBO6 manual for details.

The GENNBO executable is included in the AMS distribution. The GENNBO program can be called with:

```
#!/bin/sh
$AMSBIN/gennbo6 ams.results/dftb-nboInput.FILE47
```

CHAPTER

FIVE

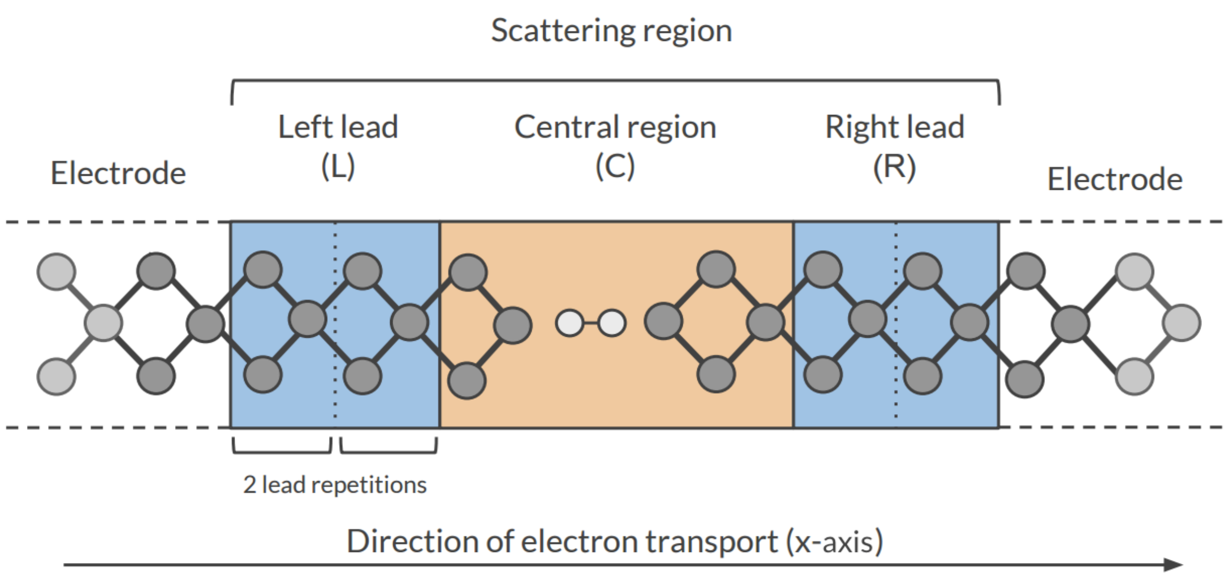
ELECTRONIC TRANSPORT (NEGF)

See also:

- DFTB-NEGF GUI tutorials
- *Example: Electronic transport with NEGF* (page 279)

5.1 Transport with NEGF in a nutshell

The **Non-Equilibrium Green's Functions** formalism (**NEGF**) is a theoretical framework for modeling electron transport through nano-scale devices. Electron transport is treated as a one-dimensional coherent scattering process in the "scattering region" for electrons coming in from the electrodes:



Our goal is to compute the **transmission function** $T(E)$, which describes the rate at which electrons of energy E are transferred from the left electrode to the right electrode by propagating through the scattering region. From the transmission function we can calculate the electric current for given **Bias Voltage** V applied between the electrodes:

$$I(V) = \frac{2e}{h} \int_{-\infty}^{\infty} T(E) \left(f(E - \mu_L) - f(E - \mu_R) \right) dE$$

where $f(E)$ is the Fermi-Dirac distribution function for a given temperature, and μ_L (μ_R) is $\epsilon_F + eV/2$ ($\epsilon_F - eV/2$), ϵ_F being the Fermi energy of the electrodes.

The transmission function $T(E)$ can be computed from the **Green's function** of our system.

The Green's function $G(E)$ of the scattering region is obtained solving the following equation:

$$(ES - H)G(E) = I$$

where S is the overlap matrix, H is the Hamiltonian and I is the identity matrix. The Hamiltonian is composed as follows (**L**, **C** and **R** denote the **left lead**, the **central region** and the **right lead** respectively):

$$H = \begin{pmatrix} H_L + \Sigma_L & H_{LC} & 0 \\ H_{LC} & H_C & H_{RC} \\ 0 & H_{RC} & H_R + \Sigma_R \end{pmatrix}$$

The two *self-energies* Σ_L and Σ_R model the two semi-infinite electrodes.

The transmission function $T(E)$ can be calculated from the Green's function $G(E)$ and the so-called *coupling matrices* $\Gamma_L(E)$ and $\Gamma_R(E)$ (which are related to Σ_L and Σ_R):

$$T(E) = Tr[G(E)\Gamma_R(E)G(E)\Gamma_L(E)]$$

See also:

PhD Thesis (https://opus.jacobs-university.de/frontdoor/index/index/docId/478) of Mahdi Ghorbani-Asl (DFTB-NEGF developer)

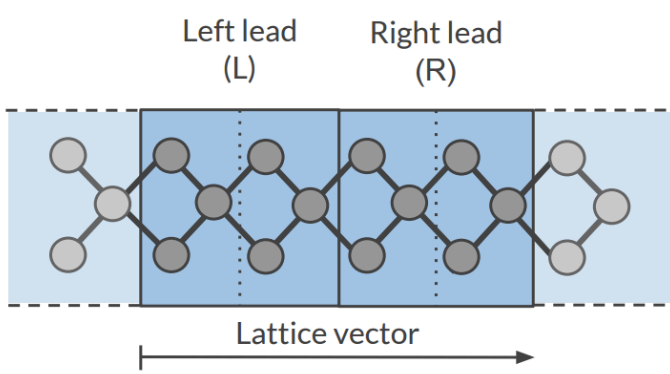
5.2 Simulation workflow

The computation of the transmission function $T(E)$ within the DFTB-NEGF formalism requires three individual simulations.

Tip: Use ADFInput (GUI) to set up your DFTB-NEGF calculation (see the DFTB-NEGF GUI tutorials)

1): DFTB leads calculation

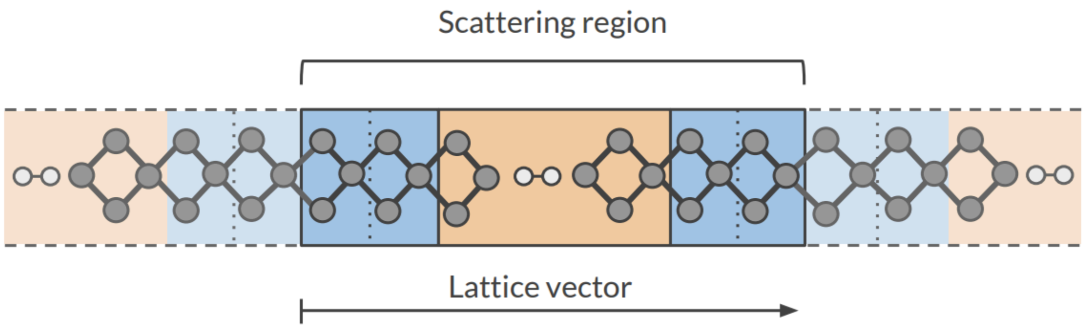
A 1D-periodic DFTB calculation of the leads (*StoreMatrices* (page 39): yes, *KSpace* (page 33) sampling 13):



The Hamiltonian matrices H_L and H_R and the Fermi energy of the electrode ϵ_F are computed in this calculation (H_L, H_R and H_{LR} are also used to compute the surface Green's functions g_L and g_R of the semi-infinite electrodes).

2): DFTB scattering-region calculation

A 1D-periodic DFTB calculation of the scattering region (*StoreMatrices* (page 39): yes, gamma-only, *i.e.*, no *KSpace* (page 33) sampling):



The Hamiltonian matrices H_{LC} and H_{RC} and H_C are computed in this calculation.

3): Conductance calculation

The **Conductance program** computes the NEGF transmission function $T(E)$ using the Hamiltonians and overlap matrices from the previous two DFTB calculations.

5.3 Conductance input options

The **Conductance** program computes the transmission function using the NEGF approach. This is the input structure of the **conductance** program:

```
$AMSBIN/conductance <<EOF > conductance.out

  EnergyGrid
     Min value
     Max value
     Num value

  Files
     Leads       /path/DFTB_lead_filename.rkf
     Scattering  /path/DFTB_scattering_filename.rkf
  End

  Technical
     Eta                    value
     OverwriteLeads         [True|False]
     SetOffDiagonalToZero   [True|False]
  End

  end input
EOF
```

EnergyGrid

Type
Block

Description
Energy grid for Transmission Function

Max

Type
Float

Default value
5.0

Unit
eV

Description
Max Energy (relative to Fermi energy)

`Min`

Type
Float

Default value
-5.0

Unit
eV

Description
Min energy (relative to Fermi energy)

`Num`

Type
Integer

Default value
200

Description
Number of energy values in which the interval Min-Max is subdivided

`Technical`

Type
Block

Description
options describing technical parts of the calculation

`Eta`

Type
Float

Default value
1e-05

Description
To avoid poles of the Green's function, a small imaginary number is added to the energy

`overwriteLeads`

Type
Bool

Default value
Yes

Description
If true, Hamiltonians H_L and H_R are taken from the DFTB-leads calculation. If False, they are taken from the DFTB scattering-region calculation

setOffDiagonalToZero

Type
Bool

Default value
Yes

Description
If true, H_LR and S_LR are explicitly set to zero. If False, they are taken from the DFTB scattering-region calculation.

Files

Type
Block

Description
path of files

Leads

Type
String

Default value

Description
Path (either absolute or relative) of the lead results file

Scattering

Type
String

Default value

Description
Path (either absolute or relative) of the scattering region results

5.4 Miscellaneous remarks on DFTB-NEGF

- You should make sure that your results are converged with respect to the number of lead repetitions; the results should not change significantly if you increase the number of lead repetitions.
- It's good practice to include at least one lead repetition in the central region.
- The transmission function is computed at zero bias voltage. The zero-bias transmission function is then used for computing the electric current for non-zero bias voltage.

CHAPTER

SIX

CHARGE TRANSPORT (TRANSFER INTEGRALS)

DFTB can provide input parameters, such as charge transfer integrals, that are needed in approximate methods that model charge transport properties in the hopping regime. Note that DFTB is an approximate method. You might use ADF to calculate more accurate charge transfer integrals, or use specifically optimized DFTB parameters.

See also:

- ADF tutorial on charge transfer integrals
- *Example: Charge transfer integrals Alq3 dimer* (page 282)

In theoretical models of charge transport in organic materials, see Refs.[1][2][3], the whole system is divided into fragments, in which an electron or hole is localized on a fragment, and can hop from one fragment to another. In the tight-binding approximation that is used in these models the electron or hole is approximated with a single orbital, and it is assumed that only the nearest neighboring fragments can couple. The models require accurate values of electronic couplings for charge transfer (also referred to as charge transfer integrals or hopping matrix elements) and site energies (energy of a charge when it is localized at a particular molecule) as a function of the geometric conformation of adjacent molecules. Charge transfer integrals for hole transport can be calculated from the energetic splitting of the two highest-occupied molecular orbitals (HOMO and HOMO-1) in a system consisting of two adjacent molecules, also called "energy splitting in dimer" (ESID) method. For electron transport these can be calculated from the two lowest-unoccupied orbitals (LUMO and LUMO+1) in this ESID method. DFTB can also calculate transfer integrals based on the direct method by using a fragment approach. The charge transfer integrals obtained in this way may differ significantly from values estimated from the energy splitting between the highest occupied molecular orbitals in a dimer. The difference is due to the nonzero spatial overlap between the molecular orbitals on adjacent molecules. Also, the direct method is applicable in cases where an orbital on one molecule couples with two or more orbitals on another molecule.

6.1 Charge transfer integrals direct method

In this method the matrix elements of the molecular DFTB Hamiltonian H^{DFTB} in the basis of fragment orbitals is used to calculate site energies and charge transfer integrals. Likewise the overlap integrals between fragment orbitals are calculated. No explicit electrons are removed or added in this method. For electron mobility calculations the fragment LUMOs are considered. For hole mobility calculations the fragment HOMOs are considered.

To calculate the charge transfer integrals, spatial overlap integrals, and site energies, the molecular system typically should be built from two fragments. See also the section on *Fragment orbital analysis* (page 54). In the `Engine DFTB` block, specify

[1] M.D. Newton, *Quantum chemical probes of electron-transfer kinetics: the nature of donor-acceptor interactions*, Chemical Reviews 91, 767 (1991) (https://doi.org/10.1021/cr00005a007).

[2] K. Senthilkumar, F.C. Grozema, F.M. Bickelhaupt, and L.D.A. Siebbeles, *Charge transport in columnar stacked triphenylenes: Effects of conformational fluctuations on charge transfer integrals and site energies*, Journal of Chemical Physics 119, 9809 (2003) (https://doi.org/10.1063/1.1615476).

[3] K. Senthilkumar, F.C. Grozema, C. Fonseca Guerra, F.M. Bickelhaupt, F.D. Lewis, Y.A. Berlin, M.A. Ratner, and L.D.A. Siebbeles, *Absolute Rates of Hole Transfer in DNA*, Journal of the American Chemical Society 127, 14894 (2005) (https://doi.org/10.1021/ja054257e)

```
Properties
   Fragments
      File frag1.results/dftb.rkf
      File frag2.results/dftb.rkf
      TransferIntegrals
   End
End
```

By default, integrals are calculated only for the HOMO (LUMO) of the fragments, and possibly HOMO-1, HOMO-2 (LUMO+1, LUMO+2) if the energy of those fragment orbitals are close to the HOMO (LUMO) of that fragment.

If two fragments are used, the electronic coupling V (also known as effective (generalized) transfer integrals J_eff) for hole transfer or electron transfer is calculated as V = (J-S(e1+e2)/2)/(1-S^2). Here e1 and e2 are the site energies of fragment 1 and 2, respectively. J is the charge transfer integral, and S the overlap integral.

$$e_1 = \langle\phi_1|H^{DFTB}|\phi_1\rangle$$
$$e_2 = \langle\phi_2|H^{DFTB}|\phi_2\rangle$$
$$J = \langle\phi_1|H^{DFTB}|\phi_2\rangle$$
$$S = \langle\phi_1|\phi_2\rangle$$
$$V = \frac{J - S(e1 + e2)/2}{1 - S^2}$$

In case of electron mobility calculations ϕ_1 is the LUMO of fragment 1 and ϕ_2 is the LUMO of fragment 2. In case of hole mobility calculations ϕ_1 is the HOMO of fragment 1 and ϕ_2 is the HOMO of fragment 2. The electronic coupling between the HOMO of the donor fragment and the LUMO of the acceptor fragment and vice-versa is also calculated, which represents the probability of a charge recombination process.

If there is (near) degeneracy in the fragment HOMO and/or LUMO, multiple electronic couplings V_i are printed. A total electronic coupling is calculated as

$$V_{tot} = \sqrt{\sum_{deg} {V_i}^2}$$

```
Properties
   Fragments
      Analysis Yes/No
      EMax float
      Emin float
      File string
      TIDegeneracyThreshold float
      TransferIntegrals Yes/No
   End
End
```

Properties

Fragments

Type
Block

Description
Fragment files

Analysis

Type
Bool

Default value
Yes

GUI name
Fragment analysis

Description
Mulliken population analysis in terms of fragment orbitals.

`EMax`

Type
Float

Default value
0.25

Unit
Hartree

Description
Upper end of the energy interval for which the orbitals are analyzed.

`Emin`

Type
Float

Default value
-0.75

Unit
Hartree

Description
Lower end of the energy interval for which the orbitals are analyzed.

`File`

Type
String

Recurring
True

Description
Path (either absolute or relative) of fragment file

`TIDegeneracyThreshold`

Type
Float

Default value
0.1

Unit
eV

Description
If the orbital energy of the fragment MO is within this threshold with fragment HOMO or LUMO energy, then this fragment MO is included in the calculation of the transfer integrals. Relevant in case there is (near) degeneracy.

`TransferIntegrals`

Type
Bool

Default value
No

GUI name
Charge transfer integrals

Description
Calculate the charge transfer integrals, spatial overlap integrals and site energies.

Charge transfer integrals can be used in models that calculate transport properties.

CHAPTER

SEVEN

PARAMETERIZATIONS

7.1 Parameter meta-info

There is a file named `metainfo.yaml` in each resources directory (see *ResourcesDir* (page 10)), for example *DFTB.org/3ob-3-1/metainfo.yaml*, which contains information about the capabilities of a parameter set. The file is in accordance with the YAML (https://www.yaml.org) syntax convention. In older versions of AMS this file was optional and its format was slightly different. Starting with the 2017 release of ADF/AMS, the `metainfo.yaml` file is required to use a parameter set.

The following entries in `metainfo.yaml` specify the capabilities of the parameter set:

`supports: [dftb0, scc-dftb, dftb3, gfn-xtb]`
A comma-separated list of model Hamiltonians for which the parameter set can be used. If the parameter set only supports a single model Hamiltonian, the enclosing `[ ]` can be dropped. This entry is mandatory. Without it, DFTB will refuse to use the parameter set.

`format: txt|txtq`
Specifies which format is used for the Slater-Koster files of the parameter set. Use `txt` for normal text files with extension `.skf`. `txtq` is used for the encrypted Slater-Koster files from the QUASINANO parameter sets. Encrypted Slater-Koster files have the extension `.ske`. If the `format` entry is not there, normal (unencrypted) text files are assumed. Note that this entry is only relevant for Slater-Koster based DFTB and not used by the extended tight-binding model Hamiltonians.

`repulsion: no|partial|yes`
Specifies whether the parameter set has repulsive potentials for all pairs of elements. Parameter sets that do not have repulsive potentials (e.g. QUASINANO2013.1) cannot be used in geometry optimizations, molecular dynamics or frequency calculations. However, they can still be used in single point calculations, e.g. for UV/Vis absorption spectra of molecules or band structures of solids. Some parameter sets (e.g. DFTB.org/halorg-0-1) have most, *but not quite all* repulsive potentials. If `repulsion` is set to `partial`, DFTB will allow calculations with run-types normally requiring repulsive potentials and will only print a warning about which pairs are missing. It is then the user's responsibility to ensure that element pairs for which the repulsion is missing do not get too close during the calculation. If the `repulsion` entry is not found, DFTB will assume that there are repulsive potentials for all element pairs.

`spin_polarization: no|yes`
Whether the parameter set supports unrestricted calculations. The default value is `no`.

`orbital_dependence: [ noldep, ldep ]`
Whether the parameter set supports an atomic and/or shell-resolved SCC cycle. If only one of the two is supported, the enclosing `[ ]` can be dropped and the `default_orbital_dependence` entry (see below) does not need to be specified. If the `orbital_dependence` key is not found, DFTB assumes that the parameter set only supports atomic SCC cycles.

default_orbital_dependence: noldep|ldep
The default mode for the SCC cycle.

dispersion: [uff, ulg, d2, d3-bj, d4]
A comma-separated list of London dispersion corrections supported by the parameter set. If only one method is supported, the enclosing `[ ]` can be dropped and the `default_dispersion` entry (see below) does not need to be specified.

default_dispersion: uff|ulg|d2|d3-bj|d4
The default dispersion method to be used if the user enables dispersion but does not specify a method explicitly. If the `default_dispersion` entry is not found and more than one method is supported according to `dispersion` entry, **no** dispersion correction will be used by default. The user then has to select a dispersion method explicitly in the input file.

In addition to specifying the parameter set's capabilities, the `metainfo.yaml` file should also contain references to the scientific publication describing the parameter set:

```
url: https://www.scm.com

reference: |
  M. Wahiduzzaman, A. F. Oliveira, P. Philipsen, L. Zhechkov, E. van Lenthe, H. Witek,
↪ T. Heine
  "DFTB Parameters for the Periodic Table: Part 1, Electronic Structure",
  J. Chem. Theory Comput., 9, 2013, 4006-4017, DOI: 10.1021/ct4004959

short_reference: J. Chem. Theory Comput., 9, 2013, 4006-4017
```

All these entries are optional and at the moment only the `reference` entry is read by DFTB (and reproduced verbatim in its output). Note that the pipe symbol `|` is necessary to start a multiline entry (with preserved line breaks) and that the following lines have to be indented by at least one space.

7.2 Slater-Koster based DFTB

The most popular parameter sets for Slater-Koster based DFTB are *distributed with the AMS package* (page 68). Other parameter sets can easily be *added* (page 70).

Often parameter files are designed for a specific purpose, which may be different from your application, and therefore may not give the desired accuracy. Note that parameter files coming from different parameter sets are in general not compatible with each other and should not be mixed.

Additional licenses may be required to use some of the distributed parameter sets. Please contact us at license@scm.com for details.

7.2.1 Available parameter sets

DFTB.org

The DFTB implementation shipped by SCM provides the most up-to-date parameter sets available on the DFTB.org website. The following sets are currently shipped:

- 3ob-3-1 (Br, C, Ca, Cl, F, H, I, K, Mg, N, Na, O, P, S, Zn): general purpose set for the DFTB3 method
- mio-1-1 (H, C, N, O, S, P): for bio and organic molecules with SCC-DFTB
- 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, we ship the following specific purpose parameter sets:

- 3ob-freq: modified 3ob parameters for a better description of vibrational frequencies
- 3ob-hhmod: modified H-H for 3ob (for a better description of H2)
- 3ob-nhmod: modified N-H for 3ob (improves sp3-N proton affinities)
- 3ob-ophyd: modified O-P for 3ob (improves description of pentavalent phosphorus species)
- auorg (Au + mio): for gold-thiolate compounds
- borg (B, H): boron systems (solids and molecules)
- chalc-0-1 (As + mio): for chalcogenide glasses
- halorg (F, Cl, Br, I + mio): for halogens
- hyb-0-1 (Ag, Ga, As, Si + mio): for organic and inorganic hybrid systems
- magsil (Mg, Si, O, H, Mg): for chrisotyle nanotubes
- miomod-hh: contains a modified parameter set for H2
- miomod-nh: contains a modified parameter set for N-H to improve N-H binding energies
- siband (Si, O, H): electronic parameters for accurate silicon and silicon dioxide band structures
- tiorg-0-1 (Ti + mio): for Ti bulk, TiO2 bulk, TiO2 surfaces, and TiO2 with organic molecules
- trans3d-0-1 (Sc, Ti, Fe, Co, Ni + mio): transition metal elements for biological systems
- znorg-0-1 (Zn + mio): for Zn bulk, ZnO bulk, ZnO surfaces, and ZnO with organic molecules

We recommend visiting the DFTB.org (https://www.dftb.org) website for more detailed information about each set. We are committed to shipping all DFTB.org parameter sets in their latest version. If you miss one of the DFTB.org parameter sets in our distribution, please contact us at support@scm.com. Please note that our implementation of DFTB currently does not support parameter sets containing f-functions, such as the "rare" set.

QUASINANO

The *QUASINANO2013.1* (page 76) set of DFTB parameter files available in the AMS package is designed by Mohammad Wahiduzzaman et al. and contains parameters for a large part of the periodic table (no f-elements). Note that the QUASINANO2013.1 set only contains the electronic part of the interaction, so that only the spectrum for a given geometry can be calculated, but no total energy, and thus also no forces. These parameters can be used in TD-DFTB calculations, for example.

The *QUASINANO2015* (page 76) parameter set extends the QUASINANO2013.1 parameter set, and includes terms that are needed to compute the total energy and its gradient.

Dresden

The so-called Dresden set of DFTB parameter files available in the AMS 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* (page 76). These parameter files are kept in the directory $AMSHOME/atomicdata/DFTB/Dresden.

7.2.2 Files in the resources directory

This section contains a technical description of all the files and their formats which together constitute a DFTB parameter set. The parameter sets *distributed with the AMS package* (page 68) are ready to be used out of the box, and no knowledge about their format should be necessary to run DFTB calculations. However, users who want to use their own DFTB parameters with our implementation will need to package them in a way that is understood by it.

DFTB parameter sets in the AMS package have up to four components: The *Slater-Koster files* (page 70), the *metainfo.yaml file* (page 67) and optionally some *additional .yaml files* (page 70) as well as *binary .rkf files containing the basis functions* (page 71).

Slater-Koster files

Most of the data constituting a DFTB parameter set is contained in the so-called Slater-Koster files. These are typically text files with the file extension `.skf`. For legal reasons, some parameter sets that are shipped with AMS have encrypted Slater-Koster files, in which case their file extension is `.ske`.

There is generally a Slater-Koster file per **pair of elements** supported by the parameter set, e.g. for a set supporting the four elements C,H,O,N there will be 16 Slater-Koster files in total. The Slater-Koster file names contain the symbols of the elements, e.g. `C-H.skf`, `H-O.skf` and `C-C.skf`. Note that files for both element orders, e.g. `C-H.skf` and `H-C.skf`, are needed and differ in general. The Slater-Koster files contain the matrix elements of the Hamiltonian operator and the overlap between basis functions centered on two atoms, tabulated for different distances. They also contain a description of a repulsive potential between the two atoms. Furthermore the one-element Slater-Koster files (like `H-H.skf` and `C-C.skf`) contain some information about the individual atom, e.g. orbital energies of the atomic orbitals. A detailed description (https://www.dftb.org/parameters/introduction.html) of the Slater-Koster file format can be found at DFTB.org (https://www.dftb.org).

Additional .yaml files

The Slater-Koster file format (https://www.dftb.org/parameters/introduction.html) is relatively old and very inflexible. Over the years extensions of the DFTB method (e.g. spin-polarization, DFTB3, dispersion corrections) have been developed that require parameters which do not have a place in the Slater-Koster files. In the AMS implementation of DFTB, these parameters are stored in additional `.yaml` files in the resources directory of the parameter set: The `additional_parameters.yaml` file as well as per element `.yaml` files, e.g. `H.yaml` and `C.yaml`.

The `additional_parameters.yaml` file contains anything that applies to the entire parameter set and does not depend on the individual elements. At the moment this is:

`grimme_d3bj_params: s6 s8 a1 a2`
The fitting parameters for Grimme's D3-BJ dispersion correction. This entry is mandatory if the `metainfo.yaml` file lists D3-BJ as a supported dispersion correction method.

`grimme_d4_params: s6 s8 a1 a2`
The fitting parameters for Grimme's D4 dispersion correction. This entry is mandatory if the `metainfo.yaml` file lists D4 as a supported dispersion correction method.

zeta_Hcorr: zeta
A single number `zeta` used in the HX-damping usually applied in DFTB3 calculations.

The per element `.yaml` files may contain the following entries:

hubbard: U_atom
The atomic Hubbard parameter used in a normal, atomic SCC cycle is specified in the element's `.yaml` file as the `hubbard` entry. It is quite surprising that such a commonly used parameter does not have its place in the Slater-Koster files, which only hold the shell-dependent Hubbard parameters. For atomic SCC cycles it is common practice to use the Hubbard parameter of the s-shell as the atomic Hubbard parameter, even though the two values are not strictly related. For consistency with other DFTB implementations, AMS DFTB will do the same if the atomic Hubbard parameter is not found in the element's `.yaml` file. However, it will also notify the user about this potentially questionable behavior.

hubbard_derivative: dUdq
The derivative of the atomic Hubbard parameter with respect to the atomic charge. This information is required to perform DFTB3 calculations.

magnetic_hubbard and magnetic_hubbard_ldep
The magnetic Hubbard parameters (often abbreviated W in the literature). These are required for unrestricted calculations and TD-DFTB singlet-triplet excitations. Depending on whether the parameter set allows atomic and/or shell resolved SCC cycles, the magnetic Hubbard parameter is given as a single number and/or a small matrix:

```
magnetic_hubbard: W_atom

magnetic_hubbard_ldep: >
    W_ss  W_sp
    W_ps  W_pp
```

The size of the matrix is determined by the number of basis functions on the element. Note that the > is essential to start a multiline entry (in which line breaks are ignored).

Basis function information in .rkf files

Many parameter sets additionally have per element `.rkf` files in the resources directory, e.g. `H.rkf` and `C.rkf`. These binary files, which can be opened in the GUI with KFBrowser, contain information about the basis functions used to calculate the matrix elements in the Slater-Koster files. While this information is not needed to perform the DFTB calculation itself, it is used by the GUI in order to visualize properties like molecular orbitals or densities in AMSview.

7.3 Extended tight-binding (xTB)

The AMS package comes with the GFN1-xTB parameterization of the extended tight-binding Hamiltonian. This is the parameterization published in the original article on GFN1-xTB, which is optimized for accurate geometries, frequencies and non-covalent interactions.

In contrast to Slater-Koster based DFTB, the extended tight-binding (xTB) method does not store precalculated matrix elements in Slater-Koster files. Instead there is a parameter file which contains information about the basis functions themselves, which is used to calculate matrix elements at run-time. The entire parameterization of GFN1-xTB is stored in simple text files found in `$AMSHOME/atomicdata/DFTB/GFN1-xTB`. Expert users can copy this directory, modify the parameterization to their needs, and use the *ResourcesDir* (page 10) keyword to load their modified parameterization.

elements.xtbpar
Contains most the element specific parameters, e.g. the Hubbard parameters and their derivative, as well as the parameters used for the repulsive potential.

basis.xtbpar
Contains the definition of the used basis functions. Note that one can add or remove basis functions for an element by adding or deleting lines in this file, as long as there is at most one set of basis functions per angular momentum for each element. For example one can not have two sets of p-functions with a different main quantum number on an atom. (The only exception here is hydrogen, which has both a `1s` and `2s` function. Hydrogen is treated in a special way in the GFN1-xTB implementation in AMS, which allows this. However, one should not change the hydrogen basis by editing the `basis.xtbpar` file. DFTB will refuse to run if this is done.)

atomic_configurations.xtbpar
Contains the electron configurations of the isolated atoms.

electronegativity.xtbpar
Contains the Pauling electronegativities for all elements.

globals.xtbpar
Contains the global parameters of the method, see Table 2 of the GFN1-xTB article.

metals.xtbpar
This file defines which elements are considered metals. (The coordination induced scaling of the atomic energy levels is only used for nonmetals.)

CHAPTER

EIGHT

REQUIRED CITATIONS

When you publish results in the scientific literature that were obtained with programs in the package, you are required to include references to the program package with the appropriate release number, and a few key publications.

In addition to these general references, references to special features are mandatory if you have used them.

8.1 General references

For calculations with the Density Functional Tight Binding (DFTB) engine:
AMS DFTB 2026.1, SCM, Theoretical Chemistry, Vrije Universiteit, Amsterdam, The Netherlands, https://www.scm.com. Optionally, you may add the following list of authors and contributors: R. Rüger, A. Yakovlev, P. Philipsen, S. Borini, P. Melix, A.F. Oliveira, M. Franchini, T. van Vuren, T. Soini, M. de Reus, M. Ghorbani Asl, T. Q. Teodoro, D. McCormack, S. Patchkovskii, T. Heine.

For TD-DFTB, cite:
R. Rüger, E. van Lenthe, Y. Lu, J. Frenzel, T. Heine, and L. Visscher, *Efficient Calculation of Electronic Absorption Spectra by Means of Intensity-Selected Time-Dependent Density Functional Tight Binding*, J. Chem. Theory Comp., 2015, 11 (1), pp 157-167 (https://doi.org/10.1021/ct500838h).

For DFTB-NEGF, cite:
Mahdi Ghorbani-Asl, *Electronic transport through two-dimensional transition-metal chalcogenides*, PhD Thesis (2014) (https://opus.jacobs-university.de/frontdoor/index/index/docId/478)

8.2 Parameter references

If you use one of the included parameter sets you must also add the proper reference for it.

QUASINANO2015
A.F. Oliveira, P. Philipsen, T. Heine. *DFTB Parameters for the Periodic Table, Part 2: Energies and Energy Gradients from Hydrogen to Calcium*, Journal of Chemical Theory and Computation 11 (11), pp 5209–5218 (2015) (https://doi.org/10.1021/acs.jctc.5b00702)

QUASINANO2013.1
M. Wahiduzzaman, A.F. Oliveira, P.H.T. Philipsen, L. Zhechkov, E. van Lenthe, H.A. Witek, T. Heine, *DFTB Parameters for the Periodic Table: Part 1, Electronic Structure*, Journal of Chemical Theory and Computation 9, 4006 (2013) (https://doi.org/10.1021/ct4004959)

Dresden (same origin as matsci-0-3 parameters in DFTB.org)
J. Frenzel, A. F. Oliveira, N. Jardillier, T. Heine, 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

J. Frenzel, A. F. Oliveira, H. A. Duarte, T. Heine, G. Seifert, *Structural and electronic properties of bulk gibbsite and gibbsite surfaces*, Z. Anorg. Allg. Chem. 631, 1267-1271 (2005) (https://doi.org/10.1002/chin.200529002)

L. Guimaraes, A. N. Enyashin, J. Frenzel, T. Heine, H. A. Duarte, G. Seifert, *Imogolite Nanotubes: Stability, electronic and mechanical properties*, Nano 1, 362-368 (2007) (https://doi.org/10.1021/nn700184k)

R. Luschtinetz, A. F. Oliveira, J. Frenzel, J. Joswig, G. Seifert, H. A. Duarte, *Adsorption of phosphonic and ethylphosphonic acid on aluminum oxide surfaces*, Surf. Sci. 602, 1347-1359 (2008) (https://doi.org/10.1016/j.susc.2008.01.035)

R. Luschtinetz, J. Frenzel, T. Milek, G. Seifert, *Adsorption of phosphonic acid at the TiO2 anatase (101) and rutile (110) surface*, J. Phys. Chem. C 113, 5730-5740 (2009) (https://doi.org/10.1021/jp8110343)

DFTB.org

Required citations for the various DFTB.org parameter sets can be found on the official DFTB webpage: DFTB.org (https://www.dftb.org).

GFN1-xTB

S. Grimme, C. Bannwarth, P. Shushkov, *A Robust and Accurate Tight-Binding Quantum Chemical Method for Structures, Vibrational Frequencies, and Noncovalent Interactions of Large Molecular Systems Parametrized for All spd-Block Elements (Z = 1-86)*, J. Chem. Theory Comput., 2017, 13 (5), pp 1989–2009 (https://doi.org/10.1021/acs.jctc.7b00118)

CHAPTER

NINE

REFERENCES

9.1 Slater-Koster based DFTB

9.1.1 General Description

D. Porezag, T. Frauenheim, T. Köhler, G. Seifert, R. Kaschner, *Construction of tight-binding-like potentials on the basis of density-functional theory: Application to carbon*, Phys. Rev. B 51, 12947-12957 (1995) (https://doi.org/10.1103/PhysRevB.51.12947)

G. Seifert, D. Porezag, T. Frauenheim, *Calculations of molecules, clusters, and solids with a simplified LCAO-DFT-LDA scheme*, Int. J. Quantum Chem. 58, 185-192 (1996) (https://doi.org/10.1002/(SICI)1097-461X(1996)58:2%3C185::AID-QUA7%3E3.0.CO;2-U)

M. Elstner, D. Porezag, G. Jungnickel, J. Elsner, M. Haugk, T. Frauenheim, S. Suhai, and G. Seifert, *Self-consistent charge density functional tight-binding method for simulation of complex material properties*, Physical Review B 58, 7260 (1998) (https://link.aps.org/doi/10.1103/PhysRevB.58.7260)

T. Frauenheim, G. Seifert, M. Elstner, Z. Hajnal, G. Jungnickel, D. Porezag, S. Suhai, and 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) (https://onlinelibrary.wiley.com/doi/10.1002/(SICI)1521-3951(200001)217:1%3C41::AID-PSSB41%3E3.0.CO;2-V/abstract)

M. Elstner, T. Frauenheim, E. Kaxiras, G. Seifert, and S. Suhai, *A self-consistent charge density-functional based tight-binding scheme for large biomolecules*, Physica Status Solidi (b) 217, 357 (2000) (https://onlinelibrary.wiley.com/doi/10.1002/(SICI)1521-3951(200001)217:1%3C357::AID-PSSB357%3E3.0.CO;2-J/abstract)

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) (https://doi.org/10.1039/B105782K)

T. Frauenheim, G. Seifert, M. Elstner, T. Niehaus, C. Kohler, M. Armkreutz, M. Sternberg, Z. Hajnal, A. di Carlo, and S. Suhai, *Atomistic Simulations of complex materials: ground and excited state properties*, Journal of Physics: Condensed Matter 14, 3015 (2002) (https://www.iop.org/EJ/abstract/0953-8984/14/11/313)

M. Gaus, Q. Cui, and M. Elstner, *DFTB3: Extension of the Self-Consistent-Charge Density-Functional Tight-Binding Method (SCC-DFTB)*, Journal of Chemical Theory and Computation 7, 931 (2011) (https://pubs.acs.org/doi/abs/10.1021/ct100684s)

T. A. Niehaus, S. Suhai, F. Della Sala, P. Lugli, M. Elstner, G. Seifert, and Th. Frauenheim, *Tight-binding approach to time-dependent density-functional response theory*, Phys. Rev. B 63, 085108 (2001) (https://doi.org/10.1103/PhysRevB.63.085108)

D. Heringer, T. A. Niehaus, M. Wanko, Th. Frauenheim, *Analytical excited state forces for the time-dependent density-functional tight-binding method*, J. Comput. Chem., 28: 2589-2601 (https://doi.org/10.1002/jcc.20697)

9.1.2 Parameter sets

QUASINANO2013.1

The DFTB parameter files in $AMSHOME/atomicdata/DFTB/QUASINANO2013.1 are distributed with the AMS package. These are parameters only for the electronic part of the DFTB method that covers almost the complete periodic table (no f-elements). No forces can be calculated. These parameters can be used in TD-DFTB calculations, for example.

M. Wahiduzzaman, A.F. Oliveira, P.H.T. Philipsen, L. Zhechkov, E. van Lenthe, H.A. Witek, T. Heine, *DFTB Parameters for the Periodic Table: Part 1, Electronic Structure*, Journal of Chemical Theory and Computation 9, 4006 (2013) (https://doi.org/10.1021/ct4004959)

9.1.3 QUASINANO2015

The DFTB parameter files in $AMSHOME/atomicdata/DFTB/QUASINANO2015 are distributed with the AMS package. The QUASINANO2015 parameter set extends the QUASINANO2013.1 parameter set, and includes terms that are needed to compute the total energy and its gradient.

A. F. Oliveira, P. Philipsen, T. Heine, *DFTB Parameters for the Periodic Table, Part 2: Energies and Energy Gradients from Hydrogen to Calcium*, Journal of Chemical Theory and Computation 11 (11), pp 5209–5218 (2015) (https://doi.org/10.1021/acs.jctc.5b00702)

9.1.4 Dresden

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

General reference for the construction of all integral tables in $AMSHOME/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 fr Anorganische und Allgemeine Chemie 631, 1267 (2005) (https://doi.org/10.1002/zaac.200500051)

For construction and application of integral tables for Al-Si-O-H: L. Guimares, A. N. Enyashin, J. Frenzel, T. Heine, H. A. Duarte, and G. Seifert, *Imogolite Nanotubes: Stability, electronic and mechanical properties*, Nano 1, 362 (2007) (https://doi.org/10.1021/nn700184k)

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) (https://doi.org/10.1016/j.susc.2008.01.035)

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) (https://doi.org/10.1021/jp8110343)

9.1.5 DFTB.org

For detailed information, please visit the official DFTB website: www.dftb.org (https://www.dftb.org/parameters/). Detailed references of each specific parameter set are available in the corresponding *metainfo.yaml* file.

9.2 Extended tight-binding (xTB)

S. Grimme, C. Bannwarth, P. Shushkov, *A Robust and Accurate Tight-Binding Quantum Chemical Method for Structures, Vibrational Frequencies, and Noncovalent Interactions of Large Molecular Systems Parametrized for All spd-Block Elements (Z = 1-86)*, J. Chem. Theory Comput., 2017, 13 (5), pp 1989–2009 (https://doi.org/10.1021/acs.jctc.7b00118)

9.3 External programs and Libraries

Third-party software used in the 2026.1 version of the Amsterdam Modeling Suite can be found in the file titled “third-party-software.txt” in the root of your AMS installation.

CHAPTER

TEN

EXAMPLES

The *$AMSHOME/examples/dftb* directory contains many example files that cover various DFTB options.

10.1 Model Hamiltonians

10.1.1 Example: SCC-DFTB aspirin

Download SP_aspirin_SCC.run

```
#!/bin/sh

$AMSBIN/ams << eor

Task SinglePoint

Engine DFTB
   Model SCC-DFTB
   ResourcesDir Dresden
   SCC
       Iterations 200
       Converge charge=1.0e-8
   End
   DispersionCorrection Auto
EndEngine

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
```

(continues on next page)

(continued from previous page)

```
        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

eor
```

10.1.2 Example: Smeared Fermi-Dirac occupations

Download SP_aspirin_fermi.run

```
#!/bin/sh

$AMSBIN/ams << eor

Task SinglePoint

System
    Atoms [Bohr]
    C     1.05960877221036       -4.29661605444804      -0.634037783371545
    C     3.70944109230336       -4.29661605444804      -0.634037783371545
    C     5.01105409669631       -1.99043606903162      -0.634037783371545
    C     3.65522107511068        0.286575996219979     -0.625747555592921
    C    0.994311181450713        0.336536571102876     -0.603233360526924
    C   -0.284455036107599       -2.00337880211933      -0.623649959779319
    O   -0.281193369103746        2.57767407876400      -0.596339640231410
    C    -2.98801415491818       -2.09305007828785      -0.642322341972295
    O    -4.09533876437070      -0.211143806102700       -1.93967968350738
    C   -0.320197312880997        4.26468724370209        1.32592550924302
    C    0.933554602168619        3.32259649258268        3.72681289050655
    H    5.555390692156803E-002  -6.12434199368563      -0.648191830798464
    H     4.76167074144455       -6.09597720705304      -0.642072898145812
    H     7.09553143269668       -1.96900279721371      -0.645115356938515
    H     4.71261912474754        2.08377152287689      -0.639226970852763
    O    -4.22220929602639       -3.71173831148125       0.403176103305787
    H    -3.05020881565447        1.05602705297610       -2.76001350141399
    O    -1.32857587116215        6.31113951397156        1.15028115060619
    H    0.422139955826862        4.57364609951207        5.33966942939295
    H     3.02803425766575        3.36265301371865        3.55019154354933
    H    10.292508534546246        1.38261705197608        4.22808915708257
    End
End

Engine DFTB
   Model SCC-DFTB
   ResourcesDir Dresden
   Occupation Strategy=fermi temperature=1000
   DispersionCorrection Auto
EndEngine

eor
```

10.1.3 Example: Periodic aspirin

Download SP_aspirin_GP_SCC.run

```
#!/bin/sh

$AMSBIN/ams << eor

Task SinglePoint

Engine DFTB
   Model SCC-DFTB
   ResourcesDir Dresden
   SCC
       Iterations 200
       Converge charge=1.0e-8
   End
EndEngine

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
    Lattice
        40.0   0.0   0.0
         0.0  40.0   0.0
         0.0   0.0  40.0
    End
End

eor
```

10.1.4 Example: GO aspirin DFTB-SCC

Download GO_CG_aspirin_SCC.run

```
#!/bin/sh

$AMSBIN/ams << eor

Task GeometryOptimization

GeometryOptimization
    Method ConjugateGradients
    MaxIterations 1000
    Convergence Gradients=0.0001 Step=1.0e-3
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

Engine DFTB
   Model SCC-DFTB
   ResourcesDir Dresden
   DispersionCorrection Auto
EndEngine

eor
```

10.1.5 Example: DFTB3 CH3COO-

Download SP_CH3COOminus_3rdOrder.run

```
#!/bin/sh

$AMSBIN/ams << eor

Task SinglePoint

Properties
   Gradients true
End

System
    Atoms
      C    0.00000 0.21555 0.00000
      O    1.10974 0.79418 0.00000
      O    -1.15239 0.70584 0.00000
      C    0.04178 -1.35041 0.00000
      H    -0.48762 -1.73081 0.87864
      H    -0.48762 -1.73081 -0.87864
      H    1.06573 -1.72936 0.00000
    End
    Charge -1
End

Engine DFTB
   ResourcesDir DFTB.org/3ob-3-1
   Model DFTB3
   DispersionCorrection UFF
EndEngine

eor
```

10.1.6 Example: DFTB3 dispersion

Download SP_dispersion.run

```
#! /bin/sh

echo "DFTB3 + UFF"

AMS_JOBNAME=UFF $AMSBIN/ams << eor

Task SinglePoint

Properties
   Gradients True
End

System
    Atoms
        C -0.429616 1.62129 0.448687
        C -1.6565 0.945987 0.447048
        C -1.68511 -0.45418 0.44573
```

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```
        C -0.486837 -1.17904 0.446051
        C 0.740044 -0.50373 0.447689
        C 0.768654 0.89643 0.449007
        H -2.57203 1.49981 0.446804
        H -2.6225 -0.97013 0.444478
        H -0.508696 -2.24881 0.445044
        H 1.65557 -1.05755 0.447934
        H 1.70604 1.41239 0.450259
        H -0.40755 2.70106 0.449704
        C -0.380193 0.689878 -2.96514
        C -1.60708 0.014575 -2.96678
        C -1.63569 -1.38559 -2.9681
        C -0.437414 -2.11045 -2.96778
        C 0.789467 -1.43514 -2.96614
        C 0.818077 -0.034982 -2.96482
        H -2.5226 0.568394 -2.96702
        H -2.57307 -1.90154 -2.96935
        H -0.459273 -3.18022 -2.96878
        H 1.705 -1.98896 -2.96589
        H 1.75547 0.480974 -2.96357
        H -0.358124 1.76965 -2.96412
    End
End

Engine DFTB
   ResourcesDir DFTB.org/3ob-3-1
   Model DFTB3
   DispersionCorrection UFF
EndEngine

eor


echo "DFTB3 + ULG"

AMS_JOBNAME=ULG $AMSBIN/ams << eor

Task SinglePoint

Properties
   Gradients True
End

System
    Atoms
        C -0.429616 1.62129 0.448687
        C -1.6565 0.945987 0.447048
        C -1.68511 -0.45418 0.44573
        C -0.486837 -1.17904 0.446051
        C 0.740044 -0.50373 0.447689
        C 0.768654 0.89643 0.449007
        H -2.57203 1.49981 0.446804
        H -2.6225 -0.97013 0.444478
        H -0.508696 -2.24881 0.445044
        H 1.65557 -1.05755 0.447934
        H 1.70604 1.41239 0.450259
        H -0.40755 2.70106 0.449704
```

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```
        C -0.380193 0.689878 -2.96514
        C -1.60708 0.014575 -2.96678
        C -1.63569 -1.38559 -2.9681
        C -0.437414 -2.11045 -2.96778
        C 0.789467 -1.43514 -2.96614
        C 0.818077 -0.034982 -2.96482
        H -2.5226 0.568394 -2.96702
        H -2.57307 -1.90154 -2.96935
        H -0.459273 -3.18022 -2.96878
        H 1.705 -1.98896 -2.96589
        H 1.75547 0.480974 -2.96357
        H -0.358124 1.76965 -2.96412
    End
End

Engine DFTB
   ResourcesDir DFTB.org/3ob-3-1
   Model DFTB3
   DispersionCorrection ULG
EndEngine

eor


echo "DFTB3 + D2"

AMS_JOBNAME=D2 $AMSBIN/ams << eor

Task SinglePoint

Properties
   Gradients True
End

System
    Atoms
        C -0.429616 1.62129 0.448687
        C -1.6565 0.945987 0.447048
        C -1.68511 -0.45418 0.44573
        C -0.486837 -1.17904 0.446051
        C 0.740044 -0.50373 0.447689
        C 0.768654 0.89643 0.449007
        H -2.57203 1.49981 0.446804
        H -2.6225 -0.97013 0.444478
        H -0.508696 -2.24881 0.445044
        H 1.65557 -1.05755 0.447934
        H 1.70604 1.41239 0.450259
        H -0.40755 2.70106 0.449704
        C -0.380193 0.689878 -2.96514
        C -1.60708 0.014575 -2.96678
        C -1.63569 -1.38559 -2.9681
        C -0.437414 -2.11045 -2.96778
        C 0.789467 -1.43514 -2.96614
        C 0.818077 -0.034982 -2.96482
        H -2.5226 0.568394 -2.96702
        H -2.57307 -1.90154 -2.96935
        H -0.459273 -3.18022 -2.96878
```

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```
        H 1.705 -1.98896 -2.96589
        H 1.75547 0.480974 -2.96357
        H -0.358124 1.76965 -2.96412
    End
End

Engine DFTB
   ResourcesDir DFTB.org/3ob-3-1
   Model DFTB3
   DispersionCorrection D2
EndEngine

eor


echo "DFTB3 + D3-BJ"

AMS_JOBNAME=D3BJ $AMSBIN/ams << eor

Task SinglePoint

Properties
   Gradients True
End

System
    Atoms
        C -0.429616 1.62129 0.448687
        C -1.6565 0.945987 0.447048
        C -1.68511 -0.45418 0.44573
        C -0.486837 -1.17904 0.446051
        C 0.740044 -0.50373 0.447689
        C 0.768654 0.89643 0.449007
        H -2.57203 1.49981 0.446804
        H -2.6225 -0.97013 0.444478
        H -0.508696 -2.24881 0.445044
        H 1.65557 -1.05755 0.447934
        H 1.70604 1.41239 0.450259
        H -0.40755 2.70106 0.449704
        C -0.380193 0.689878 -2.96514
        C -1.60708 0.014575 -2.96678
        C -1.63569 -1.38559 -2.9681
        C -0.437414 -2.11045 -2.96778
        C 0.789467 -1.43514 -2.96614
        C 0.818077 -0.034982 -2.96482
        H -2.5226 0.568394 -2.96702
        H -2.57307 -1.90154 -2.96935
        H -0.459273 -3.18022 -2.96878
        H 1.705 -1.98896 -2.96589
        H 1.75547 0.480974 -2.96357
        H -0.358124 1.76965 -2.96412
    End
End

Engine DFTB
   ResourcesDir DFTB.org/3ob-3-1
   Model DFTB3
```

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```
   DispersionCorrection D3-BJ
EndEngine

eor


echo "DFTB3 + D4"

AMS_JOBNAME=D4 $AMSBIN/ams << eor

Task SinglePoint

Properties
   Gradients True
End

System
    Atoms
        C -0.429616 1.62129 0.448687
        C -1.6565 0.945987 0.447048
        C -1.68511 -0.45418 0.44573
        C -0.486837 -1.17904 0.446051
        C 0.740044 -0.50373 0.447689
        C 0.768654 0.89643 0.449007
        H -2.57203 1.49981 0.446804
        H -2.6225 -0.97013 0.444478
        H -0.508696 -2.24881 0.445044
        H 1.65557 -1.05755 0.447934
        H 1.70604 1.41239 0.450259
        H -0.40755 2.70106 0.449704
        C -0.380193 0.689878 -2.96514
        C -1.60708 0.014575 -2.96678
        C -1.63569 -1.38559 -2.9681
        C -0.437414 -2.11045 -2.96778
        C 0.789467 -1.43514 -2.96614
        C 0.818077 -0.034982 -2.96482
        H -2.5226 0.568394 -2.96702
        H -2.57307 -1.90154 -2.96935
        H -0.459273 -3.18022 -2.96878
        H 1.705 -1.98896 -2.96589
        H 1.75547 0.480974 -2.96357
        H -0.358124 1.76965 -2.96412
    End
End

Engine DFTB
   ResourcesDir DFTB.org/3ob-3-1
   Model DFTB3
   DispersionCorrection D4
EndEngine

eor
```

10.1.7 Example: DFTB3 dispersion periodic

Download SP_dispersion_periodic.run

```
#! /bin/sh

echo "DFTB3 + UFF"

AMS_JOBNAME=UFF $AMSBIN/ams << eor

Task SinglePoint

Properties
   Gradients True
   StressTensor True
End

System
    Atoms
       C  0.0 0.0 0.0
       C  0.0 0.0 -3.355
       C  1.23 0.7101408312 0.0
       C -1.23 -0.7101408311 -3.355
    End
    Lattice
       2.46 0.000000 0
       1.23 2.130422493 0
    End
End

Engine DFTB
   Model SCC-DFTB
   ResourcesDir DFTB.org/3ob-3-1
   DispersionCorrection UFF
   KSpace
     Type Symmetric
     Symmetric KInteg=5
   End
EndEngine

eor


echo "DFTB3 + ULG"

AMS_JOBNAME=ULG $AMSBIN/ams << eor

Task SinglePoint

Properties
   Gradients True
   StressTensor True
End

System
    Atoms
       C  0.0 0.0 0.0
       C  0.0 0.0 -3.355
```

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```
        C  1.23 0.7101408312 0.0
        C -1.23 -0.7101408311 -3.355
    End
    Lattice
        2.46 0.000000 0
        1.23 2.130422493 0
    End
End

Engine DFTB
   Model SCC-DFTB
   ResourcesDir DFTB.org/3ob-3-1
   DispersionCorrection ULG
   KSpace
     Type Symmetric
     Symmetric KInteg=5
   End
EndEngine

eor


echo "DFTB3 + D2"

AMS_JOBNAME=D2 $AMSBIN/ams << eor

Task SinglePoint

Properties
   Gradients True
   StressTensor True
End

System
    Atoms
        C  0.0 0.0 0.0
        C  0.0 0.0 -3.355
        C  1.23 0.7101408312 0.0
        C -1.23 -0.7101408311 -3.355
    End
    Lattice
        2.46 0.000000 0
        1.23 2.130422493 0
    End
End

Engine DFTB
   Model SCC-DFTB
   ResourcesDir DFTB.org/3ob-3-1
   DispersionCorrection D2
   KSpace
     Type Symmetric
     Symmetric KInteg=5
   End
EndEngine

eor
```

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```
echo "DFTB3 + D3-BJ"

AMS_JOBNAME=D3 $AMSBIN/ams << eor

Task SinglePoint

Properties
   Gradients True
   StressTensor True
End

System
    Atoms
       C  0.0 0.0 0.0
       C  0.0 0.0 -3.355
       C  1.23 0.7101408312 0.0
       C -1.23 -0.7101408311 -3.355
    End
    Lattice
       2.46 0.000000 0
       1.23 2.130422493 0
    End
End

Engine DFTB
   Model SCC-DFTB
   ResourcesDir DFTB.org/3ob-3-1
   DispersionCorrection D3-BJ
   KSpace
     Type Symmetric
     Symmetric KInteg=5
   End
EndEngine

eor


echo "DFTB3 + D4"

AMS_JOBNAME=D4 $AMSBIN/ams << eor

Task SinglePoint

Properties
   Gradients True
   StressTensor True
End

System
    Atoms
       C  0.0 0.0 0.0
       C  0.0 0.0 -3.355
       C  1.23 0.7101408312 0.0
       C -1.23 -0.7101408311 -3.355
    End
```

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```
    Lattice
       2.46 0.000000 0
       1.23 2.130422493 0
    End
End

Engine DFTB
   Model SCC-DFTB
   ResourcesDir DFTB.org/3ob-3-1
   DispersionCorrection D4
   KSpace
     Type Symmetric
     Symmetric KInteg=5
   End
EndEngine

eor
```

10.1.8 Example: Unpaired electrons cyclobutadiene

Download SP_Cyclobutadiene_triplet_spin.run

```
#!/bin/sh

$AMSBIN/ams << eor

Task SinglePoint

Properties
   Gradients true
End

System
    Atoms
        C         0.73022709  0.73022709  0.00000000
        C        -0.73022709  0.73022709  0.00000000
        C        -0.73022709 -0.73022709  0.00000000
        C         0.73022709 -0.73022709  0.00000000
        H         1.50475790  1.50475790  0.00000000
        H        -1.50475790  1.50475790  0.00000000
        H        -1.50475790 -1.50475790  0.00000000
        H         1.50475790 -1.50475790  0.00000000
    End
End

Engine DFTB
   Model SCC-DFTB
   ResourcesDir DFTB.org/mio-1-1
   SCC
      Iterations 200
      Unrestricted Yes
   End
   Occupation Strategy=aufbau
   UnpairedElectrons 2
EndEngine
```

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```
eor
```

10.1.9 Example: Spin polarized O2

Download SP_o2_spin.run

```
#!/bin/sh

echo ''
echo 'Reality: O2 triplet state'
echo '+++++++++++++++++++++++++'
echo ''

AMS_JOBNAME=O2_triplet $AMSBIN/ams << eor

Task SinglePoint

Properties
   Gradients true
End

System
    Atoms
        O         0.00000000   0.00000000   0.00000000
        O         1.20000000   0.00000000   0.00000000
    End
End

Engine DFTB
   Model SCC-DFTB
   ResourcesDir DFTB.org/mio-1-1
   SCC
       Unrestricted Yes
   End
   UnpairedElectrons 2
   Occupation Strategy=aufbau
EndEngine

eor


echo ''
echo 'Technical test: O2 singlet as a restricted and unrestricted calculation should␣
↪give the same result'
echo
↪'++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
↪'
echo ''

AMS_JOBNAME=O2_restricted $AMSBIN/ams << eor

Task SinglePoint

Properties
```

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```
   Gradients true
End

System
    Atoms
        O         0.00000000  0.00000000  0.00000000
        O         1.20000000  0.00000000  0.00000000
    End
End

Engine DFTB
   Model SCC-DFTB
   ResourcesDir DFTB.org/mio-1-1
   SCC
       Unrestricted No
   End
   UnpairedElectrons 0
   Occupation Strategy=aufbau
EndEngine

eor

AMS_JOBNAME=O2_unrestricted $AMSBIN/ams << eor

Task SinglePoint

Properties
   Gradients true
End

System
    Atoms
        O         0.00000000  0.00000000  0.00000000
        O         1.20000000  0.00000000  0.00000000
    End
End

Engine DFTB
   Model SCC-DFTB
   ResourcesDir DFTB.org/mio-1-1
   SCC
       Unrestricted Yes
   End
   UnpairedElectrons 0
   Occupation Strategy=aufbau
EndEngine

eor
```

10.1.10 Example: Orbital dependent spin-polarized CH

Download SP_CH_spin_ldep.run

```
#!/bin/sh

$AMSBIN/ams << eor

Task SinglePoint

Properties
   Gradients True
End

System
    Atoms
        H        -0.500000      0.000000  0.000000
        C         0.5           0.000000  0.000000
    End
End

Engine DFTB
   Model SCC-DFTB
   ResourcesDir DFTB.org/mio-1-1
   SCC
       Iterations 100
       Converge charge=1e-7
       OrbitalDependent Yes
       Unrestricted Yes
   End
   UnpairedElectrons 3
EndEngine

eor
```

10.1.11 Example: NaCl fractional coordinates

Download NaCl_natural.run

```
#!/bin/sh

$AMSBIN/ams << eor

Task SinglePoint

Properties
   Gradients True
End

System
   ATOMS
      Na  0   0   0
      Cl  0.5 0.5 0.5
   END
   FractionalCoords yes
   Lattice
```

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```
      0.000 2.285 2.285
      2.285 0.000 2.285
      2.285 2.285 0.000
   End
End

Engine DFTB
   ResourcesDir Demo
   Model DFTB0
   DispersionCorrection Auto
   KSpace
     Type Symmetric
     Symmetric KInteg=3
   End
EndEngine

eor
```

10.1.12 Example: NaCl slab

Download SP_NaClSlab_SCC.run

```
#! /bin/sh

$AMSBIN/ams << eor

Task SinglePoint

Properties
   Gradients True
End

System
   Atoms
      Na 0 0 0
      Cl 0 2.23 0
      Na 0 0 40
      Cl 0 2.23 40
   End
   Charge 0
   Lattice
      6 0 0
      0 6 0
   End
End

Engine DFTB
   Model SCC-DFTB
   ResourcesDir Demo
   useSymmetry yes
   KSpace
     Type Symmetric
     Symmetric KInteg=8
   End
   Technical
```

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```
      Screening
         rMadel 40
         DirectionalScreening yes
      End
   End
EndEngine

eor
```

10.1.13 Example: OH- noSCC

Download SP_OHminus_noSCC.run

```
#!/bin/sh

$AMSBIN/ams << eor

Task SinglePoint

Properties
   Gradients True
End

System
    Atoms
        H         0.000000      0.000000   0.000000
        O         0.98          0.000000   0.000000
    End
    Charge -1
End

Engine DFTB
   ResourcesDir Dresden
   Model DFTB0
   DispersionCorrection Auto
EndEngine

eor
```

10.1.14 Example: OH- SCC

Download SP_OHminus_SCC.run

```
#!/bin/sh

$AMSBIN/ams << eor

Task SinglePoint

Properties
   Gradients True
End
```

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```
System
    Atoms
        H         0.000000     0.000000   0.000000
        O         0.8          0.000000   0.000000
    End
    Charge -1
End

Engine DFTB
   Model SCC-DFTB
   ResourcesDir Dresden
   DispersionCorrection Auto
EndEngine

eor
```

10.1.15 Example: Single Point H2 MOF

Download SP_H2_MOF.run

```
#! /bin/sh

$AMSBIN/ams << eor

Task SinglePoint

System
    Atoms
        H 0.38282500  0.00000000   5.60000000000
        H -0.3828250  0.00000000  5.60000000000
        O 0.00000000 0.00000000 0.00000000
        Zn 0.00000000 0.00000000 2.07033600
        Zn 1.95221700 0.00000000 -0.68941100
        Zn -0.97572100 -1.69053600 -0.69042000
        Zn -0.97586100 1.69056900 -0.69039900
        O -1.70780800 2.79082900 0.92154600
        C -1.54771500 2.71021500 2.20701300
        O -0.89790100 1.74274000 2.77774100
        H -1.98764400 3.50247700 2.84643000
        O 0.35029100 2.87568900 -1.77812900
        C 1.55929600 2.69704500 -2.21508600
        O 2.26769700 1.64993000 -1.92250000
        H 2.00771600 3.47493600 -2.86611400
        O -2.56050700 1.13810100 -1.92604400
        C -3.11277300 0.00091100 -2.21896700
        O -2.66351100 -1.13524300 -1.78104000
        H -4.00986100 0.00010300 -2.87107900
        O -1.56072200 -2.87595200 0.92089600
        C -1.56969400 -2.69789300 2.20650400
        O -1.05725600 -1.65122100 2.77740000
        H -2.03424700 -3.47599200 2.84591000
        O 0.29643200 -2.78842800 -1.92295400
        C 1.55740800 -2.69772600 -2.21571900
        O 2.31610200 -1.73959500 -1.77889300
        H 2.00724200 -3.47483300 -2.86672100
```

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```
        O 1.95801500 -0.09214100 2.77853700
        C 3.12091400 -0.01368100 2.20790300
        O 3.27101900 0.08318800 0.92238000
        H 4.02685600 -0.02795200 2.84752500
    End

End

Engine DFTB
   ResourcesDir DFTB.org/znorg-0-1
   Model DFTB0
   DispersionCorrection Auto
EndEngine

eor
```

10.1.16 Example: Single point COF5

Download SP_COF5.run

```
#!/bin/sh

$AMSBIN/ams << eor

Task SinglePoint

System
    Atoms
        B       38.63248800       32.59377000        0.91194600
        C       36.09458800       35.44149000        0.92444600
        C       34.85617800       34.77408000        0.92199600
        C       34.89652800       33.36791000        0.92484600
        C       36.09798800       32.67391000        0.92531600
        C       37.33626800       33.34130000        0.92419600
        C       37.29612800       34.74734000        0.92611600
        H       33.95059800       32.80183000        0.92439600
        H       36.08021800       31.57168000        0.92504600
        H       38.24223800       35.31352000        0.92657600
        H       36.11240200       36.54401000        0.92374600
        C       29.28170700       37.19760000        0.85329600
        C       29.97484700       35.99389000        0.87646600
        C       31.36465700       35.99214000        0.88762600
        C       32.06076700       37.19435000        0.87479600
        O       29.02497700       34.89896000        0.88401600
        O       32.31174700       34.89496000        0.91024600
        O       33.48383700       36.91940000        0.88909600
        O       27.85778700       36.92589000        0.84604600
        B       33.56100700       35.52326000        0.90899600
        C       37.29593700       52.17899000        0.86629600
        C       37.33667700       53.58514000        0.86421600
        C       36.09870700       54.25318000        0.86022600
        C       34.89691700       53.55963000        0.85949600
        C       34.85601700       52.15338000        0.86069600
        C       36.09417700       51.48538000        0.86332600
        H       36.08146700       55.35543000        0.85847600
```

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        H       33.95121700       54.12617000        0.85664600
        H       36.11128700       50.38306000        0.86407600
        H       38.24167700       51.61260000        0.86954600
        C       31.87386700       44.15720700        0.79794600
        C       30.67636700       44.89542800        0.80012600
        C       29.47895800       44.15705700        0.79609600
        C       29.47894800       42.76949400        0.79519600
        C       30.67646700       42.03134900        0.79957600
        C       31.87388700       42.76958800        0.79849600
        H       28.51565800       44.69324600        0.79534600
        H       28.51578800       42.23324900        0.79376600
        H       32.83719700       42.23353100        0.80019600
        H       32.83738700       44.69300100        0.79887600
        C       31.36431700       50.93490000        0.87506600
        C       29.97459800       50.93282000        0.88854600
        C       29.28148800       49.72897000        0.87776600
        C       29.97798800       48.52647000        0.85291600
        C       31.36707700       48.52853000        0.83951600
        C       32.06050700       49.73297000        0.85087600
        O       27.85751800       50.00036000        0.89359600
        O       29.50464800       47.15628500        0.83719600
        O       33.48353700       50.00819000        0.84179600
        O       32.31147700       52.03219000        0.88159600
        O       31.84369700       47.15959500        0.81491600
        O       29.02457800       52.02737000        0.91129600
        B       49.48807800       51.39620000        0.91194600
        B       33.56072700       51.40425000        0.86106600
        B       30.67512700       46.39172500        0.81511600
        C       46.95017800       54.24392000        0.92444600
        C       45.71176800       53.57651000        0.92199600
        C       45.75211800       52.17034000        0.92484600
        C       46.95357800       51.47634000        0.92531600
        C       48.19185800       52.14373000        0.92419600
        C       48.15171800       53.54977000        0.92611600
        H       44.80618800       51.60426000        0.92439600
        H       46.93580800       50.37411000        0.92504600
        H       49.09782800       54.11595000        0.92657600
        H       46.96799200       55.34644000        0.92374600
        C       29.97819800       38.40024300        0.84009600
        C       40.13729700       56.00003000        0.85329600
        C       40.83043700       54.79632000        0.87646600
        C       42.22024700       54.79457000        0.88762600
        C       42.91635700       55.99678000        0.87479600
        C       31.36743700       38.39862600        0.85042600
        O       39.88056700       53.70139000        0.88401600
        O       43.16733700       53.69739000        0.91024600
        O       31.84405700       39.76748000        0.83267600
        O       29.50498800       39.77018800        0.81591600
        O       44.33942700       55.72183000        0.88909600
        O       38.71337700       55.72832000        0.84604600
        B       38.63298700       54.33249000        0.86504600
        B       30.67547700       40.53503300        0.81349600
        B       44.41659700       54.32569000        0.90899600
        C       48.15152700       33.37656000        0.86629600
        C       48.19226700       34.78271000        0.86421600
        C       46.95429700       35.45075000        0.86022600
        C       45.75250700       34.75720000        0.85949600
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        C       45.71160700       33.35095000        0.86069600
        C       46.94976700       32.68295000        0.86332600
        H       46.93705700       36.55300000        0.85847600
        H       44.80680700       35.32374000        0.85664600
        H       46.96687700       31.58063000        0.86407600
        H       49.09726700       32.81017000        0.86954600
        H       41.62620000       58.78560000        4.00763000
        B       75.27970000       41.26000000        4.40091000
        O       76.44790000       47.88460000        4.40233000
        C       72.88540000       44.19030000        0.93922800
        C       72.88540000       42.80270000        0.93832800
        C       74.08290000       42.06460000        0.94270800
        O       73.62880000       52.75230000        4.49871000
        C       72.68820000       37.23080000        0.99642800
        C       73.38130000       36.02710000        1.01960000
        C       75.28040000       42.80280000        0.94162800
        C       42.21990700       32.13247000        0.87506600
        C       40.83018800       32.13039000        0.88854600
        C       40.13707800       30.92654000        0.87776600
        C       40.83357800       29.72404000        0.85291600
        C       42.22266700       29.72610000        0.83951600
        C       42.91609700       30.93054000        0.85087600
        O       38.71310800       31.19793000        0.89359600
        H       71.92210000       44.72650000        0.93847800
        O       44.33912700       31.20576000        0.84179600
        O       43.16706700       33.22976000        0.88159600
        H       71.92230000       42.26650000        0.93689800
        O       39.88016800       33.22494000        0.91129600
        B       60.34366800       32.59377000        0.91194600
        B       44.41631700       32.60182000        0.86106600
        C       63.66180000       58.00260000        4.03379000
        C       57.80576800       35.44149000        0.92444600
        C       56.56735800       34.77408000        0.92199600
        C       56.60770800       33.36791000        0.92484600
        C       57.80916800       32.67391000        0.92531600
        C       59.04744800       33.34130000        0.92419600
        C       59.00730800       34.74734000        0.92611600
        H       55.66177800       32.80183000        0.92439600
        H       57.79139800       31.57168000        0.92504600
        H       59.95341800       35.31352000        0.92657600
        H       57.82358200       36.54401000        0.92374600
        C       65.05090000       58.00470000        4.02039000
        C       50.99288700       37.19760000        0.85329600
        C       51.68602700       35.99389000        0.87646600
        C       53.07583700       35.99214000        0.88762600
        C       53.77194700       37.19435000        0.87479600
        C       76.66470000       50.45790000        4.43829000
        O       50.73615700       34.89896000        0.88401600
        O       54.02292700       34.89496000        0.91024600
        O       75.25050000       39.80070000        0.97580800
        H       75.92730000       34.70460000        1.96327000
        O       55.19501700       36.91940000        0.88909600
        O       49.56896700       36.92589000        0.84604600
        B       49.48857700       35.53006000        0.86504600
        H       40.42870000       58.09420000        0.56339100
        B       55.27218700       35.52326000        0.90899600
        C       59.00711700       52.17899000        0.86629600
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        C       59.04785700       53.58514000        0.86421600
        C       57.80988700       54.25318000        0.86022600
        C       56.60809700       53.55963000        0.85949600
        C       56.56719700       52.15338000        0.86069600
        C       57.80535700       51.48538000        0.86332600
        H       57.79264700       55.35543000        0.85847600
        H       55.66239700       54.12617000        0.85664600
        H       57.82246700       50.38306000        0.86407600
        H       59.95285700       51.61260000        0.86954600
        C       53.58504700       44.15720700        0.79794600
        C       52.38754700       44.89542800        0.80012600
        C       51.19013800       44.15705700        0.79609600
        C       51.19012800       42.76949400        0.79519600
        C       52.38764700       42.03134900        0.79957600
        C       53.58506700       42.76958800        0.79849600
        H       50.22683800       44.69324600        0.79534600
        H       50.22696800       42.23324900        0.79376600
        H       54.54837700       42.23353100        0.80019600
        H       54.54856700       44.69300100        0.79887600
        C       53.07549700       50.93490000        0.87506600
        C       51.68577800       50.93282000        0.88854600
        C       50.99266800       49.72897000        0.87776600
        C       51.68916800       48.52647000        0.85291600
        C       53.07825700       48.52853000        0.83951600
        C       53.77168700       49.73297000        0.85087600
        O       49.56869800       50.00036000        0.89359600
        O       51.21582800       47.15628500        0.83719600
        O       55.19471700       50.00819000        0.84179600
        O       54.02265700       52.03219000        0.88159600
        O       53.55487700       47.15959500        0.81491600
        O       50.73575800       52.02737000        0.91129600
        B       71.19925800       51.39620000        0.91194600
        B       55.27190700       51.40425000        0.86106600
        B       52.38630700       46.39172500        0.81511600
        C       68.66135800       54.24392000        0.92444600
        C       67.42294800       53.57651000        0.92199600
        C       67.46329800       52.17034000        0.92484600
        C       68.66475800       51.47634000        0.92531600
        C       69.90303800       52.14373000        0.92419600
        C       69.86289800       53.54977000        0.92611600
        H       66.51736800       51.60426000        0.92439600
        H       68.64698800       50.37411000        0.92504600
        H       70.80900800       54.11595000        0.92657600
        H       68.67917200       55.34644000        0.92374600
        C       51.68937800       38.40024300        0.84009600
        C       61.84847700       56.00003000        0.85329600
        C       62.54161700       54.79632000        0.87646600
        C       63.93142700       54.79457000        0.88762600
        C       64.62753700       55.99678000        0.87479600
        C       53.07861700       38.39862600        0.85042600
        O       61.59174700       53.70139000        0.88401600
        O       64.87851700       53.69739000        0.91024600
        O       53.55523700       39.76748000        0.83267600
        O       51.21616800       39.77018800        0.81591600
        O       66.05060700       55.72183000        0.88909600
        O       60.42455700       55.72832000        0.84604600
        B       60.34416700       54.33249000        0.86504600
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```
B       52.38665700      40.53503300      0.81349600
B       66.12777700      54.32569000      0.90899600
C       69.86270700      33.37656000      0.86629600
C       69.90344700      34.78271000      0.86421600
C       68.66547700      35.45075000      0.86022600
C       67.46368700      34.75720000      0.85949600
C       67.42278700      33.35095000      0.86069600
C       68.66094700      32.68295000      0.86332600
H       68.64823700      36.55300000      0.85847600
H       66.51798700      35.32374000      0.85664600
H       68.67805700      31.58063000      0.86407600
H       70.80844700      32.81017000      0.86954600
O       71.26400000      50.03360000      1.03673000
O       72.91110000      47.18950000      0.98032800
O       76.89000000      50.04140000      0.98492800
O       75.71790000      52.06540000      1.02473000
H       40.29530000      28.78780000      0.84401700
C       75.46720000      37.22760000      1.01793000
H       42.76340000      28.79140000      0.82026900
H       78.40770000      50.79390000      5.33228000
H       77.19540000      36.89190000      1.94043000
O       72.46180000      50.72530000      4.48101000
C       63.93108700      32.13247000      0.87506600
C       62.54136800      32.13039000      0.88854600
C       61.84825800      30.92654000      0.87776600
C       62.54475800      29.72404000      0.85291600
C       63.93384700      29.72610000      0.83951600
C       64.62727700      30.93054000      0.85087600
O       60.42428800      31.19793000      0.89359600
C       75.28060000      45.62040000      4.38754000
O       66.05030700      31.20576000      0.84179600
O       64.87824700      33.22976000      0.88159600
C       73.38110000      50.96600000      1.03168000
O       61.59134800      33.22494000      0.91129600
B       66.12749700      32.60182000      0.86106600
H       42.91950000      58.02730000      0.51287600
O       75.25020000      47.19280000      0.95804800
O       72.43100000      52.06060000      1.05443000
H       28.73060000      50.75160000      3.43629000
C       74.08320000      44.88200000      4.38351000
B       71.19975700      35.53006000      0.86504600
H       27.53310000      50.06030000     -0.00795049
B       39.82995800      33.28513000      4.35618600
C       37.29205800      36.13285000      4.36868600
C       36.05364800      35.46544000      4.36623600
C       36.09399800      34.05927000      4.36908600
C       37.29545800      33.36527000      4.36955600
C       38.53373800      34.03266000      4.36843600
C       38.49359800      35.43870000      4.37035600
H       35.14806800      33.49319000      4.36863600
H       37.27768800      32.26304000      4.36928600
H       39.43970800      36.00488000      4.37081600
H       37.30987200      37.23537000      4.36798600
C       30.47917700      37.88896000      4.29753600
C       31.17231700      36.68525000      4.32070600
C       32.56212700      36.68350000      4.33186600
C       33.25823700      37.88571000      4.31903600
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```
O      30.22244700      35.59032000      4.32825600
O      33.50921700      35.58632000      4.35448600
O      34.68130700      37.61076000      4.33333600
O      29.05525700      37.61725000      4.29028600
B      34.75847700      36.21462000      4.35323600
C      38.49340700      52.87035000      4.31053600
C      38.53414700      54.27650000      4.30845600
C      37.29617700      54.94454000      4.30446600
C      36.09438700      54.25099000      4.30373600
C      36.05348700      52.84474000      4.30493600
C      37.29164700      52.17674000      4.30756600
H      37.27893700      56.04679000      4.30271600
H      35.14868700      54.81753000      4.30088600
H      37.30875700      51.07442000      4.30831600
H      39.43914700      52.30396000      4.31378600
C      33.07133700      44.84856700      4.24218600
C      31.87383700      45.58678800      4.24436600
C      30.67642800      44.84841700      4.24033600
C      30.67641800      43.46085400      4.23943600
C      31.87393700      42.72270900      4.24381600
C      33.07135700      43.46094800      4.24273600
H      29.71312800      45.38460600      4.23958600
H      29.71325800      42.92460900      4.23800600
H      34.03466700      42.92489100      4.24443600
H      34.03485700      45.38436100      4.24311600
C      32.56178700      51.62626000      4.31930600
C      31.17206800      51.62418000      4.33278600
C      30.47895800      50.42033000      4.32200600
C      31.17545800      49.21783000      4.29715600
C      32.56454700      49.21989000      4.28375600
C      33.25797700      50.42433000      4.29511600
O      29.05498800      50.69172000      4.33783600
O      30.70211800      47.84764500      4.28143600
O      34.68100700      50.69955000      4.28603600
O      33.50894700      52.72355000      4.32583600
O      33.04116700      47.85095500      4.25915600
O      30.22204800      52.71873000      4.35553600
B      50.68554800      52.08756000      4.35618600
B      34.75819700      52.09561000      4.30530600
B      31.87259700      47.08308500      4.25935600
C      48.14764800      54.93528000      4.36868600
C      46.90923800      54.26787000      4.36623600
C      46.94958800      52.86170000      4.36908600
C      48.15104800      52.16770000      4.36955600
C      49.38932800      52.83509000      4.36843600
C      49.34918800      54.24113000      4.37035600
H      46.00365800      52.29562000      4.36863600
H      48.13327800      51.06547000      4.36928600
H      50.29529800      54.80731000      4.37081600
H      48.16546200      56.03780000      4.36798600
C      31.17566800      39.09160300      4.28433600
C      41.33476700      56.69139000      4.29753600
C      42.02790700      55.48768000      4.32070600
C      43.41771700      55.48593000      4.33186600
C      44.11382700      56.68814000      4.31903600
C      32.56490700      39.08998600      4.29466600
O      41.07803700      54.39275000      4.32825600
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      O      44.36480700      54.38875000      4.35448600
      O      33.04152700      40.45884000      4.27691600
      O      30.70245800      40.46154800      4.26015600
      O      45.53689700      56.41319000      4.33333600
      O      39.91084700      56.41968000      4.29028600
      B      39.83045700      55.02385000      4.30928600
      B      31.87294700      41.22639300      4.25773600
      B      45.61406700      55.01705000      4.35323600
      C      49.34899700      34.06792000      4.31053600
      C      49.38973700      35.47407000      4.30845600
      C      48.15176700      36.14211000      4.30446600
      C      46.94997700      35.44856000      4.30373600
      C      46.90907700      34.04231000      4.30493600
      C      48.14723700      33.37431000      4.30756600
      H      48.13452700      37.24436000      4.30271600
      H      46.00427700      36.01510000      4.30088600
      H      48.16434700      32.27199000      4.30831600
      H      50.29473700      33.50153000      4.31378600
      H      77.12510000      35.39640000      5.40756000
      H      75.92700000      52.31300000      0.12108900
      H      76.24370000      42.26670000      0.94332800
      H      27.54810000      36.86590000     -0.06063940
      H      28.74550000      37.55730000      3.38360000
      H      76.24390000      44.72620000      0.94200800
      H      41.49270000      29.47920000      4.28826000
      B      75.27940000      47.11670000      4.40253000
      H      62.00640000      28.78780000      0.84401700
      H      64.47460000      28.79140000      0.82026900
      C      43.41737700      32.82383000      4.31930600
      C      42.02765800      32.82175000      4.33278600
      C      41.33454800      31.61790000      4.32200600
      C      42.03104800      30.41540000      4.29715600
      C      43.42013700      30.41746000      4.28375600
      C      44.11356700      31.62190000      4.29511600
      O      39.91057800      31.88929000      4.33783600
      C      75.28030000      44.19040000      0.94107800
      O      45.53659700      31.89712000      4.28603600
      O      44.36453700      33.92112000      4.32583600
      C      74.58240000      39.12520000      4.42751000
      O      41.07763800      33.91630000      4.35553600
      B      61.54113800      33.28513000      4.35618600
      B      45.61378700      33.29318000      4.30530600
      C      74.77080000      50.96810000      1.01820000
      C      59.00323800      36.13285000      4.36868600
      C      57.76482800      35.46544000      4.36623600
      C      57.80517800      34.05927000      4.36908600
      C      59.00663800      33.36527000      4.36955600
      C      60.24491800      34.03266000      4.36843600
      C      60.20477800      35.43870000      4.37035600
      H      56.85924800      33.49319000      4.36863600
      H      58.98886800      32.26304000      4.36928600
      H      61.15088800      36.00488000      4.37081600
      H      59.02105200      37.23537000      4.36798600
      H      63.20390000      29.47920000      4.28826000
      C      52.19035700      37.88896000      4.29753600
      C      52.88349700      36.68525000      4.32070600
      C      54.27330700      36.68350000      4.33186600
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C     54.96941700     37.88571000     4.31903600
H     65.67210000     29.48280000     4.26451000
O     51.93362700     35.59032000     4.32825600
O     55.22039700     35.58632000     4.35448600
C     74.08280000     44.92860000     0.94325800
C     73.88590000     37.92260000     4.44071000
O     56.39248700     37.61076000     4.33333600
O     50.76643700     37.61725000     4.29028600
B     50.68604700     36.22142000     4.30928600
C     74.57910000     36.71890000     4.46388000
B     56.46965700     36.21462000     4.35323600
C     60.20458700     52.87035000     4.31053600
C     60.24532700     54.27650000     4.30845600
C     59.00735700     54.94454000     4.30446600
C     57.80556700     54.25099000     4.30373600
C     57.76466700     52.84474000     4.30493600
C     59.00282700     52.17674000     4.30756600
H     58.99011700     56.04679000     4.30271600
H     56.85986700     54.81753000     4.30088600
H     59.01993700     51.07442000     4.30831600
H     61.15032700     52.30396000     4.31378600
C     54.78251700     44.84856700     4.24218600
C     53.58501700     45.58678800     4.24436600
C     52.38760800     44.84841700     4.24033600
C     52.38759800     43.46085400     4.23943600
C     53.58511700     42.72270900     4.24381600
C     54.78253700     43.46094800     4.24273600
H     51.42430800     45.38460600     4.23958600
H     51.42443800     42.92460900     4.23800600
H     55.74584700     42.92489100     4.24443600
H     55.74603700     45.38436100     4.24311600
C     54.27296700     51.62626000     4.31930600
C     52.88324800     51.62418000     4.33278600
C     52.19013800     50.42033000     4.32200600
C     52.88663800     49.21783000     4.29715600
C     54.27572700     49.21989000     4.28375600
C     54.96915700     50.42433000     4.29511600
O     50.76616800     50.69172000     4.33783600
O     52.41329800     47.84764500     4.28143600
O     56.39218700     50.69955000     4.28603600
O     55.22012700     52.72355000     4.32583600
O     54.75234700     47.85095500     4.25915600
O     51.93322800     52.71873000     4.35553600
B     72.39672800     52.08756000     4.35618600
B     56.46937700     52.09561000     4.30530600
B     53.58377700     47.08308500     4.25935600
C     69.85882800     54.93528000     4.36868600
C     68.62041800     54.26787000     4.36623600
C     68.66076800     52.86170000     4.36908600
C     69.86222800     52.16770000     4.36955600
C     71.10050800     52.83509000     4.36843600
C     71.06036800     54.24113000     4.37035600
H     67.71483800     52.29562000     4.36863600
H     69.84445800     51.06547000     4.36928600
H     72.00647800     54.80731000     4.37081600
H     69.87664200     56.03780000     4.36798600
C     52.88684800     39.09160300     4.28433600
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C      63.04594700      56.69139000      4.29753600
C      63.73908700      55.48768000      4.32070600
C      65.12889700      55.48593000      4.33186600
C      65.82500700      56.68814000      4.31903600
C      54.27608700      39.08998600      4.29466600
O      62.78921700      54.39275000      4.32825600
O      66.07598700      54.38875000      4.35448600
O      54.75270700      40.45884000      4.27691600
O      52.41363800      40.46154800      4.26015600
O      67.24807700      56.41319000      4.33333600
O      61.62202700      56.41968000      4.29028600
B      61.54163700      55.02385000      4.30928600
B      53.58412700      41.22639300      4.25773600
B      67.32524700      55.01705000      4.35323600
C      71.06017700      34.06792000      4.31053600
C      71.10091700      35.47407000      4.30845600
C      69.86294700      36.14211000      4.30446600
C      68.66115700      35.44856000      4.30373600
C      68.62025700      34.04231000      4.30493600
C      69.85841700      33.37431000      4.30756600
H      69.84570700      37.24436000      4.30271600
H      67.71545700      36.01510000      4.30088600
H      69.87552700      32.27199000      4.30831600
H      72.00591700      33.50153000      4.31378600
O      72.43140000      34.93220000      1.02715000
H      43.96090000      29.48280000      4.26451000
C      74.08320000      43.49450000      4.38261000
C      72.68800000      49.76220000      1.02090000
O      74.10890000      47.88130000      4.42461000
O      75.71820000      34.92820000      1.05338000
O      78.08780000      50.73320000      4.42921000
O      72.91150000      39.80340000      0.95904800
O      76.89030000      36.95260000      1.03223000
O      71.26430000      36.95910000      0.98917800
C      65.12855700      32.82383000      4.31930600
C      63.73883800      32.82175000      4.33278600
C      63.04572800      31.61790000      4.32200600
C      63.74222800      30.41540000      4.29715600
C      65.13131700      30.41746000      4.28375600
C      65.82474700      31.62190000      4.29511600
O      61.62175800      31.88929000      4.33783600
C      73.38450000      48.55970000      0.99604800
O      67.24777700      31.89712000      4.28603600
O      66.07571700      33.92112000      4.32583600
C      74.77350000      48.56170000      0.98264800
O      62.78881800      33.91630000      4.35553600
B      67.32496700      33.29318000      4.30530600
B      74.08190000      40.56820000      0.95662800
C      63.85340000      57.31330000      0.57615000
H      78.39320000      37.58370000      5.38472000
H      61.92230000      58.22880000      0.41410100
C      75.28070000      42.75630000      4.38699000
B      72.39722700      36.22142000      4.30928600
H      44.11700000      58.71860000      3.95712000
C      75.46700000      49.76620000      0.99400800
H      64.29970000      58.27030000      0.34965600
H      77.21000000      50.10220000      1.88799000
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        H      77.12480000      53.00480000       3.56537000
        C      76.47810000      43.49460000       4.38591000
        H      30.01230000      52.97920000       3.45566000
        H      28.81480000      52.28780000       0.01141710
        H      73.11990000      45.41820000       4.38276000
        H      73.12000000      42.95820000       4.38118000
        C      40.92710000      57.14440000       0.68893000
        C      42.31620000      57.14640000       0.67553000
        H      63.11980000      58.92010000       3.85833000
        H      77.44140000      42.95850000       4.38761000
        H      65.49720000      58.96170000       3.79392000
        B      74.08160000      46.42490000       0.95824800
        H      28.81530000      34.66350000       1.79076000
        H      30.01280000      35.35480000       5.23500000
        C      42.12450000      57.83570000       4.13317000
        C      43.51360000      57.83780000       4.11977000
        C      75.96890000      36.71710000       4.47504000
        C      76.66500000      37.91930000       4.46221000
        O      73.62920000      35.62390000       4.47143000
        O      76.91600000      35.61990000       4.49766000
        O      74.10920000      40.49520000       4.40333000
        O      78.08810000      37.64440000       4.47651000
        O      72.46200000      37.65090000       4.43346000
        C      75.97170000      39.12360000       4.43784000
        C      76.47810000      44.88220000       4.38536000
        O      76.44830000      40.49250000       4.42009000
        O      76.91570000      52.75720000       4.46901000
        C      62.46430000      57.31130000       0.58955000
        H      77.44160000      45.41800000       4.38629000
        C      75.96860000      51.65990000       4.46248000
        C      74.57880000      51.65780000       4.47596000
        C      73.38470000      38.43350000       0.98322800
        C      73.88570000      50.45390000       4.46518000
        C      74.58220000      49.25140000       4.44033000
        C      74.77390000      38.43180000       0.99355800
        C      75.97130000      49.25350000       4.42693000
        C      74.77110000      36.02540000       1.03076000
    End
End

Engine DFTB
   Model SCC-DFTB
   ResourcesDir DFTB.org/matsci-0-3
   SCC
       Iterations 200
   End
   DispersionCorrection UFF
EndEngine

eor
```

10.1.17 Example: Single point COF5, 2D

Download SP_COF5_2D.run

```
#! /bin/sh

$AMSBIN/ams << eor

Task SinglePoint

System
    Atoms
        B  -3.51910545  -7.26102175   8.66010017
        C  -6.05700545  -4.41330175   8.67260017
        C  -7.29541545  -5.08071175   8.67015017
        C  -7.25506545  -6.48688175   8.67300017
        C  -6.05360545  -7.18088175   8.67347017
        C  -4.81532545  -6.51349175   8.67235017
        C  -4.85546545  -5.10745175   8.67427017
        H  -8.20099545  -7.05296175   8.67255017
        H  -6.07137545  -8.28311175   8.67320017
        H  -3.90935545  -4.54127175   8.67473017
        H  -6.03919145  -3.31078175   8.67190017
        C -12.86988645  -2.65719175   8.60145017
        C -12.17674645  -3.86090175   8.62462017
        C -10.78693645  -3.86265175   8.63578017
        C -10.09082645  -2.66044175   8.62295017
        O -13.12661645  -4.95583175   8.63217017
        O  -9.83984645  -4.95983175   8.65840017
        O  -8.66775645  -2.93539175   8.63725017
        O -14.29380645  -2.92890175   8.59420017
        B  -8.59058645  -4.33153175   8.65715017
        C  -4.85565645  12.32419825   8.61445017
        C  -4.81491645  13.73034825   8.61237017
        C  -6.05288645  14.39838825   8.60838017
        C  -7.25467645  13.70483825   8.60765017
        C  -7.29557645  12.29858825   8.60885017
        C  -6.05741645  11.63058825   8.61148017
        H  -6.07012645  15.50063825   8.60663017
        H  -8.20037645  14.27137825   8.60480017
        H  -6.04030645  10.52826825   8.61223017
        H  -3.90991645  11.75780825   8.61770017
        C -10.27772645   4.30241525   8.54610017
        C -11.47522645   5.04063625   8.54828017
        C -12.67263545   4.30226525   8.54425017
        C -12.67264545   2.91470225   8.54335017
        C -11.47512645   2.17655725   8.54773017
        C -10.27770645   2.91479625   8.54665017
        H -13.63593545   4.83845425   8.54350017
        H -13.63580545   2.37845725   8.54192017
        H  -9.31439645   2.37873925   8.54835017
        H  -9.31420645   4.83820925   8.54703017
        C -10.78727645  11.08010825   8.62322017
        C -12.17699545  11.07802825   8.63670017
        C -12.87010545   9.87417825   8.62592017
        C -12.17360545   8.67167825   8.60107017
        C -10.78451645   8.67373825   8.58767017
        C -10.09108645   9.87817825   8.59903017
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O -14.29407545  10.14556825   8.64175017
O -12.64694545   7.30149325   8.58535017
O  -8.66805645  10.15339825   8.58995017
O  -9.84011645  12.17739825   8.62975017
O -10.30789645   7.30480325   8.56307017
O -13.12701545  12.17257825   8.65945017
B   7.33648455  11.54140825   8.66010017
B  -8.59086645  11.54945825   8.60922017
B -11.47646645   6.53693325   8.56327017
C   4.79858455  14.38912825   8.67260017
C   3.56017455  13.72171825   8.67015017
C   3.60052455  12.31554825   8.67300017
C   4.80198455  11.62154825   8.67347017
C   6.04026455  12.28893825   8.67235017
C   6.00012455  13.69497825   8.67427017
H   2.65459455  11.74946825   8.67255017
H   4.78421455  10.51931825   8.67320017
H   6.94623455  14.26115825   8.67473017
H   4.81639855  15.49164825   8.67190017
C -12.17339545  -1.45454875   8.58825017
C  -2.01429645  16.14523825   8.60145017
C  -1.32115645  14.94152825   8.62462017
C   0.06865355  14.93977825   8.63578017
C   0.76476355  16.14198825   8.62295017
C -10.78415645  -1.45616575   8.59858017
O  -2.27102645  13.84659825   8.63217017
O   1.01574355  13.84259825   8.65840017
O -10.30753645  -0.08731175   8.58083017
O -12.64660545  -0.08460375   8.56407017
O   2.18783355  15.86703825   8.63725017
O  -3.43821645  15.87352825   8.59420017
B  -3.51860645  14.47769825   8.61320017
B -11.47611645   0.68024125   8.56165017
B   2.26500355  14.47089825   8.65715017
C   5.99993355  -6.47823175   8.61445017
C   6.04067355  -5.07208175   8.61237017
C   4.80270355  -4.40404175   8.60838017
C   3.60091355  -5.09759175   8.60765017
C   3.56001355  -6.50384175   8.60885017
C   4.79817355  -7.17184175   8.61148017
H   4.78546355  -3.30179175   8.60663017
H   2.65521355  -4.53105175   8.60480017
H   4.81528355  -8.27416175   8.61223017
H   6.94567355  -7.04462175   8.61770017
C   0.57786355 -14.50001475   8.54610017
C  -0.61963645 -13.76179375   8.54828017
C  -1.81704545 -14.50016475   8.54425017
C  -1.81705545 -15.88772775   8.54335017
C  -0.61953645 -16.62587275   8.54773017
C   0.57788355 -15.88763375   8.54665017
H  -2.78034545 -13.96397575   8.54350017
H  -2.78021545 -16.42397275   8.54192017
H   1.54119355 -16.42369075   8.54835017
H   1.54138355 -13.96422075   8.54703017
C   0.06831355  -7.72232175   8.62322017
C  -1.32140545  -7.72440175   8.63670017
C  -2.01451545  -8.92825175   8.62592017
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        C  -1.31801545 -10.13075175   8.60107017
        C   0.07107355 -10.12869175   8.58767017
        C   0.76450355  -8.92425175   8.59903017
        O  -3.43848545  -8.65686175   8.64175017
        O  -1.79135545 -11.50093675   8.58535017
        O   2.18753355  -8.64903175   8.58995017
        O   1.01547355  -6.62503175   8.62975017
        O   0.54769355 -11.49762675   8.56307017
        O  -2.27142545  -6.62985175   8.65945017
        B  18.19207455  -7.26102175   8.66010017
        B   2.26472355  -7.25297175   8.60922017
        B  -0.62087645 -12.26549675   8.56327017
        C  15.65417455  -4.41330175   8.67260017
        C  14.41576455  -5.08071175   8.67015017
        C  14.45611455  -6.48688175   8.67300017
        C  15.65757455  -7.18088175   8.67347017
        C  16.89585455  -6.51349175   8.67235017
        C  16.85571455  -5.10745175   8.67427017
        H  13.51018455  -7.05296175   8.67255017
        H  15.63980455  -8.28311175   8.67320017
        H  17.80182455  -4.54127175   8.67473017
        H  15.67198855  -3.31078175   8.67190017
        C  -1.31780545  17.34788125   8.58825017
        C   8.84129355  -2.65719175   8.60145017
        C   9.53443355  -3.86090175   8.62462017
        C  10.92424355  -3.86265175   8.63578017
        C  11.62035355  -2.66044175   8.62295017
        C   0.07143355  17.34626425   8.59858017
        O   8.58456355  -4.95583175   8.63217017
        O  11.87133355  -4.95983175   8.65840017
        O   0.54805355  18.71511825   8.58083017
        O  -1.79101545  18.71782625   8.56407017
        O  13.04342355  -2.93539175   8.63725017
        O   7.41737355  -2.92890175   8.59420017
        B   7.33698355  -4.32473175   8.61320017
        B  -0.62052645 -18.12218875   8.56165017
        B  13.12059355  -4.33153175   8.65715017
        C  16.85552355  12.32419825   8.61445017
        C  16.89626355  13.73034825   8.61237017
        C  15.65829355  14.39838825   8.60838017
        C  14.45650355  13.70483825   8.60765017
        C  14.41560355  12.29858825   8.60885017
        C  15.65376355  11.63058825   8.61148017
        H  15.64105355  15.50063825   8.60663017
        H  13.51080355  14.27137825   8.60480017
        H  15.67087355  10.52826825   8.61223017
        H  17.80126355  11.75780825   8.61770017
        C  11.43345355   4.30241525   8.54610017
        C  10.23595355   5.04063625   8.54828017
        C   9.03854455   4.30226525   8.54425017
        C   9.03853455   2.91470225   8.54335017
        C  10.23605355   2.17655725   8.54773017
        C  11.43347355   2.91479625   8.54665017
        H   8.07524455   4.83845425   8.54350017
        H   8.07537455   2.37845725   8.54192017
        H  12.39678355   2.37873925   8.54835017
        H  12.39697355   4.83820925   8.54703017
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C  10.92390355  11.08010825   8.62322017
C   9.53418455  11.07802825   8.63670017
C   8.84107455   9.87417825   8.62592017
C   9.53757455   8.67167825   8.60107017
C  10.92666355   8.67373825   8.58767017
C  11.62009355   9.87817825   8.59903017
O   7.41710455  10.14556825   8.64175017
O   9.06423455   7.30149325   8.58535017
O  13.04312355  10.15339825   8.58995017
O  11.87106355  12.17739825   8.62975017
O  11.40328355   7.30480325   8.56307017
O   8.58416455  12.17257825   8.65945017
B -14.37469545  11.54140825   8.66010017
B  13.12031355  11.54945825   8.60922017
B  10.23471355   6.53693325   8.56327017
C -16.91259545  14.38912825   8.67260017
C -18.15100545  13.72171825   8.67015017
C -18.11065545  12.31554825   8.67300017
C -16.90919545  11.62154825   8.67347017
C -15.67091545  12.28893825   8.67235017
C -15.71105545  13.69497825   8.67427017
H -19.05658545  11.74946825   8.67255017
H -16.92696545  10.51931825   8.67320017
H -14.76494545  14.26115825   8.67473017
H -16.89478145  15.49164825   8.67190017
C   9.53778455  -1.45454875   8.58825017
C  19.69688355  16.14523825   8.60145017
C  20.39002355  14.94152825   8.62462017
C  21.77983355  14.93977825   8.63578017
C  22.47594355  16.14198825   8.62295017
C  10.92702355  -1.45616575   8.59858017
O  19.44015355  13.84659825   8.63217017
O  22.72692355  13.84259825   8.65840017
O  11.40364355  -0.08731175   8.58083017
O   9.06457455  -0.08460375   8.56407017
O  23.89901355  15.86703825   8.63725017
O  18.27296355  15.87352825   8.59420017
B  18.19257355  14.47769825   8.61320017
B  10.23506355   0.68024125   8.56165017
B  23.97618355  14.47089825   8.65715017
C -15.71124645  -6.47823175   8.61445017
C -15.67050645  -5.07208175   8.61237017
C -16.90847645  -4.40404175   8.60838017
C -18.11026645  -5.09759175   8.60765017
C -18.15116645  -6.50384175   8.60885017
C -16.91300645  -7.17184175   8.61148017
H -16.92571645  -3.30179175   8.60663017
H -19.05596645  -4.53105175   8.60480017
H -16.89589645  -8.27416175   8.61223017
H -14.76550645  -7.04462175   8.61770017
C  22.28904355 -14.50001475   8.54610017
C  21.09154355 -13.76179375   8.54828017
C  19.89413455 -14.50016475   8.54425017
C  19.89412455 -15.88772775   8.54335017
C  21.09164355 -16.62587275   8.54773017
C  22.28906355 -15.88763375   8.54665017
H  18.93083455 -13.96397575   8.54350017
```

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```
        H  18.93096455 -16.42397275   8.54192017
        H  23.25237355 -16.42369075   8.54835017
        H  23.25256355 -13.96422075   8.54703017
        C  21.77949355  -7.72232175   8.62322017
        C  20.38977455  -7.72440175   8.63670017
        C  19.69666455  -8.92825175   8.62592017
        C  20.39316455 -10.13075175   8.60107017
        C  21.78225355 -10.12869175   8.58767017
        C  22.47568355  -8.92425175   8.59903017
        O  18.27269455  -8.65686175   8.64175017
        O  19.91982455 -11.50093675   8.58535017
        O  23.89871355  -8.64903175   8.58995017
        O  22.72665355  -6.62503175   8.62975017
        O  22.25887355 -11.49762675   8.56307017
        O  19.43975455  -6.62985175   8.65945017
        B  23.97590355  -7.25297175   8.60922017
        B  21.09030355 -12.26549675   8.56327017
        C  20.39337455  17.34788125   8.58825017
        C  21.78261355  17.34626425   8.59858017
        O  22.25923355  18.71511825   8.58083017
        O  19.92016455  18.71782625   8.56407017
        B -14.37419645  -4.32473175   8.61320017
        B  21.09065355 -18.12218875   8.56165017
    End

    Lattice
        43.42236000 0.0 0.0
        0.0 37.60486000 0.0
    End
End

Engine DFTB
   Model SCC-DFTB
   ResourcesDir DFTB.org/matsci-0-3
EndEngine

eor
```

10.1.18 Example: Single point COF5, 3D

Download SP_COF5_3D.run

```
#! /bin/sh

$AMSBIN/ams << eor

Task SinglePoint

System
    Atoms
        B  -3.51910545  -7.26102175   8.66010017
        C  -6.05700545  -4.41330175   8.67260017
        C  -7.29541545  -5.08071175   8.67015017
        C  -7.25506545  -6.48688175   8.67300017
        C  -6.05360545  -7.18088175   8.67347017
```

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```
        C  -4.81532545  -6.51349175   8.67235017
        C  -4.85546545  -5.10745175   8.67427017
        H  -8.20099545  -7.05296175   8.67255017
        H  -6.07137545  -8.28311175   8.67320017
        H  -3.90935545  -4.54127175   8.67473017
        H  -6.03919145  -3.31078175   8.67190017
        C -12.86988645  -2.65719175   8.60145017
        C -12.17674645  -3.86090175   8.62462017
        C -10.78693645  -3.86265175   8.63578017
        C -10.09082645  -2.66044175   8.62295017
        O -13.12661645  -4.95583175   8.63217017
        O  -9.83984645  -4.95983175   8.65840017
        O  -8.66775645  -2.93539175   8.63725017
        O -14.29380645  -2.92890175   8.59420017
        B  -8.59058645  -4.33153175   8.65715017
        C  -4.85565645  12.32419825   8.61445017
        C  -4.81491645  13.73034825   8.61237017
        C  -6.05288645  14.39838825   8.60838017
        C  -7.25467645  13.70483825   8.60765017
        C  -7.29557645  12.29858825   8.60885017
        C  -6.05741645  11.63058825   8.61148017
        H  -6.07012645  15.50063825   8.60663017
        H  -8.20037645  14.27137825   8.60480017
        H  -6.04030645  10.52826825   8.61223017
        H  -3.90991645  11.75780825   8.61770017
        C -10.27772645   4.30241525   8.54610017
        C -11.47522645   5.04063625   8.54828017
        C -12.67263545   4.30226525   8.54425017
        C -12.67264545   2.91470225   8.54335017
        C -11.47512645   2.17655725   8.54773017
        C -10.27770645   2.91479625   8.54665017
        H -13.63593545   4.83845425   8.54350017
        H -13.63580545   2.37845725   8.54192017
        H  -9.31439645   2.37873925   8.54835017
        H  -9.31420645   4.83820925   8.54703017
        C -10.78727645  11.08010825   8.62322017
        C -12.17699545  11.07802825   8.63670017
        C -12.87010545   9.87417825   8.62592017
        C -12.17360545   8.67167825   8.60107017
        C -10.78451645   8.67373825   8.58767017
        C -10.09108645   9.87817825   8.59903017
        O -14.29407545  10.14556825   8.64175017
        O -12.64694545   7.30149325   8.58535017
        O  -8.66805645  10.15339825   8.58995017
        O  -9.84011645  12.17739825   8.62975017
        O -10.30789645   7.30480325   8.56307017
        O -13.12701545  12.17257825   8.65945017
        B   7.33648455  11.54140825   8.66010017
        B  -8.59086645  11.54945825   8.60922017
        B -11.47646645   6.53693325   8.56327017
        C   4.79858455  14.38912825   8.67260017
        C   3.56017455  13.72171825   8.67015017
        C   3.60052455  12.31554825   8.67300017
        C   4.80198455  11.62154825   8.67347017
        C   6.04026455  12.28893825   8.67235017
        C   6.00012455  13.69497825   8.67427017
        H   2.65459455  11.74946825   8.67255017
```

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```
        H   4.78421455  10.51931825   8.67320017
        H   6.94623455  14.26115825   8.67473017
        H   4.81639855  15.49164825   8.67190017
        C -12.17339545  -1.45454875   8.58825017
        C  -2.01429645  16.14523825   8.60145017
        C  -1.32115645  14.94152825   8.62462017
        C   0.06865355  14.93977825   8.63578017
        C   0.76476355  16.14198825   8.62295017
        C -10.78415645  -1.45616575   8.59858017
        O  -2.27102645  13.84659825   8.63217017
        O   1.01574355  13.84259825   8.65840017
        O -10.30753645  -0.08731175   8.58083017
        O -12.64660545  -0.08460375   8.56407017
        O   2.18783355  15.86703825   8.63725017
        O  -3.43821645  15.87352825   8.59420017
        B  -3.51860645  14.47769825   8.61320017
        B -11.47611645   0.68024125   8.56165017
        B   2.26500355  14.47089825   8.65715017
        C   5.99993355  -6.47823175   8.61445017
        C   6.04067355  -5.07208175   8.61237017
        C   4.80270355  -4.40404175   8.60838017
        C   3.60091355  -5.09759175   8.60765017
        C   3.56001355  -6.50384175   8.60885017
        C   4.79817355  -7.17184175   8.61148017
        H   4.78546355  -3.30179175   8.60663017
        H   2.65521355  -4.53105175   8.60480017
        H   4.81528355  -8.27416175   8.61223017
        H   6.94567355  -7.04462175   8.61770017
        C   0.57786355 -14.50001475   8.54610017
        C  -0.61963645 -13.76179375   8.54828017
        C  -1.81704545 -14.50016475   8.54425017
        C  -1.81705545 -15.88772775   8.54335017
        C  -0.61953645 -16.62587275   8.54773017
        C   0.57788355 -15.88763375   8.54665017
        H  -2.78034545 -13.96397575   8.54350017
        H  -2.78021545 -16.42397275   8.54192017
        H   1.54119355 -16.42369075   8.54835017
        H   1.54138355 -13.96422075   8.54703017
        C   0.06831355  -7.72232175   8.62322017
        C  -1.32140545  -7.72440175   8.63670017
        C  -2.01451545  -8.92825175   8.62592017
        C  -1.31801545 -10.13075175   8.60107017
        C   0.07107355 -10.12869175   8.58767017
        C   0.76450355  -8.92425175   8.59903017
        O  -3.43848545  -8.65686175   8.64175017
        O  -1.79135545 -11.50093675   8.58535017
        O   2.18753355  -8.64903175   8.58995017
        O   1.01547355  -6.62503175   8.62975017
        O   0.54769355 -11.49762675   8.56307017
        O  -2.27142545  -6.62985175   8.65945017
        B  18.19207455  -7.26102175   8.66010017
        B   2.26472355  -7.25297175   8.60922017
        B  -0.62087645 -12.26549675   8.56327017
        C  15.65417455  -4.41330175   8.67260017
        C  14.41576455  -5.08071175   8.67015017
        C  14.45611455  -6.48688175   8.67300017
        C  15.65757455  -7.18088175   8.67347017
```

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```
        C  16.89585455  -6.51349175   8.67235017
        C  16.85571455  -5.10745175   8.67427017
        H  13.51018455  -7.05296175   8.67255017
        H  15.63980455  -8.28311175   8.67320017
        H  17.80182455  -4.54127175   8.67473017
        H  15.67198855  -3.31078175   8.67190017
        C  -1.31780545  17.34788125   8.58825017
        C   8.84129355  -2.65719175   8.60145017
        C   9.53443355  -3.86090175   8.62462017
        C  10.92424355  -3.86265175   8.63578017
        C  11.62035355  -2.66044175   8.62295017
        C   0.07143355  17.34626425   8.59858017
        O   8.58456355  -4.95583175   8.63217017
        O  11.87133355  -4.95983175   8.65840017
        O   0.54805355  18.71511825   8.58083017
        O  -1.79101545  18.71782625   8.56407017
        O  13.04342355  -2.93539175   8.63725017
        O   7.41737355  -2.92890175   8.59420017
        B   7.33698355  -4.32473175   8.61320017
        B  -0.62052645 -18.12218875   8.56165017
        B  13.12059355  -4.33153175   8.65715017
        C  16.85552355  12.32419825   8.61445017
        C  16.89626355  13.73034825   8.61237017
        C  15.65829355  14.39838825   8.60838017
        C  14.45650355  13.70483825   8.60765017
        C  14.41560355  12.29858825   8.60885017
        C  15.65376355  11.63058825   8.61148017
        H  15.64105355  15.50063825   8.60663017
        H  13.51080355  14.27137825   8.60480017
        H  15.67087355  10.52826825   8.61223017
        H  17.80126355  11.75780825   8.61770017
        C  11.43345355   4.30241525   8.54610017
        C  10.23595355   5.04063625   8.54828017
        C   9.03854455   4.30226525   8.54425017
        C   9.03853455   2.91470225   8.54335017
        C  10.23605355   2.17655725   8.54773017
        C  11.43347355   2.91479625   8.54665017
        H   8.07524455   4.83845425   8.54350017
        H   8.07537455   2.37845725   8.54192017
        H  12.39678355   2.37873925   8.54835017
        H  12.39697355   4.83820925   8.54703017
        C  10.92390355  11.08010825   8.62322017
        C   9.53418455  11.07802825   8.63670017
        C   8.84107455   9.87417825   8.62592017
        C   9.53757455   8.67167825   8.60107017
        C  10.92666355   8.67373825   8.58767017
        C  11.62009355   9.87817825   8.59903017
        O   7.41710455  10.14556825   8.64175017
        O   9.06423455   7.30149325   8.58535017
        O  13.04312355  10.15339825   8.58995017
        O  11.87106355  12.17739825   8.62975017
        O  11.40328355   7.30480325   8.56307017
        O   8.58416455  12.17257825   8.65945017
        B -14.37469545  11.54140825   8.66010017
        B  13.12031355  11.54945825   8.60922017
        B  10.23471355   6.53693325   8.56327017
        C -16.91259545  14.38912825   8.67260017
```

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```
        C -18.15100545  13.72171825   8.67015017
        C -18.11065545  12.31554825   8.67300017
        C -16.90919545  11.62154825   8.67347017
        C -15.67091545  12.28893825   8.67235017
        C -15.71105545  13.69497825   8.67427017
        H -19.05658545  11.74946825   8.67255017
        H -16.92696545  10.51931825   8.67320017
        H -14.76494545  14.26115825   8.67473017
        H -16.89478145  15.49164825   8.67190017
        C   9.53778455  -1.45454875   8.58825017
        C  19.69688355  16.14523825   8.60145017
        C  20.39002355  14.94152825   8.62462017
        C  21.77983355  14.93977825   8.63578017
        C  22.47594355  16.14198825   8.62295017
        C  10.92702355  -1.45616575   8.59858017
        O  19.44015355  13.84659825   8.63217017
        O  22.72692355  13.84259825   8.65840017
        O  11.40364355  -0.08731175   8.58083017
        O   9.06457455  -0.08460375   8.56407017
        O  23.89901355  15.86703825   8.63725017
        O  18.27296355  15.87352825   8.59420017
        B  18.19257355  14.47769825   8.61320017
        B  10.23506355   0.68024125   8.56165017
        B  23.97618355  14.47089825   8.65715017
        C -15.71124645  -6.47823175   8.61445017
        C -15.67050645  -5.07208175   8.61237017
        C -16.90847645  -4.40404175   8.60838017
        C -18.11026645  -5.09759175   8.60765017
        C -18.15116645  -6.50384175   8.60885017
        C -16.91300645  -7.17184175   8.61148017
        H -16.92571645  -3.30179175   8.60663017
        H -19.05596645  -4.53105175   8.60480017
        H -16.89589645  -8.27416175   8.61223017
        H -14.76550645  -7.04462175   8.61770017
        C  22.28904355 -14.50001475   8.54610017
        C  21.09154355 -13.76179375   8.54828017
        C  19.89413455 -14.50016475   8.54425017
        C  19.89412455 -15.88772775   8.54335017
        C  21.09164355 -16.62587275   8.54773017
        C  22.28906355 -15.88763375   8.54665017
        H  18.93083455 -13.96397575   8.54350017
        H  18.93096455 -16.42397275   8.54192017
        H  23.25237355 -16.42369075   8.54835017
        H  23.25256355 -13.96422075   8.54703017
        C  21.77949355  -7.72232175   8.62322017
        C  20.38977455  -7.72440175   8.63670017
        C  19.69666455  -8.92825175   8.62592017
        C  20.39316455 -10.13075175   8.60107017
        C  21.78225355 -10.12869175   8.58767017
        C  22.47568355  -8.92425175   8.59903017
        O  18.27269455  -8.65686175   8.64175017
        O  19.91982455 -11.50093675   8.58535017
        O  23.89871355  -8.64903175   8.58995017
        O  22.72665355  -6.62503175   8.62975017
        O  22.25887355 -11.49762675   8.56307017
        O  19.43975455  -6.62985175   8.65945017
        B  23.97590355  -7.25297175   8.60922017
```

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```
        B  21.09030355 -12.26549675   8.56327017
        C  20.39337455  17.34788125   8.58825017
        C  21.78261355  17.34626425   8.59858017
        O  22.25923355  18.71511825   8.58083017
        O  19.92016455  18.71782625   8.56407017
        B -14.37419645  -4.32473175   8.61320017
        B  21.09065355 -18.12218875   8.56165017
    End

    Lattice
        43.42236000 0.0 0.0
        0.0 37.60486000 0.0
        7.18482000 4.14816000 20.66544000
    End
End

Engine DFTB
   Model SCC-DFTB
   ResourcesDir DFTB.org/matsci-0-3
EndEngine

eor
```

10.1.19 Example: H+

Download SP_Hplus.run

```
#!/bin/sh

# Neutral H atom

AMS_JOBNAME=H_DFTB0 $AMSBIN/ams << eor
Task SinglePoint
System
    Atoms
        H 0.0 0.0 0.0
    End
End
Engine DFTB
   ResourcesDir DFTB.org/3ob-3-1
   Model DFTB0
EndEngine
eor

AMS_JOBNAME=H_SCC $AMSBIN/ams << eor
Task SinglePoint
System
    Atoms
        H 0.0 0.0 0.0
    End
End
Engine DFTB
   ResourcesDir DFTB.org/3ob-3-1
   Model SCC-DFTB
EndEngine
```

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```
eor

AMS_JOBNAME=H_DFTB3 $AMSBIN/ams << eor
Task SinglePoint
System
    Atoms
        H 0.0 0.0 0.0
    End
End
Engine DFTB
   ResourcesDir DFTB.org/3ob-3-1
   Model DFTB3
EndEngine
eor


# H+ ion

AMS_JOBNAME=Hplus_DFTB0 $AMSBIN/ams << eor
Task SinglePoint
System
    Atoms
        H 0.0 0.0 0.0
    End
    Charge 1
End
Engine DFTB
   ResourcesDir DFTB.org/3ob-3-1
   Model DFTB0
EndEngine
eor

AMS_JOBNAME=Hplus_SCC $AMSBIN/ams << eor
Task SinglePoint
System
    Atoms
        H 0.0 0.0 0.0
    End
    Charge 1
End
Engine DFTB
   ResourcesDir DFTB.org/3ob-3-1
   Model SCC-DFTB
EndEngine
eor

AMS_JOBNAME=Hplus_DFTB3 $AMSBIN/ams << eor
Task SinglePoint
System
    Atoms
        H 0.0 0.0 0.0
    End
    Charge 1
End
Engine DFTB
   ResourcesDir DFTB.org/3ob-3-1
   Model DFTB3
```

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```
EndEngine
eor
```

10.1.20 Example: geometry optimizations in solution

Download GBSA_solvation.run

```
#!/bin/sh


# 1. Test: Correct geometry in solution. Proton should stay where it is.
# ======================================================================

AMS_JOBNAME=insolution $AMSBIN/ams << eor

Task GeometryOptimization

GeometryOptimization
   Convergence Step=1.0e-3
End

System
    Atoms
        C -2.952658582657874 0.04645901178988775 -0.2265370925256049
        C -1.525681082568581 -0.0632256145142199 0.3253833614393568
        C -0.8702309998044314 1.320132595321299 0.4237615743177286
        C -1.51274965669442 -0.7747515748731322 1.675623541214415
        N -0.7585531160264641 -0.8002764137525281 -0.685002445614226
        C -0.125815059541938 -1.888404876006561 -0.5619452224652126
        H 0.3933316241384404 -2.297780064591292 -1.420796950876057
        Cl -0.6405638449575868 0.3711605263839059 -3.386878242415801
        H -0.07954642621561822 -2.433755645332853 0.3716143879666342
        H 0.1593861124853071 1.224674178285476 0.7663389629840952
        H -1.425551586480803 1.930381023229107 1.134028455207074
        H -0.8766051564206533 1.814252585786801 -0.5466890218510505
        H -3.562314031052068 0.6219838361677803 0.4680147715674572
        H -3.387932028293341 -0.9453294765130141 -0.3430211448005557
        H -2.950029479645555 0.5481307479235709 -1.193069533171342
        H -0.4972001484798669 -0.8666401271795375 2.059424124249443
        H -1.960500983176193 -1.765112626081995 1.59927019965761
        H -2.095961597315341 -0.1875167889244935 2.38340332667977
        H -0.7534711472929415 -0.3338452271177779 -1.625750861563839
    End
End

Engine DFTB
    Model GFN1-xTB
    Solvation Solvent=chcl3
EndEngine

eor
echo "N-H bond distance"
$AMSBIN/amsreport insolution.results/ams.rkf distance#5#19
echo "H-Cl distance"
$AMSBIN/amsreport insolution.results/ams.rkf distance#19#8
```

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```
# 2. Test: Same with DFTB3
# ========================

AMS_JOBNAME=insolution_DFTB3 $AMSBIN/ams << eor

Task GeometryOptimization

GeometryOptimization
   Convergence Step=1.0e-3
End

System
    Atoms
        C -2.952658582657874 0.04645901178988775 -0.2265370925256049
        C -1.525681082568581 -0.0632256145142199 0.3253833614393568
        C -0.8702309998044314 1.320132595321299 0.4237615743177286
        C -1.51274965669442 -0.7747515748731322 1.675623541214415
        N -0.7585531160264641 -0.8002764137525281 -0.685002445614226
        C -0.125815059541938 -1.888404876006561 -0.5619452224652126
        H 0.3933316241384404 -2.297780064591292 -1.420796950876057
        Cl -0.6405638449575868 0.3711605263839059 -3.386878242415801
        H -0.07954642621561822 -2.433755645332853 0.3716143879666342
        H 0.1593861124853071 1.224674178285476 0.7663389629840952
        H -1.425551586480803 1.930381023229107 1.134028455207074
        H -0.8766051564206533 1.814252585786801 -0.5466890218510505
        H -3.562314031052068 0.6219838361677803 0.4680147715674572
        H -3.387932028293341 -0.9453294765130141 -0.3430211448005557
        H -2.950029479645555 0.5481307479235709 -1.193069533171342
        H -0.4972001484798669 -0.8666401271795375 2.059424124249443
        H -1.960500983176193 -1.765112626081995 1.59927019965761
        H -2.095961597315341 -0.1875167889244935 2.38340332667977
        H -0.7534711472929415 -0.3338452271177779 -1.625750861563839
    End
End

Engine DFTB
    Model DFTB3
    ResourcesDir DFTB.org/3ob-3-1
    DispersionCorrection D3-BJ
    Solvation Solvent=chcl3
EndEngine

eor
echo "N-H bond distance"
$AMSBIN/amsreport insolution_DFTB3.results/ams.rkf distance#5#19
echo "H-Cl distance"
$AMSBIN/amsreport insolution_DFTB3.results/ams.rkf distance#19#8


# 3. Test: No solvation model. Proton should move to the Cl.
# ==========================================================

AMS_JOBNAME=invacuum $AMSBIN/ams << eor

Task GeometryOptimization
```

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```
GeometryOptimization
   Convergence Step=1.0e-3
End

System
    Atoms
        C -2.952658582657874 0.04645901178988775 -0.2265370925256049
        C -1.525681082568581 -0.0632256145142199 0.3253833614393568
        C -0.8702309998044314 1.320132595321299 0.4237615743177286
        C -1.51274965669442 -0.7747515748731322 1.675623541214415
        N -0.7585531160264641 -0.8002764137525281 -0.685002445614226
        C -0.125815059541938 -1.888404876006561 -0.5619452224652126
        H 0.3933316241384404 -2.297780064591292 -1.420796950876057
        Cl -0.6405638449575868 0.3711605263839059 -3.386878242415801
        H -0.07954642621561822 -2.433755645332853 0.3716143879666342
        H 0.1593861124853071 1.224674178285476 0.7663389629840952
        H -1.425551586480803 1.930381023229107 1.134028455207074
        H -0.8766051564206533 1.814252585786801 -0.5466890218510505
        H -3.562314031052068 0.6219838361677803 0.4680147715674572
        H -3.387932028293341 -0.9453294765130141 -0.3430211448005557
        H -2.950029479645555 0.5481307479235709 -1.193069533171342
        H -0.4972001484798669 -0.8666401271795375 2.059424124249443
        H -1.960500983176193 -1.765112626081995 1.59927019965761
        H -2.095961597315341 -0.1875167889244935 2.38340332667977
        H -0.7534711472929415 -0.3338452271177779 -1.625750861563839
    End
End

Engine DFTB
    Model GFN1-xTB
EndEngine

eor
echo "N-H bond distance"
$AMSBIN/amsreport invacuum.results/ams.rkf distance#5#19
echo "H-Cl distance"
$AMSBIN/amsreport invacuum.results/ams.rkf distance#19#8
```

10.1.21 Example: Precision: k-space integration

Download KSpace_sampling.run

```
#! /bin/sh

# Calculate bulk Al with different k-space integration qualities.

# Regular grid (new default)
for q in GammaOnly Basic Normal Good VeryGood Excellent ; do
AMS_JOBNAME=quality_$q $AMSBIN/ams << EOF

   Task SinglePoint

   System
      Atoms
```

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```
            Al 0.0 0.0 0.0
        End
        Lattice
            0.0 2.025 2.025
            2.025 0.0 2.025
            2.025 2.025 0.0
        End
    End

    Engine DFTB
        Model DFTB0
        ResourcesDir QUASINANO2013.1
        KSpace Quality=$q
    EndEngine

EOF
done

# Super accurate regular grid
AMS_JOBNAME=reg_31 $AMSBIN/ams << EOF

    Task SinglePoint

    System
        Atoms
            Al 0.0 0.0 0.0
        End
        Lattice
            0.0 2.025 2.025
            2.025 0.0 2.025
            2.025 2.025 0.0
        End
    End

    Engine DFTB
        Model DFTB0
        ResourcesDir QUASINANO2013.1
        KSpace
            Type Regular
            Regular
                NumberOfPoints 31 31 31
            End
        End
    EndEngine

EOF

# Symmetric grid (old default in AMS<=2018)
for i in 1 3 5 7 9 11 13 15 ; do
AMS_JOBNAME=sym_$i $AMSBIN/ams << EOF

    Task SinglePoint

    System
        Atoms
            Al 0.0 0.0 0.0
        End
```

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```
      Lattice
          0.0 2.025 2.025
          2.025 0.0 2.025
          2.025 2.025 0.0
      End
   End

   Engine DFTB
       Model DFTB0
       ResourcesDir QUASINANO2013.1
       KSpace
         Type Symmetric
         Symmetric KInteg=$i
       End
   EndEngine

EOF
done
```

10.1.22 Example: External potential at nuclei

Download SP_extpotential.run

```
#!/bin/sh

$AMSBIN/ams << eor

Task SinglePoint

Properties
   Gradients True
End

System
    Atoms
      H   0.0    0.0   0.0    DFTB.Vext=-0.01
      H   0.75   0.0   0.0    DFTB.Vext=0.01
    End
End

Engine DFTB
    Model SCC-DFTB
    ResourcesDir DFTB.org/mio-1-1
EndEngine

eor
```

10.1.23 Example: Restart DFTB

Download SP_DFTB_restart.run

```
#!/bin/sh

# ===============================================
# Generate shell-resolved spin populations
# ===============================================

AMS_JOBNAME=gen_ldepsp $AMSBIN/ams <<EOF > out.trash

Task SinglePoint

System
    Atoms
        O -1.361332295 -0.04735246111 -0.02869152269
        O -0.09790358374 0.6673459552 0.06152027535
        H -1.738074016 0.103293031 0.8758691702
        H 0.2801603051 0.514241345 -0.8420753829
    End
End

Engine DFTB
   Model SCC-DFTB
   ResourcesDir DFTB.org/mio-1-1
   SCC
       OrbitalDependent Yes
       Unrestricted Yes
   End
   Occupation Strategy=aufbau
   UnpairedElectrons 2
EndEngine

EOF

# ===============================================
# Restart from shell-resolved spin populations
# ===============================================
AMS_JOBNAME=res_ldepsp $AMSBIN/ams <<EOF

Task SinglePoint

System
    Atoms
        O -1.361332295 -0.04735246111 -0.02869152269
        O -0.09790358374 0.6673459552 0.06152027535
        H -1.738074016 0.103293031 0.8758691702
        H 0.2801603051 0.514241345 -0.8420753829
    End
End

Engine DFTB
   Model SCC-DFTB
   ResourcesDir DFTB.org/mio-1-1
   SCC
       OrbitalDependent Yes
       Unrestricted Yes
```

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```
   End
   Occupation Strategy=aufbau
   UnpairedElectrons 2
EndEngine

EngineRestart gen_ldepsp.results/dftb.rkf

EOF




# ===============================================
# Generate shell-resolved Mulliken charges
# ===============================================

AMS_JOBNAME=gen_ldepq $AMSBIN/ams <<EOF > out.trash

Task SinglePoint

System
    Atoms
        O -1.361332295 -0.04735246111 -0.02869152269
        O -0.09790358374 0.6673459552 0.06152027535
        H -1.738074016 0.103293031 0.8758691702
        H 0.2801603051 0.514241345 -0.8420753829
    End
End

Engine DFTB
   Model SCC-DFTB
   ResourcesDir DFTB.org/mio-1-1
   SCC
       OrbitalDependent Yes
   End
EndEngine

EOF

# ===============================================
# Restart from shell-resolved Mulliken charges
# ===============================================

AMS_JOBNAME=res_ldepq $AMSBIN/ams <<EOF

Task SinglePoint

System
    Atoms
        O -1.361332295 -0.04735246111 -0.02869152269
        O -0.09790358374 0.6673459552 0.06152027535
        H -1.738074016 0.103293031 0.8758691702
        H 0.2801603051 0.514241345 -0.8420753829
    End
End

Engine DFTB
```

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```
   Model SCC-DFTB
   ResourcesDir DFTB.org/mio-1-1
   SCC
       OrbitalDependent Yes
   End
EndEngine

EngineRestart gen_ldepq.results/dftb.rkf

EOF




# ===============================================
# Generate atom-resolved spin populations
# ===============================================

AMS_JOBNAME=gen_asp $AMSBIN/ams <<EOF > out.trash

Task SinglePoint

System
    Atoms
        O -1.361332295 -0.04735246111 -0.02869152269
        O -0.09790358374 0.6673459552 0.06152027535
        H -1.738074016 0.103293031 0.8758691702
        H 0.2801603051 0.514241345 -0.8420753829
    End
End

Engine DFTB
   Model SCC-DFTB
   ResourcesDir DFTB.org/mio-1-1
   SCC
       Unrestricted Yes
   End
   Occupation Strategy=aufbau
   UnpairedElectrons 2
EndEngine

EOF

# ===============================================
# Restart from atom-resolved spin populations
# ===============================================

AMS_JOBNAME=res_asp $AMSBIN/ams <<EOF

Task SinglePoint

System
    Atoms
        O -1.361332295 -0.04735246111 -0.02869152269
        O -0.09790358374 0.6673459552 0.06152027535
        H -1.738074016 0.103293031 0.8758691702
        H 0.2801603051 0.514241345 -0.8420753829
```

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```
    End
End

Engine DFTB
   Model SCC-DFTB
   ResourcesDir DFTB.org/mio-1-1
   SCC
       Unrestricted Yes
   End
   Occupation Strategy=aufbau
   UnpairedElectrons 2
EndEngine

EngineRestart gen_asp.results/dftb.rkf

EOF




# ===============================================
# Generate atom-resolved Mulliken charges
# ===============================================

AMS_JOBNAME=gen_aq $AMSBIN/ams <<EOF > out.trash

Task SinglePoint

System
    Atoms
        O -1.361332295 -0.04735246111 -0.02869152269
        O -0.09790358374 0.6673459552 0.06152027535
        H -1.738074016 0.103293031 0.8758691702
        H 0.2801603051 0.514241345 -0.8420753829
    End
End

Engine DFTB
   Model SCC-DFTB
   ResourcesDir DFTB.org/mio-1-1
EndEngine

EOF

# ===============================================
# Restart from atom-resolved Mulliken charges
# ===============================================

AMS_JOBNAME=res_aq $AMSBIN/ams <<EOF

Task SinglePoint

System
    Atoms
        O -1.361332295 -0.04735246111 -0.02869152269
        O -0.09790358374 0.6673459552 0.06152027535
        H -1.738074016 0.103293031 0.8758691702
```

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```
        H 0.2801603051 0.514241345 -0.8420753829
    End
End

Engine DFTB
   Model SCC-DFTB
   ResourcesDir DFTB.org/mio-1-1
EndEngine

EngineRestart gen_aq.results/dftb.rkf

EOF
```

10.1.24 Example: System input from file

Download TECH_systeminput.run

```
#!/bin/sh

cp $AMSHOME/examples/dftb/TECH_systeminput/*.xyz .

AMS_JOBNAME=bc_standard $AMSBIN/ams << EOF
Task SinglePoint
Engine DFTB
   Resourcesdir DFTB.org/mio-1-1
   Model DFTB0
EndEngine
System
   GeometryFile bc_standard.xyz
End
EOF

AMS_JOBNAME=bc_lattice1 $AMSBIN/ams << EOF
Task SinglePoint
Engine DFTB
   Resourcesdir DFTB.org/mio-1-1
   Model DFTB0
EndEngine
System
   GeometryFile bc_lattice1.xyz
End
EOF

AMS_JOBNAME=bc_lattice2 $AMSBIN/ams << EOF
Task SinglePoint
Engine DFTB
   Resourcesdir DFTB.org/mio-1-1
   Model DFTB0
EndEngine
System
   GeometryFile bc_lattice2.xyz
End
EOF

AMS_JOBNAME=bc_lattice3 $AMSBIN/ams << EOF
```

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```
Task SinglePoint
Engine DFTB
   Resourcesdir DFTB.org/mio-1-1
   Model DFTB0
EndEngine
System
   GeometryFile bc_lattice3.xyz
End
EOF

AMS_JOBNAME=bc_lattice3_blanklines $AMSBIN/ams << EOF
Task SinglePoint
Engine DFTB
   Resourcesdir DFTB.org/mio-1-1
   Model DFTB0
EndEngine
System
   GeometryFile bc_lattice3_blanklines.xyz
End
EOF
```

10.2 Geometry Optimization

10.2.1 Example: GO formaldehyde noSCC

Download GO_formaldehyde_noSCC.run

```
#!/bin/sh

$AMSBIN/ams << EOF

   Task GeometryOptimization

   System
       Atoms [Bohr]
          C    0.0    0.0     -1.0
          O    0.0    0.0      1.247
          H    0.0   -1.738   -2.097
          H    0.0    1.738   -2.097
       End
   End

   Engine DFTB
       ResourcesDir Dresden
       Model DFTB0
       DispersionCorrection Auto
   EndEngine

EOF
```

10.2.2 Example: GO formaldehyde SCC

Download GO_formaldehyde_SCC.run

```
#!/bin/sh

$AMSBIN/ams << eor

Task GeometryOptimization

GeometryOptimization
  Convergence Gradients=1.0e-5
End

System
    Atoms [Bohr]
      C      0.0  0.0  -1.00
      O      0.0  0.0   1.247
      H      0.0 -1.738 -2.097
      H      0.0  1.738 -2.097
    End
End

Engine DFTB
    Model SCC-DFTB
    ResourcesDir Dresden
    SCC
        Converge charge=1.0e-8
    End
    DispersionCorrection UFF
EndEngine

eor
```

10.2.3 Example: GO H3COO- DFTB3

Download GO_CH3COOminus_3rdOrder.run

```
#!/bin/sh

$AMSBIN/ams << eor

Task GeometryOptimization

System
    Atoms
      C    0.00000 0.21555 0.00000
      O    1.10974 0.79418 0.00000
      O    -1.15239 0.70584 0.00000
      C    0.04178 -1.35041 0.00000
      H    -0.48762 -1.73081 0.87864
      H    -0.48762 -1.73081 -0.87864
      H    1.06573 -1.72936 0.00000
    End
    Charge -1
End
```

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```
Engine DFTB
   ResourcesDir DFTB.org/3ob-3-1
   Model DFTB3
   DispersionCorrection UFF
EndEngine

eor
```

10.2.4 Example: GO cyclobutadiene spin-polarized

Download constraints.run

```
#!/bin/sh

AMS_JOBNAME=triplet $AMSBIN/ams << eor

Task GeometryOptimization

GeometryOptimization
    MaxIterations 100
    Convergence Gradients=1.0e-4
End

System
    Atoms
        C         0.64000000  0.74000000  0.00000000
        C        -0.64000000  0.74000000  0.00000000
        C        -0.64000000 -0.74000000  0.00000000
        C         0.64000000 -0.74000000  0.00000000
        H         1.50000000  1.50000000  0.00000000
        H        -1.50000000  1.50000000  0.00000000
        H        -1.50000000 -1.50000000  0.00000000
        H         1.50000000 -1.50000000  0.00000000
    End
End

Engine DFTB
   Model SCC-DFTB
   ResourcesDir DFTB.org/mio-1-1
   SCC
       DIIS MixingFactor=0.1
       Unrestricted Yes
   End
   Occupation
      Strategy fermi
      temperature 10
   End
   UnpairedElectrons 2
EndEngine

eor


AMS_JOBNAME=singlet $AMSBIN/ams << eor
```

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```
Task GeometryOptimization

GeometryOptimization
    MaxIterations 100
    Convergence Gradients=1.0e-4
End

System
    Atoms
        C         0.64000000  0.74000000  0.00000000
        C        -0.64000000  0.74000000  0.00000000
        C        -0.64000000 -0.74000000  0.00000000
        C         0.64000000 -0.74000000  0.00000000
        H         1.50000000  1.50000000  0.00000000
        H        -1.50000000  1.50000000  0.00000000
        H        -1.50000000 -1.50000000  0.00000000
        H         1.50000000 -1.50000000  0.00000000
    End
End

Engine DFTB
   Model SCC-DFTB
   ResourcesDir DFTB.org/mio-1-1
   SCC
       DIIS MixingFactor=0.1
       Unrestricted Yes
   End
   Occupation
      Strategy fermi
      temperature 10
   End
   UnpairedElectrons 0
EndEngine

eor
```

10.2.5 Example: GO cyclobutadiene unpaired electrons

Download GO_cyclobutadiene_unpairedelectrons.run

```
#!/bin/sh

AMS_JOBNAME=singlet $AMSBIN/ams << eor

Task GeometryOptimization

GeometryOptimization
   Convergence Gradients=1.0e-5
   CoordinateType Cartesian
End

System
    Atoms
        C         0.6  0.8  0.00000000
```

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```
        C        -0.6  0.8  0.00000000
        C        -0.6 -0.8  0.00000000
        C         0.6 -0.8  0.00000000
        H         1.4  1.4  0.00000000
        H        -1.4  1.4  0.00000000
        H        -1.4 -1.4  0.00000000
        H         1.4 -1.4  0.00000000
    End
End

Engine DFTB
   Model SCC-DFTB
   ResourcesDir DFTB.org/mio-1-1
   Occupation
      Strategy aufbau
   End
   UnpairedElectrons 0
EndEngine

eor


AMS_JOBNAME=triplet $AMSBIN/ams << eor

Task GeometryOptimization

GeometryOptimization
   Convergence Gradients=1.0e-5
   CoordinateType Cartesian
End

System
    Atoms
        C         0.6  0.8  0.00000000
        C        -0.6  0.8  0.00000000
        C        -0.6 -0.8  0.00000000
        C         0.6 -0.8  0.00000000
        H         1.4  1.4  0.00000000
        H        -1.4  1.4  0.00000000
        H        -1.4 -1.4  0.00000000
        H         1.4 -1.4  0.00000000
    End
End

Engine DFTB
   Model SCC-DFTB
   ResourcesDir DFTB.org/mio-1-1
   Occupation
      Strategy aufbau
   End
   UnpairedElectrons 2
EndEngine

eor
```

10.2.6 Example: GO ethane 0D, 1D, 2D, 3D

Download GO_ethane.run

```
#!/bin/sh

AMS_JOBNAME=0D $AMSBIN/ams << EOF

Task GeometryOptimization

GeometryOptimization
   Convergence Gradients=1.0e-5
End

Properties
   NormalModes true
End

System
   Atoms
      C       0.000000000000       0.000000000000       0.767685465031
      C       0.000000000000       0.000000000000      -0.767685465031
      H       0.964354016767       0.347635559279       1.177128271450
      H      -0.181115782790      -1.008972856410       1.177128271450
      H      -0.783238233981       0.661337297125       1.177128271450
      H      -0.500471876676       0.894626767091      -1.177128271450
      H      -0.524533568868      -0.880734742626      -1.177128271450
      H       1.025005445540      -0.013892024465      -1.177128271450
   End
End

Engine DFTB
   Model SCC-DFTB
   ResourcesDir DFTB.org/mio-1-1
EndEngine

EOF

echo "Relevant frequencies after optimisation"
$AMSBIN/amsreport 0D.results/dftb.rkf "Vibrations%Frequencies[cm-1]#1:18##1"
echo "End relevant frequencies"

AMS_JOBNAME=1D $AMSBIN/ams << EOF

Task GeometryOptimization

GeometryOptimization
   Convergence Gradients=1.0e-5
End

Properties
   NormalModes true
End

System
   Atoms
      C       0.000000000000       0.000000000000       0.767685465031
      C       0.000000000000       0.000000000000      -0.767685465031
```

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```
      H       0.964354016767       0.347635559279       1.177128271450
      H      -0.181115782790      -1.008972856410       1.177128271450
      H      -0.783238233981       0.661337297125       1.177128271450
      H      -0.500471876676       0.894626767091      -1.177128271450
      H      -0.524533568868      -0.880734742626      -1.177128271450
      H       1.025005445540      -0.013892024465      -1.177128271450
   End
   Lattice
      50.0   0.0   0.0
   End
End

Engine DFTB
   Model SCC-DFTB
   ResourcesDir DFTB.org/mio-1-1
EndEngine

EOF

echo "Relevant frequencies after optimisation"
$AMSBIN/amsreport 1D.results/dftb.rkf "Vibrations%Frequencies[cm-1]#3:20##1"
echo "End relevant frequencies"

AMS_JOBNAME=2D $AMSBIN/ams << EOF

Task GeometryOptimization

GeometryOptimization
   Convergence Gradients=1.0e-5
End

Properties
   NormalModes true
End

System
   Atoms
      C       0.000000000000       0.000000000000       0.767685465031
      C       0.000000000000       0.000000000000      -0.767685465031
      H       0.964354016767       0.347635559279       1.177128271450
      H      -0.181115782790      -1.008972856410       1.177128271450
      H      -0.783238233981       0.661337297125       1.177128271450
      H      -0.500471876676       0.894626767091      -1.177128271450
      H      -0.524533568868      -0.880734742626      -1.177128271450
      H       1.025005445540      -0.013892024465      -1.177128271450
   End
   Lattice
      50.0   0.0   0.0
      0.0   50.0   0.0
   End
End

Engine DFTB
   Model SCC-DFTB
   ResourcesDir DFTB.org/mio-1-1
EndEngine
```

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```
EOF

echo "Relevant frequencies after optimisation"
$AMSBIN/amsreport 2D.results/dftb.rkf "Vibrations%Frequencies[cm-1]#4:21##1"
echo "End relevant frequencies"

AMS_JOBNAME=3D $AMSBIN/ams << EOF

Task GeometryOptimization

GeometryOptimization
   Convergence Gradients=1.0e-5
End

Properties
   NormalModes true
End

System
   Atoms
      C       0.000000000000       0.000000000000       0.767685465031
      C       0.000000000000       0.000000000000      -0.767685465031
      H       0.964354016767       0.347635559279       1.177128271450
      H      -0.181115782790      -1.008972856410       1.177128271450
      H      -0.783238233981       0.661337297125       1.177128271450
      H      -0.500471876676       0.894626767091      -1.177128271450
      H      -0.524533568868      -0.880734742626      -1.177128271450
      H       1.025005445540      -0.013892024465      -1.177128271450
   End
   Lattice
      50.0   0.0   0.0
      0.0   50.0   0.0
      0.0    0.0  50.0
   End
End

Engine DFTB
   Model SCC-DFTB
   ResourcesDir DFTB.org/mio-1-1
EndEngine

EOF

echo "Relevant frequencies after optimisation"
$AMSBIN/amsreport 3D.results/dftb.rkf "Vibrations%Frequencies[cm-1]#4:21##1"
echo "End relevant frequencies"
```

10.2.7 Example: GO poly-ethyleen

Download GO_PEChain.run

```
#!/bin/sh


# first run: optimize coordinates with a fixed unit cell

AMS_JOBNAME=fixed $AMSBIN/ams << eor

Task GeometryOptimization

GeometryOptimization
  Convergence Gradients=0.0001
End

System
    Atoms [Bohr]
        C  -1.20630475   0.00000000   0.80181600
        C   1.20630475   0.00000000  -0.80181600
        H  -1.20630475   1.68180819   1.99106085
        H  -1.20630475  -1.68180819   1.99106085
        H   1.20630475   1.68180819  -1.99106085
        H   1.20630475  -1.68180819  -1.99106085
    End
    Lattice [Bohr]
       5.7 0 0
    End
End

Engine DFTB
   ResourcesDir Dresden
   Model DFTB0
   KSpace
       Type Symmetric
       Symmetric KInteg=5
   End
   Technical AnalyticalStressTensor=False # Not yet supported with symmetric k-space␣
↪grid ...
EndEngine

eor


# second run: also optimize lattice vectors

AMS_JOBNAME=lattice $AMSBIN/ams << eor

Task GeometryOptimization

GeometryOptimization
  Convergence Gradients=0.0001
  OptimizeLattice yes
End

System
    Atoms [Bohr]
```

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```
        C  -1.20630475   0.00000000   0.80181600
        C   1.20630475   0.00000000  -0.80181600
        H  -1.20630475   1.68180819   1.99106085
        H  -1.20630475  -1.68180819   1.99106085
        H   1.20630475   1.68180819  -1.99106085
        H   1.20630475  -1.68180819  -1.99106085
    End
    Lattice [Bohr]
       5.7 0 0
    End
End

Engine DFTB
   ResourcesDir Dresden
   Model DFTB0
   KSpace
       Type Symmetric
       Symmetric KInteg=5
   End
   Technical AnalyticalStressTensor=False # Not yet supported with symmetric k-space␣
↪grid ...
EndEngine

eor
```

10.2.8 Example: Restarting a geometry optimization

Download GO_restart.run

```
#!/bin/sh

# Step 1: Run the entire optimization in one go to get the reference result.

AMS_JOBNAME=reference $AMSBIN/ams 2>&1 << EOF

Task GeometryOptimization

System
    Atoms
        Mg      0.00000000       0.00000000       0.00000000
        H      -1.27917000       4.11016000       4.72389000
        O       2.16655000      -0.38813000      -7.10271000
        H      -1.42939000       1.48933000      -2.39439000
        H       1.09521000       1.50513000     -11.11199000
        C      -1.73924000      -3.56815000      -7.25491000
        O       1.13468000       2.30574000      -6.31297000
        H      -1.00635000      -3.89600000       0.57440000
        C       2.39949000       1.96079000      -8.76280000
        H      -0.50312000      -2.26723000       5.55260000
        H       0.50312000       2.26723000      -5.55260000
        C      -1.58070000       0.43033000       8.37317000
        C       1.68553000       0.69328000      -9.20655000
        H       3.10514000       2.27128000      -9.54815000
        C      -2.12273000       1.75783000       3.90134000
        C      -1.41195000      -3.08564000       8.52014000
```

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```
        C      -0.80701000      1.55547000      8.71125000
        H       2.96787000      1.75892000     -7.84715000
        H      -3.10514000     -2.27128000      9.54815000
        H       1.41484000     -2.74396000     -7.00335000
        H       1.12426000     -3.20203000      2.78552000
        C      -0.17468000      1.56294000      9.95926000
        C      -0.72719000     -2.63659000     -6.99325000
        C      -1.09765000     -3.99973000      9.52904000
        H      -0.25814000     -8.23193000     -3.30969000
        C       1.14520000     -2.61556000     -3.22986000
        O       0.72583000     -0.95806000     -1.56717000
        H      -2.36816000     -5.34341000     -4.50996000
        H      -2.96787000     -1.75892000      7.84715000
        H      -2.25336000      0.75053000      3.46787000
        N       2.80755000     -2.14965000     -4.91471000
        C      -0.30154000      0.48014000     10.82965000
        C       0.54101000     -2.17341000     -2.01004000
        C       2.39908000      0.51189000      4.29012000
        H      -1.63623000     -3.94265000     10.47839000
        H       0.19490000      0.50042000     11.80153000
        N       0.47889000      1.91215000     -0.81627000
        C      -0.66060000     -2.05093000      2.26021000
        H      -0.20633000     -7.24015000     -5.59602000
        H       1.49008000      0.40226000      3.68367000
        H      -0.39995000      4.15871000     -4.93170000
        H      -1.12426000      3.20203000     -2.78552000
        C      -1.03828000     -0.64018000     10.44800000
        H       1.56169000      4.33269000      8.01583000
        C      -0.11223000     -4.97150000      9.34588000
        C      -0.03554000      7.26375000      2.87602000
        H      -1.09521000     -1.50513000     11.11199000
        H       3.22983000      0.79151000      3.62424000
        C       3.45382000     -1.03521000     -6.98441000
        O      -0.72583000      0.95806000      1.56717000
        H       2.36816000      5.34341000      4.50996000
        C      -1.68553000     -0.69328000      9.20655000
        H       4.21952000     -0.40168000     -7.46345000
        H      -1.28611000     -2.92413000      2.51305000
        C       1.07673000     -4.19100000      5.79908000
        C       0.46002000      6.10723000      3.76764000
        H       0.19942000      5.47949000      5.84797000
        H      -0.11989000      5.68080000    -10.14146000
        N      -2.80755000      2.14965000      4.91471000
        H       1.23144000     -6.29513000     -5.15638000
        C       3.74078000     -1.20712000     -5.50076000
        N      -0.47889000     -1.91215000      0.81627000
        C      -0.57607000      5.02038000     -8.13428000
        H       1.60192000     -5.15615000      5.75895000
        H      -1.13094000     -1.13799000      2.64965000
        C      -0.23845000     -3.15299000     -1.28978000
        C      -0.05550000     -4.76579000     -3.14405000
        H      -1.35753000      5.76910000     -7.98196000
        H       3.72395000     -0.21480000     -5.00525000
        H      -1.13142000      7.24453000      2.78458000
        H      -4.76310000      1.61527000      5.41439000
        H       4.76310000     -1.61527000     -5.41439000
        C       2.12273000     -1.75783000     -3.90134000
```

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```
        C      -0.28104000      4.13616000      -7.08959000
        C       0.73514000      3.17615000      -7.28394000
        C       0.81335000     -3.86199000      -3.77035000
        C      -2.39908000     -0.51189000      -4.29012000
        H       2.25336000     -0.75053000      -3.46787000
        C       1.41195000      3.08564000      -8.52014000
        C      -0.52384000     -4.40125000      -1.88411000
        C      -1.84973000      1.90289000      -4.97333000
        H       0.20633000      7.24015000       5.59602000
        C       1.09765000      3.99973000      -9.52904000
        H       0.11989000     -5.68080000      10.14146000
        H       0.25814000      8.23193000       3.30969000
        H      -1.49008000     -0.40226000      -3.68367000
        H       1.63623000      3.94265000     -10.47839000
        C      -2.10065000      3.07251000      -5.70877000
        C       0.57607000     -5.02038000       8.13428000
        H      -1.56169000     -4.33269000      -8.01583000
        C       0.11223000      4.97150000      -9.34588000
        H      -1.13449000     -5.10187000      -1.30711000
        H       0.39995000     -4.15871000       4.93170000
        H       1.35753000     -5.76910000       7.98196000
        C      -3.29750000      3.15241000      -6.42939000
        C       0.23845000      3.15299000       1.28978000
        H      -3.22983000     -0.79151000      -3.62424000
        C      -0.59486000      2.70197000       7.73655000
        C       0.28104000     -4.13616000       7.08959000
        C       0.52384000      4.40125000       1.88411000
        H       0.43755000      2.42353000      10.23864000
        H      -3.50575000      4.04950000      -7.01656000
        H       0.38971000      7.20647000       1.86361000
        H       1.13449000      5.10187000       1.30711000
        C       1.84973000     -1.90289000       4.97333000
        C      -1.07673000      4.19100000      -5.79908000
        H       0.62192000     -3.64814000      -8.29677000
        C      -4.20635000      2.09524000      -6.41695000
        C       2.10065000     -3.07251000       5.70877000
        O      -0.62968000      1.82005000      -4.28278000
        C       0.03554000     -7.26375000      -2.87602000
        C       1.99778000      6.16492000       3.88117000
        C       3.29750000     -3.15241000       6.42939000
        H      -1.41484000      2.74396000       7.00335000
        O      -0.07653000     -0.68618000      -5.67912000
        H      -5.13801000      2.17027000      -6.98038000
        H       3.50575000     -4.04950000       7.01656000
        C      -3.45382000      1.03521000       6.98441000
        C      -1.14520000      2.61556000       3.22986000
        H      -2.30900000     -7.11968000      -4.33255000
        C       4.20635000     -2.09524000       6.41695000
        H       0.78141000     -0.75072000      -6.17605000
        H       1.13142000     -7.24453000      -2.78458000
        C      -0.54101000      2.17341000       2.01004000
        H       5.13801000     -2.17027000       6.98038000
        C      -3.91320000      0.93142000      -5.70744000
        H      -1.60192000      5.15615000      -5.75895000
        H      -0.43755000     -2.42353000     -10.23864000
        C       3.91320000     -0.93142000       5.70744000
        C       0.72575000     -2.17732000       2.89574000
```

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```
H        -4.21952000        0.40168000        7.46345000
H        -4.60197000        0.08443000       -5.74068000
H         4.60197000       -0.08443000        5.74068000
H        -0.62192000        3.64814000        8.29677000
H         2.30900000        7.11968000        4.33255000
H         1.27917000       -4.11016000       -4.72389000
C         2.72586000       -0.80591000        4.97465000
C        -2.72586000        0.80591000       -4.97465000
H        -0.19942000       -5.47949000       -5.84797000
H         1.42939000       -1.48933000        2.39439000
C         0.96682000        1.65125000        6.01252000
C        -1.99778000       -6.16492000       -3.88117000
C         0.59486000       -2.70197000       -7.73655000
C        -0.96682000       -1.65125000       -6.01252000
C         2.18562000        1.61836000        5.30149000
C         0.05550000        4.76579000        3.14405000
H         3.43079000       -2.01409000       -7.48984000
C         1.58070000       -0.43033000       -8.37317000
C         3.16089000        2.57613000        5.58075000
C        -3.74078000        1.20712000        5.50076000
C        -0.81335000        3.86199000        3.77035000
H        -3.43079000        2.01409000        7.48984000
H         4.09911000        2.55793000        5.02051000
C        -2.18562000       -1.61836000       -5.30149000
C         0.80701000       -1.55547000       -8.71125000
H        -2.47896000       -6.08599000       -2.89560000
C         2.94890000        3.55128000        6.55908000
C        -0.13167000        6.28247000        5.17426000
C         0.13167000       -6.28247000       -5.17426000
C         0.17468000       -1.56294000       -9.95926000
H         3.71667000        4.29632000        6.77231000
C        -3.16089000       -2.57613000       -5.58075000
C        -0.46002000       -6.10723000       -3.76764000
C        -0.61444000       -2.98553000        0.08587000
C         1.73924000        3.56815000        7.25491000
O         0.62968000       -1.82005000        4.28278000
H        -0.38971000       -7.20647000       -1.86361000
H         2.47896000        6.08599000        2.89560000
H        -4.09911000       -2.55793000       -5.02051000
C        -0.72575000        2.17732000       -2.89574000
O         0.07653000        0.68618000        5.67912000
C         0.61444000        2.98553000       -0.08587000
O        -2.16655000        0.38813000        7.10271000
C         0.30154000       -0.48014000      -10.82965000
H        -3.72395000        0.21480000        5.00525000
H         1.00635000        3.89600000       -0.57440000
H        -0.78141000        0.75072000        6.17605000
C        -2.94890000       -3.55128000       -6.55908000
C         0.72719000        2.63659000        6.99325000
C         0.66060000        2.05093000       -2.26021000
H        -1.23144000        6.29513000        5.15638000
H        -0.19490000       -0.50042000      -11.80153000
C        -2.39949000       -1.96079000        8.76280000
H         1.28611000        2.92413000       -2.51305000
O        -1.13468000       -2.30574000        6.31297000
H        -3.71667000       -4.29632000       -6.77231000
C         1.03828000        0.64018000      -10.44800000
```

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```
        H       1.13094000       1.13799000      -2.64965000
        C      -0.73514000      -3.17615000       7.28394000
    End
End

GeometryOptimization
   CoordinateType Cartesian
End

Engine DFTB
   ResourcesDir DFTB.org/3ob-3-1
   Model DFTB3
   DispersionCorrection D3-BJ
EndEngine

EOF


# Step 2: Start the optimization but abort after 5 steps.

AMS_JOBNAME=aborted $AMSBIN/ams 2>&1 << EOF

Task GeometryOptimization

GeometryOptimization
    MaxIterations 5
    CoordinateType Cartesian
End

LoadSystem
   File reference.results/ams.rkf
   Section InputMolecule
End

LoadEngine reference.results/dftb.rkf

EOF


# Step 3: Restart the aborted optimization and finish it.

AMS_JOBNAME=resume $AMSBIN/ams 2>&1 << EOF

Task GeometryOptimization

GeometryOptimization
   CoordinateType Cartesian
End

LoadSystem
   File aborted.results/ams.rkf
End

LoadEngine aborted.results/dftb.rkf
EngineRestart aborted.results/dftb.rkf

EOF
```

10.2.9 Example: GO with constraints

Download constraints.run

```
#!/bin/sh

# This example demonstrates the setup of all different types of constraints.
# Note that all constraints types can be combined with each other, as long as
# the resulting set of constraints actually makes sense. (It must of course be
# possible to satisfy all of them at the same time. AMS is not able to check
# that and you might get really surprising results if that is not the case ...)


# 1. Angle constraints
# ====================

AMS_JOBNAME=angle "$AMSBIN/ams" << EOF

   Task GeometryOptimization

   GeometryOptimization
      Convergence Step=1.0e-3
   End

   System
       Atoms
          O   0.001356   0.000999   0.000000
          H   0.994442  -0.037855   0.000000
          H  -0.298554   0.948531   0.000000
       End
   End

   Constraints
     # Fix the H--O--H angle to 125 degrees.
     Angle  3 1 2 125.0
   End

   Engine DFTB
       Model SCC-DFTB
       ResourcesDir Dresden
       DispersionCorrection Auto
   EndEngine

EOF


# 2. Distance constraints
# =======================

AMS_JOBNAME=dist "$AMSBIN/ams" << EOF

   Task GeometryOptimization

   GeometryOptimization
      Convergence Step=1.0e-3
   End

   System
```

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```
        Atoms
           O   0.001356   0.000999   0.000000
           H   0.994442  -0.037855   0.000000
           H  -0.298554   0.948531   0.000000
        End
        BondOrders
           1 2 1.0
           1 3 1.0
        End
    End
    Constraints
       # Fix the OH bond distances to 1.03 Angstrom, for which bonds need to be␣
↪defined in the System block
       All bonds O H to 1.03
       # Alternatively you can list the distances one by one as follows
       # Distance  1 2 1.03
       # Distance  1 3 1.03
    End

    Engine DFTB
        Model SCC-DFTB
        ResourcesDir Dresden
        DispersionCorrection Auto
    EndEngine

EOF


# 3. Dihedral angle constraint
# ============================

AMS_JOBNAME=dihed "$AMSBIN/ams" << EOF

    Task GeometryOptimization

    GeometryOptimization
       Convergence Step=1.0e-3
    End

    System
        Atoms
           C   -0.004115   -0.000021    0.000023
           C    1.535711    0.000022    0.000008
           H   -0.399693    1.027812   -0.000082
           H   -0.399745   -0.513934    0.890139
           H   -0.399612   -0.513952   -0.890156
           H    1.931188    0.514066    0.890140
           H    1.931432    0.513819   -0.890121
           H    1.931281   -1.027824    0.000244
        End
    End

    Constraints
       # Fix the dihedral angle H(6)--C(2)--C(1)--H(3) to 20 degrees.
       Dihedral  6 2 1 3 20.00
    End
```

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```
   Engine DFTB
       Model SCC-DFTB
       ResourcesDir Dresden
       DispersionCorrection Auto
   EndEngine

EOF


# 4a. Fixed atom constraint (Atoms keyword)
# =========================================

AMS_JOBNAME=atom "$AMSBIN/ams" << EOF

   Task GeometryOptimization

   GeometryOptimization
      Convergence Energy=1.0e-6 Gradients=1.0e-4 Step=1.0e-3
      CoordinateType Cartesian
   End

   System
      Atoms
         C   -0.2460249052   -1.70363153     0.0005128649944
         O    1.152833576    -1.81594932    -0.0004409224206
         C    1.489235475     0.61782051    10.0004771689226
         O    0.5700116914    0.627761615   10.0005491194077
      End
   End

   Constraints
      # Fix atom 1 and 2 at their initial positions.
      Atom 1
      Atom 2
   End

   Engine DFTB
      Model SCC-DFTB
      ResourcesDir DFTB.org/mio-1-1
   EndEngine

EOF


# 4b. Fixed atom constraint (AtomList keyword)
# ============================================

AMS_JOBNAME=atomlist "$AMSBIN/ams" << EOF

   Task GeometryOptimization

   GeometryOptimization
      Convergence Energy=1.0e-6 Gradients=1.0e-4 Step=1.0e-3
      CoordinateType Cartesian
   End

   System
```

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```
      Atoms
         C   -0.2460249052   -1.70363153     0.0005128649944
         O    1.152833576    -1.81594932    -0.0004409224206
         C    1.489235475     0.61782051    10.0004771689226
         O    0.5700116914    0.627761615   10.0005491194077
      End
   End

   Constraints
      # Fix atom 1 and 2 at their initial positions.
      AtomList 1:2
   End

   Engine DFTB
      Model SCC-DFTB
      ResourcesDir DFTB.org/mio-1-1
   EndEngine

EOF


# 4c. Fixed atom constraint (FixedRegion keyword)
# ===============================================

AMS_JOBNAME=region "$AMSBIN/ams" << EOF

   Task GeometryOptimization

   GeometryOptimization
      Convergence Energy=1.0e-6 Gradients=1.0e-4 Step=1.0e-3
      CoordinateType Cartesian
   End

   System
      Atoms
         C   -0.2460249052   -1.70363153     0.0005128649944    region=fixed
         O    1.152833576    -1.81594932    -0.0004409224206    region=fixed
         C    1.489235475     0.61782051    10.0004771689226
         O    0.5700116914    0.627761615   10.0005491194077
      End
   End

   Constraints
      # Fix all atoms in region "fixed"
      FixedRegion fixed
   End

   Engine DFTB
      Model SCC-DFTB
      ResourcesDir DFTB.org/mio-1-1
   EndEngine

EOF


# 4d. Fixed atom constraint (overlapping combination)
# ===================================================
```

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```
AMS_JOBNAME=combination "$AMSBIN/ams" << EOF

   Task GeometryOptimization

   GeometryOptimization
      Convergence Energy=1.0e-6 Gradients=1.0e-4 Step=1.0e-3
      CoordinateType Cartesian
   End

   System
      Atoms
         C   -0.2460249052   -1.70363153     0.0005128649944    region=fixed
         O    1.152833576    -1.81594932    -0.0004409224206    region=fixed
         C    1.489235475     0.61782051    10.0004771689226
         O    0.5700116914    0.627761615   10.0005491194077
      End
   End

   Constraints
      Atom 1
      AtomList 1 2
      FixedRegion fixed
   End

   Engine DFTB
      Model SCC-DFTB
      ResourcesDir DFTB.org/mio-1-1
   EndEngine

EOF


# 5. Fixed coordinate constraint
# ==============================

AMS_JOBNAME=coord "$AMSBIN/ams" << EOF

   Task GeometryOptimization

   GeometryOptimization
      Convergence Energy=1.0e-6 Gradients=1.0e-4 Step=1.0e-3
      CoordinateType Cartesian
   End

   System
      Atoms
         C   -0.2460249052   -1.70363153     0.0005128649944
         O    1.152833576    -1.81594932    -0.0004409224206
         C    1.489235475     0.61782051    10.0004771689226
         O    0.5700116914    0.627761615   10.0005491194077
      End
   End

   Constraints
      # Fix the x-coordinate of all atoms.
      Coordinate 1 x
```

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```
      Coordinate 2 x
      Coordinate 3 x
      Coordinate 4 x
   End

   Engine DFTB
      Model SCC-DFTB
      ResourcesDir DFTB.org/mio-1-1
   EndEngine

EOF


# 6. Fixed atom constraint (in periodic system)
# ==============================================

AMS_JOBNAME=pbcatom "$AMSBIN/ams" << EOF

   Task GeometryOptimization

   GeometryOptimization
      Convergence Step=1.0e-3
   End

   System
       Atoms
           C  -1.23  -0.710140830   0.0
           C  -1.23  -0.710140830   3.8
           C   0.0    0.0           0.4
           C   0.0   -1.42028166    3.355
       End

       Lattice
           1.23  -2.130422493309719  0.0
           1.23   2.130422493309719  0.0
       End
   End

   Constraints
      # Fix atom 1 and 3 at their initial positions.
      Atom 1
      Atom 3
   End

   Engine DFTB
      Model SCC-DFTB
      ResourcesDir DFTB.org/mio-1-1
      KSpace Quality=GammaOnly
   EndEngine

EOF


# 7. Block constraints (with listing the atoms in a block)
# ========================================================

AMS_JOBNAME=block_list "$AMSBIN/ams" << EOF
```

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```
Task GeometryOptimization

System
    Atoms
        C   0.5584839616765542   0.5023705181144142  -0.4625483159356394
        C   1.07173137896726     0.2125484528111251  -1.892767990599312
        C   1.699248504588085   -1.006061067555322   -2.191856791501442
        C   2.242484629452111   -1.236470028363516   -3.455616615521399
        C   2.18874580207099    -0.2444337131062739  -4.435483595049287
        C   1.604409798904145    0.9866950282217637  -4.135465239465763
        C   1.061086793296828    1.217355116664161   -2.871773146851866
        H   1.763625603740592   -1.780903563899969   -1.431707209662057
        H   2.716038261390732   -2.190869049673275   -3.672115451399807
        H   2.611833078693977   -0.4241619800888815  -5.420308290235123
        H   1.578029796368043    1.774138556616255   -4.884624561698751
        H   0.6247213391616491   2.187200330357715   -2.64521108544713
        C   1.303528070245188   -0.1416812092038768   0.7303699949711653
        C   0.8164830922475474  -1.314631142230651    1.326337082260565
        C   1.531799364672407   -1.947399963062604    2.342825210379356
        C   2.757684862125068   -1.432061688813837    2.765634667957531
        C   3.271640455523863   -0.2897364031184506   2.150731553729188
        C   2.556535912403799    0.3432056352653093   1.134221563049466
        H  -0.128925843064934   -1.7366201913903      0.9939642396630857
        H   1.133600273086767   -2.849990046242235    2.799740694330775
        H   3.31486005979636    -1.925049398411132    3.557912279830031
        H   4.236604921323707    0.1064455961800578   2.457138367063388
        H   2.976510069814392    1.222131876866508    0.6510413538003352
        C  -0.930165749820548    0.9153412637395284  -0.5420710991631585
        C  -1.791729737216814    0.6892660986048864   0.5418285200469819
        C  -3.111373625199894    1.139542032267652    0.5090625363459357
        C  -3.586568528476239    1.843983986018719   -0.5977864609101087
        C  -2.726152821786783    2.111108432452229   -1.663369105880468
        C  -1.406454626777386    1.660929752085611   -1.63085383469072
        H  -1.428888457076976    0.1571120160719108   1.417905619994904
        H  -3.76723983501283     0.9462006794587581   1.35432032282366
        H  -4.614972346570283    2.194578435055282   -0.6233521468909432
        H  -3.080200905921361    2.678981846821393   -2.520207901691867
        H  -0.7413545301831963   1.891248563160919   -2.459672151335554
        C   1.235557647765805    1.735720249011045    0.1803884343948648
        C   1.377191890012647    1.826646222422494    1.573181692925026
        C   1.905898822116255    2.975086608901246    2.16214311213053
        C   2.280792642899383    4.061906342938987    1.371311861877147
        C   2.105006642447361    3.998471351380415   -0.0115253875199488
        C   1.576317094651283    2.850163227898022   -0.6007264381779673
        H   1.072424817958776    0.9937816064904853   2.202306496283991
        H   2.017471491684088    3.023369029562452    3.242524256706377
        H   2.693031233132915    4.956641734238467    1.830324484771476
        H   2.372569859099136    4.8485771293401     -0.6342066225733602
        H   1.427765851939196    2.820397327218896   -1.677480576376967
    End
End

GeometryOptimization
    Convergence
        Energy 1.0e-6
        Gradients 1.0e-4
```

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```
            Step 1.0e-4
        End
        CoordinateType Delocalized
    End

    Constraints
       # Create blocks from the 4 phenyl groups by specifying the atom indices
       # explicitly. (The indices follow the order in the System%Atoms block,
       # where we happen to have the atoms belonging to the different phenyl
       # groups consecutive.)
       BlockAtoms  2  3  4  5  6  7  8  9 10 11 12
       BlockAtoms 13 14 15 16 17 18 19 20 21 22 23
       BlockAtoms 24 25 26 27 28 29 30 31 32 33 34
       BlockAtoms 35 36 37 38 39 40 41 42 43 44 45
    End

    Engine DFTB
        Model DFTB3
        ResourcesDir DFTB.org/3ob-3-1
        DispersionCorrection D3-BJ
    EndEngine

EOF


# 8. Block constraints (with named blocks)
# ========================================

AMS_JOBNAME=block_names "$AMSBIN/ams" << EOF

    Task GeometryOptimization

    System
        Atoms
            C   0.5584839616765542   0.5023705181144142  -0.4625483159356394
            C   1.07173137896726     0.2125484528111251  -1.892767990599312      ␣
↪region=phenyl1
            C   1.699248504588085   -1.006061067555322   -2.191856791501442      ␣
↪region=phenyl1
            C   2.242484629452111   -1.236470028363516   -3.455616615521399      ␣
↪region=phenyl1
            C   2.18874580207099    -0.2444337131062739  -4.435483595049287      ␣
↪region=phenyl1
            C   1.604409798904145    0.9866950282217637  -4.135465239465763      ␣
↪region=phenyl1
            C   1.061086793296828    1.217355116664161   -2.871773146851866      ␣
↪region=phenyl1
            H   1.763625603740592   -1.780903563899969   -1.431707209662057      ␣
↪region=phenyl1
            H   2.716038261390732   -2.190869049673275   -3.672115451399807      ␣
↪region=phenyl1
            H   2.611833078693977   -0.4241619800888815  -5.420308290235123      ␣
↪region=phenyl1
            H   1.578029796368043    1.774138556616255   -4.884624561698751      ␣
↪region=phenyl1
            H   0.6247213391616491   2.187200330357715   -2.64521108544713       ␣
↪region=phenyl1
```

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```
           C   1.303528070245188   -0.1416812092038768   0.7303699949711653      ␣
↪region=phenyl2
           C   0.8164830922475474  -1.314631142230651    1.326337082260565       ␣
↪region=phenyl2
           C   1.531799364672407   -1.947399963062604    2.342825210379356       ␣
↪region=phenyl2
           C   2.757684862125068   -1.432061688813837    2.765634667957531       ␣
↪region=phenyl2
           C   3.271640455523863   -0.2897364031184506   2.150731553729188       ␣
↪region=phenyl2
           C   2.556535912403799    0.3432056352653093   1.134221563049466       ␣
↪region=phenyl2
           H  -0.128925843064934   -1.7366201913903      0.9939642396630857      ␣
↪region=phenyl2
           H   1.133600273086767   -2.849990046242235    2.799740694330775       ␣
↪region=phenyl2
           H   3.31486005979636    -1.925049398411132    3.557912279830031       ␣
↪region=phenyl2
           H   4.236604921323707    0.1064455961800578   2.457138367063388       ␣
↪region=phenyl2
           H   2.976510069814392    1.222131876866508    0.6510413538003352      ␣
↪region=phenyl2
           C  -0.930165749820548    0.9153412637395284  -0.5420710991631585      ␣
↪region=phenyl3
           C  -1.791729737216814    0.6892660986048864   0.5418285200469819      ␣
↪region=phenyl3
           C  -3.111373625199894    1.139542032267652    0.5090625363459357      ␣
↪region=phenyl3
           C  -3.586568528476239    1.843983986018719   -0.5977864609101087      ␣
↪region=phenyl3
           C  -2.726152821786783    2.111108432452229   -1.663369105880468       ␣
↪region=phenyl3
           C  -1.406454626777386    1.660929752085611   -1.63085383469072        ␣
↪region=phenyl3
           H  -1.428888457076976    0.1571120160719108   1.417905619994904       ␣
↪region=phenyl3
           H  -3.76723983501283     0.9462006794587581   1.35432032282366        ␣
↪region=phenyl3
           H  -4.614972346570283    2.194578435055282   -0.6233521468909432      ␣
↪region=phenyl3
           H  -3.080200905921361    2.678981846821393   -2.520207901691867       ␣
↪region=phenyl3
           H  -0.7413545301831963   1.891248563160919   -2.459672151335554       ␣
↪region=phenyl3
           C   1.235557647765805    1.735720249011045    0.1803884343948648      ␣
↪region=phenyl4
           C   1.377191890012647    1.826646222422494    1.573181692925026       ␣
↪region=phenyl4
           C   1.905898822116255    2.975086608901246    2.16214311213053        ␣
↪region=phenyl4
           C   2.280792642899383    4.061906342938987    1.371311861877147       ␣
↪region=phenyl4
           C   2.105006642447361    3.998471351380415   -0.0115253875199488      ␣
↪region=phenyl4
           C   1.576317094651283    2.850163227898022   -0.6007264381779673      ␣
↪region=phenyl4
           H   1.072424817958776    0.9937816064904853   2.202306496283991       ␣
```

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```
↪region=phenyl4
          H   2.017471491684088    3.023369029562452    3.242524256706377       ␣
↪region=phenyl4
          H   2.693031233132915    4.956641734238467    1.830324484771476       ␣
↪region=phenyl4
          H   2.372569859099136    4.8485771293401     -0.6342066225733602      ␣
↪region=phenyl4
          H   1.427765851939196    2.820397327218896   -1.677480576376967       ␣
↪region=phenyl4
      End
   End

   GeometryOptimization
       Convergence
           Energy 1.0e-6
           Gradients 1.0e-4
           Step 1.0e-4
       End
       CoordinateType Delocalized
   End

   Constraints
      # Use the region from System%Atoms to set up the block constraints.
      Block phenyl1
      Block phenyl2
      Block phenyl3
      Block phenyl4
   End

   Engine DFTB
       Model DFTB3
       ResourcesDir DFTB.org/3ob-3-1
       DispersionCorrection D3-BJ
   EndEngine

EOF


# 9. Frozen strain components
# ===========================

AMS_JOBNAME=freezestrain "$AMSBIN/ams" << EOF

Task GeometryOptimization

GeometryOptimization
    OptimizeLattice Yes
    Convergence Step=1.0e-3
End

Constraints
   # Keeps first two lattice vectors orthogonal to the third.  Also fixes the
   # length of the third vector, keeping the graphene layer compressed.
   FreezeStrain xz yz zz
End

System
```

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```
    Atoms
        C 1.332002504889882e-05 -0.0005830055256093706 -8.209389319526933e-06
        C -1.22799350000696 -0.7102112812520209 2.281155685325205e-06
        C -0.0006872840163290542 -0.0003386565731411325 -1.981477647175959
        C 1.2274512359848 0.7092866246929653 -1.981478017299119
        C 2.455989750017203 -0.0007676724464739l5 -5.638209535859324e-06
        C 1.227983749989149 -0.7105220051279582 3.556077144406634e-06
        C 2.455553905980411 -0.0003697961984884611 -1.981476578954899
        C 3.68349483597652 0.7093774139714127 -1.981475303736415
        C 4.912014119974971 -0.0004697689000645081 8.202057640607653e-06
        C 3.68401303002027 -0.7103327188132248 -6.644074866545941e-06
        C 4.911561265976663 -0.0002732185613776612 -1.98147535090646
        C -3.685503114025999 0.7094747213946447 -1.98147447813657
        C -2.457004890026731 -0.0008782302621621878 8.760751751649826e-06
        C -3.684994169978904 -0.710349159056094 4 -6.913500704937906e-06
        C -2.45740142402999 -0.0002120088132086839 -1.981473170030486
        C -1.229200584026242 0.709517932531879 -1.98147439816519
        C 1.227980230018157 2.127401471357515 -5.950364005944094e-06
        C 9.469984377119545e-06 1.417970232416515 5.120417805695729e-06
        C 1.227229005981529 2.127790824745807 -1.981476944534885
        C 2.45544009594217 2.837313001498961 -1.981464045820237
        C 3.683977240012926 2.127396400995821 -4.237131224100653e-06
        C 2.456019429974761 1.41770041892015 8.271514976735398e-06
        C 3.683520895940616 2.127826615636785 -1.981463536474189
        C 4.911484545967099 2.837408990674362 -1.981472216079415
        C 6.140019459971655 2.127636216669431 9.289406940173374e-06
        C 4.912011129977858 1.417969521782559 7.256699431696856e-06
        C 6.139527915931508 2.12792209328836 -1.981460550680031
        C -2.457504644023984 2.837506078460876 -1.981475136785154
        C -1.229001220032881 2.127025640069692 1.077705178964691e-05
        C -2.457025360024441 1.417788944250494 8.010947395781608e-06
        C -1.229428944072945 2.128012192586653 -1.981459091806229
        C -0.001217694074323372 2.837543459113209 -1.981458639351295
        C 2.455982410005773 4.255441598373883 -1.892083560740779e-06
        C 1.228003499971814 3.545886142064043 9.237737681677788e-06
        C 2.455221785970465 4.255792992279458 -1.981473318340598
        C -1.228386974045185 -3.547700260767117 -1.981468190394571
        C 4.911976899993052 4.255411828501257 2.27723146438149e-06
        C 3.684014579960917 3.545723396055813 1.280915829951697e-05
        C 4.911520375955087 4.255828023455356 -1.981468278811
        C 1.227655395958869 -3.54761476141838 6 -1.98146951906497
        C -2.457018900008975 4.255512695928259 2.943041159330732e-06
        C 6.140026009993287 3.545891232143294 2.20060806891485e-06
        C 7.367526315913146 4.255927240986645 -1.981454533470139
        C -6.141340994042006 -3.547511474074143 -1.981469232026619
        C -0.001002500050462096 4.255387679251578 1.654017565004685e-05
        C -1.228981830007242 3.545851372434187 2.37503105142233e-06
        C -0.00142595404759982 4.256013860539822 -1.981467396982039
        C -3.685044664049419 -3.547477052980626 -1.981466802486946
        C -1.227808819999351 -2.12938224692705 -2.127801149456805e-07
        C -2.455832350038186 -2.838708610558109 1.251523005803983e-05
        C -1.228620264037983 -2.129205540950233 -1.981470550283798
        C -0.0004192140835714842 -1.419477849521901 -1.981455609514733
        C 1.228193719957573 -2.129406616582517 1.390527520593389e-05
        C 0.0001477699611014405 -2.839255138681037 1.274825905530347e-05
        C 1.227684425953123 -2.129163359695275 -1.981467635427455
        C 2.455626385910209 -1.419413169537493 -1.981453570671329
```

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```
        C -6.140842350045955 -2.129322170430451 1.506226938282425e-05
        C 2.456153479955113 -2.839200210115958 1.47101339575357e-05
        C 3.683689305925244 -2.129064842197087 -1.981458500475127
        C -4.913374384079035 -1.419316522220884 -1.981457095053834
        C -3.684843340052955 -2.129350560151249 1.735547419229382e-05
        C -4.912808430047692 -2.839071261955975 1.563048016823986e-05
        C -3.685268534086676 -2.128978772839927 -1.98145459141338
        C -2.45712732409351 -1.419353221465499 -1.981452351546793
        C -2.996192032925579e-05 -0.000699242152149526 3.962939886687566
        C -1.228003971875175 -0.7103778453492622 3.962925088122617
        C -0.000700355908038296 -0.0003332148789394825 1.981452859744668
        C 1.227439704045832 0.7092909964964251 1.981467977918086
        C 2.455972288079895 -0.000591484995550912 3.962939812711258
        C 1.228003298120663 -0.7104549535647978 3.962926452096982
        C 2.455542044092204 -0.0003647244468015716 1.981452779807835
        C 3.683482354040657 0.7093820057289575 1.981469673526022
        C 4.912000348117807 -0.0004686671456845799 3.96292738718769
        C 3.683997778083127 -0.7103249572456309 3.962938753391991
        C 4.911548884078128 -0.0002680168299863262 1.981457393146928
        C -3.685515265933381 0.7094801331342701 1.981461165904004
        C -2.457014661901717 -0.0008761383582568633 3.962933787286889
        C -3.685007531928472 -0.7103425373777408 3.962942555784025
        C -2.457412705931413 -0.0002065770405354501 1.981460520958165
        C -1.229211335932976 0.7095228343414065 1.98146103281522
        C 1.227967348110556 2.127386193561453 3.962929764672974
        C -4.281883530521391e-06 1.417919455416095 3.96292782690195
        C 1.227218624090811 2.127796526544795 1.981453236878594
        C 2.455427384033809 2.83731889320433 1.981471917810995
        C 3.683966438104317 2.12740635268383 3.962931809362267
        C 2.456006178071116 1.417740879775001 3.962942690498066
        C 3.683508864080636 2.127831077384122 1.981456571921596
        C 4.911472874041424 2.837414422441095 1.981469423240322
        C 6.140006188100173 2.127640908364754 3.96293316778528
        C 4.912000948062944 1.417975193600739 3.962945368689221
        C 6.139515384034993 2.127928054994523 1.981471530520008
        C -2.457516635928298 2.837511270211092 1.981459501137365
        C -1.229012451945974 2.127104470095207 3.962948291371187
        C -2.457033631907664 1.417792836176979 3.962935736248542
        C -1.229441855971066 2.128017364296635 1.981473516125039
        C -0.001231065982844282 2.83754798082405 1.981477377543141
        C 2.455970918062962 4.255446730162459 3.962945363741043
        C 1.227990978068837 3.545888883850297 3.962943437699987
        C 2.455207564067417 4.255798083939164 1.981460905296909
        C -1.228397585936881 -3.54769452897796 1.981462310609218
        C 4.911964488060532 4.255420650159205 3.962946159605713
        C 3.684002968100828 3.545727757822979 3.962932953064215
        C 4.911507194030889 4.25583213519047 1.981472875202606
        C 1.22764468406568 -3.547609799614339 1.981461473160161
        C -2.457027591902453 4.255510887977889 3.962934029953071
        C 6.140011718057854 3.545898453762834 3.962947035832434
        C 7.367513404018803 4.25593209270268 1.981476837527609
        C -6.141352815949912 -3.547506482310592 1.981466583645511
        C -0.001013701916043441 4.255385511194097 3.962938483249906
        C -1.228995721948309 3.545866003895579 3.962949056786192
        C -0.001438315946372004 4.256019262267359 1.98146542401001
        C -3.68505504595736 -3.547472521146422 1.981469025022036
        C -1.227817711946263 -2.129397354545356 3.962948386486201
```

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```
        C -2.45584760189824 -2.838693919188594 3.962932647309199
        C -1.22863031596877 -2.129200899095368 1.981472763926178
        C -0.0004312259786934947 -1.419471387806733 1.981476015973903
        C 1.228183428085925 -2.129384525179524 3.962937836939656
        C 0.0001342880538246494 -2.839225227582055 3.962948356816577
        C 1.227671624025677 -2.129158527960262 1.981474583888431
        C 2.455614294015247 -1.419407657803005 1.981478001551132
        C -6.140855951953014 -2.129314868796188 3.962950599781267
        C 2.456139408049645 -2.839212628030558 3.962949726809414
        C 3.683677514018658 -2.12905939044384 1.98147688315868
        C -4.913386125957436 -1.419311390469788 1.981469050050141
        C -3.68485488196171 -2.129348928295441 3.96295344930467
        C -4.91282016191732 -2.839063750265042 3.962938899273355
        C -3.685281025994509 -2.12897353111013 1.981481200585353
        C -2.457141595966529 -1.419347949824808 1.981472029890663
    End
    Lattice
        9.825000579999999 0.0 0.0
        4.91182904 8.51302256 0.0
        0.0 0.0 8.0
    End
End

Engine DFTB
    Model DFTB
    ResourcesDir DFTB.org/mio-1-1
    KSpace
        Quality GammaOnly
    End
EndEngine

EOF


# 10. Equalized strain components
# ===============================

AMS_JOBNAME=equalstrain "$AMSBIN/ams" << EOF

Task GeometryOptimization

GeometryOptimization
    OptimizeLattice Yes
    Convergence Step=1.0e-3
End

Constraints
   # Keep the cell cubic, but allow the size of the cube to vary.
   FreezeStrain xy xz yz
   EqualStrain  xx yy zz
End

System
    Atoms
        C -0.132285 3.230196 3.399625
        H 0.67231 2.571995 3.747816
        H -0.546925 3.782407 4.25108
```

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```
        H -0.921872 2.627955 2.935193
        H 0.267346 3.938428 2.664409
        C 2.647972 3.79511 0.161215
        H 2.745753 2.707187 0.254494
        H 2.108302 4.189352 1.030219
        H 2.093026 4.03506 -0.753279
        H 3.644808 4.248843 0.113424
        C -3.290954 -3.607704 -3.419879
        H -4.099867 -4.000479 -4.046956
        H -2.386445 -3.482146 -4.026458
        H -3.088346 -4.309774 -2.602634
        H -3.589157 -2.638419 -3.003466
        C -3.900392 1.971446 -2.092972
        H -2.821972 1.97396 -1.895882
        H -4.303924 2.977719 -1.930439
        H -4.394183 1.265761 -1.414725
        H -4.081488 1.668344 -3.130841
        C -3.143958 -3.520015 3.393796
        H -3.128547 -4.088022 2.456262
        H -3.994325 -3.845525 4.004334
        H -3.24151 -2.450891 3.171766
        H -2.211449 -3.695621 3.94282
        C -0.31406 -0.626145 3.522914
        H -0.044022 0.228271 4.154493
        H -1.353702 -0.912447 3.720437
        H 0.346904 -1.471041 3.749005
        H -0.205421 -0.349364 2.467723
        C 3.411151 -3.454122 0.161835
        H 2.877462 -2.569463 0.528433
        H 4.211866 -3.141886 -0.518755
        H 2.711585 -4.107617 -0.372385
        H 3.843691 -3.997522 1.010048
        H -3.283653 -0.451758 -4.172013
        H -1.922139 0.6502520000000001 -3.802207
        H -2.586463 -0.412172 -2.523601
        C -2.360175 -0.332772 -3.593334
        H -1.648446 -1.117408 -3.875514
        C 3.046249 -3.33059 3.76859
        H 2.414628 -3.18136 2.88506
        H 2.465863 -3.831302 4.55235
        H 3.39517 -2.358701 4.136729
        H 3.909333 -3.950995 3.500222
        C -3.086408 3.73574 0.4638
        H -2.559805 3.990117 -0.463465
        H -2.394025 3.813016 1.310247
        H -3.469203 2.710618 0.397221
        H -3.922599 4.429208 0.611196
        C 3.736451 0.338903 -0.234383
        H 4.139844 -0.659226 -0.441391
        H 4.286082 0.789262 0.6004350000000001
        H 2.675343 0.256879 0.028602
        H 3.844535 0.968696 -1.125179
        C -0.953217 3.761489 -3.029722
        H -0.738671 2.687271 -2.986546
        H -2.017033 3.913231 -3.24677
        H -0.349572 4.223228 -3.819817
        H -0.707592 4.222226 -2.065757
```

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```
        C 3.438238 3.368005 3.536049
        H 3.718968 3.030104 2.531632
        H 4.305113 3.831685 4.021198
        H 3.102844 2.509703 4.129906
        H 2.62603 4.10053 3.461459
        C -0.093351 2.447961 0.147782
        H 0.412783 2.191741 -0.790311
        H -1.100739 2.015519 0.149423
        H -0.163522 3.53817 0.239205
        H 0.478074 2.046413 0.99281
        C -0.06737899999999999 -1.067744 -0.644773
        H 0.831493 -1.69444 -0.611303
        H -0.920384 -1.630791 -0.248288
        H -0.271712 -0.77696 -1.681851
        H 0.091087 -0.168785 -0.037648
        C -3.13266 0.095347 1.684164
        H -2.468956 -0.758832 1.506078
        H -3.797646 -0.127993 2.526632
        H -3.731911 0.285949 0.786162
        H -2.532126 0.982263 1.917783
        C -3.650862 -2.700373 -0.074687
        H -4.155919 -2.467829 0.87013
        H -2.740814 -3.276506 0.129574
        H -3.385824 -1.767849 -0.58654
        H -4.32089 -3.289309 -0.711913
        C 3.803884 3.754796 -3.348637
        H 3.946713 2.667857 -3.350306
        H 2.769436 3.987861 -3.626912
        H 4.48894 4.214494 -4.07059
        H 4.010448 4.148971 -2.34674
        C 2.868209 0.11231 2.894284
        H 2.317604 0.914041 2.388417
        H 2.406222 -0.09055000000000001 3.867554
        H 3.909847 0.420825 3.041412
        H 2.839161 -0.7950739999999999 2.279753
        C -0.320765 -3.560008 1.887422
        H -0.965068 -2.68183 2.011986
        H 0.02585 -3.901247 2.869895
        H 0.543227 -3.294315 1.26713
        H -0.88707 -4.36264 1.400678
        C 2.415398 -1.437717 -2.776235
        H 1.964383 -1.676188 -3.746573
        H 2.445411 -2.340763 -2.155392
        H 1.816728 -0.668767 -2.274091
        H 3.43507 -1.065149 -2.928883
        C -3.625996 2.934989 3.78523
        H -4.070333 2.734452 2.803299
        H -3.043299 2.064066 4.107404
        H -4.421782 3.131813 4.513121
        H -2.968572 3.809626 3.717096
        C 1.422335 1.538945 -3.931672
        H 0.608488 0.8054 -3.894205
        H 2.3282 1.060135 -4.321529
        H 1.616409 1.921293 -2.92272
        H 1.136242 2.368954 -4.588236
        C 0.028875 -3.521123 -2.677443
        H 0.240436 -2.624091 -3.271089
```

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```
        H -0.857142 -3.347281 -2.055678
        H 0.888225 -3.744967 -2.034598
        H -0.156019 -4.368152 -3.348409
    End
    Lattice
        10.0 0.0 0.0
        0.0 10.0 0.0
        0.0 0.0 10.0
    End
End

Engine DFTB
    Model DFTB
    ResourcesDir DFTB.org/mio-1-1
    KSpace
        Quality GammaOnly
    End
EndEngine

EOF
```

10.2.10 Example: GO with restraints

Download GO_restraints.run

```
#!/bin/sh

$AMSBIN/ams <<EOR

Task GeometryOptimization

Properties
    Gradients
End

System
  Atoms
    O    -0.73806601     0.05760021     0.28813500
    O     0.73806601    -0.05760021     0.28813500
    H     0.95903096     0.70364829    -0.28813500
    H    -0.95903096    -0.70364829    -0.28813500
  End
End

UseSymmetry False

Restraints
# Change the default profile type
   Profile Hyperbolic
# Change the asymptotic value for the restraint force
   fInfinity 10.0
#  Type      Atoms     OptValue  FC   Profile      F(Inf)
   Distance 1 2         5.0      1.0  Erf          1.0
   Angle    1 2 3      90.0
   SumDist  1 4 2 3     1.5
```

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```
   DifDist  2 3 1 4    0.2
   Dihedral 4 1 2 3  180.0     0.1
End


Engine DFTB
  Model GFN1-xTB
EndEngine
EOR
```

10.2.11 Example: geometry optimizations: automations

Download DFTBAutomations.run

```
#!/bin/bash

# the System is extremely artificial but the calculation points out something useful

# The system has two CO molecules, one of which is compressed.
# We freeze the coordinates of the compressed CO molecules

# We define a gradient dependent electronic temperature (excluding the gradient of␣
↪the constrained atoms)
# When far from convergence a higher value is used to ease SCF convergence (not␣
↪relevant to this system)
# When the gradients become small the temperature is lowered, so that is will have␣
↪negligible influence on the energy

# Here we let on purpose not converge the geometry optimization
# The final calculation should be performed as a normal single point and we␣
↪explicitly set in band the ElectronicTemperature to 0.001

report=report.txt

echo "We use a gradient dependent KT value (finite electronic temperature)" > $report

printf "\nThe value of kT gets progressively lower during the optimization\n\n" >>
↪$report

printf "\nFor two optimizers we do 3 steps and they do not converge. Yet the last␣
↪single point should be done at KTlow=0.001\n\n" >> $report

targetKT=0.001

system=test

for optim in Quasi-Newton FIRE
do

for automation in yes
do

export AMS_JOBNAME=$system.optim=$optim.automation=$automation

rm -rf $AMS_JOBNAME.results
```

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```
$AMSBIN/ams<<EOF

EngineDebugging NeverQuiet=yes

# log
#   debug AutomationInteractionModule
# end

Task GeometryOptimization

GeometryOptimization
    Method $optim
    MaxIterations 2

    EngineAutomations
       Enabled $automation
       Gradient variable=Occupation%KT InitialValue=0.01 FinalValue=$targetKT␣
↪HighGradient=0.1 LowGradient=1.0e-3
       Iteration variable=SCC%Converge%Charge InitialValue=1.0e-3 FinalValue=1.0e-8␣
↪FirstIteration=0 LastIteration=1
    End
end


Constraints
    Atom 3
    Atom 4
End

System

  Atoms
     C 0.0 0.0 0.0
     O 1.13 0.0 0.0
     C 0.0 5.0 0.0
     O 1.0 5.0 0.0
  End
End


Engine DFTB
   Occupation kT=$targetKT
EndEngine

EOF

echo "kT series for optimizer: $optim" >> $report
grep "temperature kT" $AMS_JOBNAME.results/ams.log | awk '{print $NF}' >> $report
echo "(the last kT should be 0.001)" >> $report
echo "">>$report


echo "Converge%charge for optimizer: $optim" >> $report
grep "setting SCC%Converge%Charge to" $AMS_JOBNAME.results/ams.log | awk '{print $NF}
↪' >> $report
# echo "(the last value should be 1.0e-8)" >> $report
```

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```
echo "">>$report

done
done

echo "begin report"
cat $report
echo "end report"
```

10.2.12 Example: Geometry optimization for an excited state

Download GO_LR-TDDFTB_benzene.run

```
#!/bin/sh

# This test optimizes the geometry of the lowest singlet excitation
# of benzene. This was an example from Niehaus' original paper on
# TD-DFTB gradients. See
#      D. Heringer et al. J. Comput. Chem. 28:2589-2601, 2007
# for his results and the C-C and C-H bond distances this test
# should produce.

$AMSBIN/ams << eor

Task GeometryOptimization
GeometryOptimization
   Convergence Gradients=0.0001
End

System
    Atoms
      H    0.000000       2.484212      0.000000
      H    0.000000      -2.484212      0.000000
      H    2.151390       1.242106      0.000000
      H   -2.151390      -1.242106      0.000000
      H   -2.151390       1.242106      0.000000
      H    2.151390      -1.242106      0.000000
      C    0.000000       1.396792      0.000000
      C    0.000000      -1.396792      0.000000
      C    1.209657       0.698396      0.000000
      C   -1.209657      -0.698396      0.000000
      C   -1.209657       0.698396      0.000000
      C    1.209657      -0.698396      0.000000
    End
End


Engine DFTB
   Model SCC-DFTB
   ResourcesDir DFTB.org/mio-1-1
   Properties
       Excitations
           TDDFTB
               Calc singlet
               Lowest 1
```

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```
                Diagonalization exact
            End
            TDDFTBGradients
                Excitation 1
            End
        End
    End
EndEngine

eor
```

10.2.13 Example: Geometry optimization following a specific excited state

Download GO_LR-TDDFTB_CO_eigenfollow.run

```
#!/bin/sh

# This test optimizes the 1st and 3rd triplet excitation of
# carbon monoxide. The difficult thing about these two is
# that they change character during the optimization. What
# is the lowest triplet at the ground state equilibrium will
# become the third triplet during the optimization and vice
# versa. We are using the eigenfollow keyword to follow the
# excitations during the geometry optimization.

AMS_JOBNAME=followT1 $AMSBIN/ams << eor

Task GeometryOptimization

System
    Atoms
      C    0.0000    0.0000    0.0000
      O    1.1000    0.0000    0.0000
    End
End

Engine DFTB

   Model SCC-DFTB
   ResourcesDir DFTB.org/mio-1-1

   Properties
       Excitations
           TDDFTB
               Calc triplet
               Lowest 10
               Print EVContribs
           End
           TDDFTBGradients
               Excitation 1
               Eigenfollow true
           End
       End
   End
```

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```
EndEngine

Log
   Info TDDFTBExcitationFollowerModule
End

eor


AMS_JOBNAME=followT3 $AMSBIN/ams << eor

Task GeometryOptimization

System
    Atoms
      C    0.0000    0.0000    0.0000
      O    1.1000    0.0000    0.0000
    End
End

Engine DFTB

   Model SCC-DFTB
   ResourcesDir DFTB.org/mio-1-1

   Properties
       Excitations
           TDDFTB
               Calc triplet
               Lowest 10
               Print EVContribs
           End
           TDDFTBGradients
               Excitation 3
               Eigenfollow true
           End
       End
   End

EndEngine

Log
   Info TDDFTBExcitationFollowerModule
End

eor
```

10.3 PESScan, Linear Transit, Transition State, NEB

10.3.1 Example: Linear transit

Download LinearTransit.run

```
#!/bin/sh



echo "================="
echo "HCN isomerization"
echo "================="
echo

AMS_JOBNAME=HCN_isomerization $AMSBIN/ams << EOF

   Task PESScan
   # (Linear transit is just a PES scan with 1 scan coordinate.)

   System
      Atoms
         C       0.00000000       0.00000000       1.04219000
         H       0.00000000       0.00000000      -0.03324000
         N       0.00000000       0.00000000       2.20064000
      End
   End

   PESScan
      ScanCoordinate
         nPoints 25
         Angle  2 1 3  180.0 0.0
      End
   End

   Engine DFTB
      Model DFTB0
      ResourcesDir DFTB.org/mio-1-1
   EndEngine

EOF



echo
echo "==================="
echo "Water angle transit"
echo "==================="
echo

AMS_JOBNAME=water_angle $AMSBIN/ams << EOF

   Task PESScan

   System
      Atoms
         O       0.00000000       0.00000000       0.59372000
```

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```
         H       0.00000000       0.76544000      -0.00836000
         H       0.00000000      -0.76544000      -0.00836000
      End
   End

   PESScan
      ScanCoordinate
         nPoints 25
         Angle  2 1 3  80.0 180.0
      End
   End

   GeometryOptimization
      ! Delocalized coordinates currently have a problem with linear systems.
      ! So we will use cartesian coordinates here.
      CoordinateType Cartesian
   End

   Engine DFTB
      Model DFTB0
      ResourcesDir DFTB.org/mio-1-1
   EndEngine

EOF



echo
echo "===================="
echo "Hydrocarbon reaction"
echo "===================="
echo

AMS_JOBNAME=hydcarb $AMSBIN/ams << EOF

   Task PESScan

   System
      Atoms
         C       0.14667300      -0.21503500       0.40053800
         C       1.45297400      -0.07836900       0.12424400
         C       2.23119700       1.15868100       0.12912100
         C       1.78331500       2.39701500       0.38779700
         H      -0.48348000       0.63110600       0.67664100
         H      -0.33261900      -1.19332100       0.35411600
         H       2.01546300      -0.97840100      -0.14506700
         H       3.29046200       1.03872500      -0.12139700
         H       2.45728900       3.25301000       0.35150400
         H       0.74193400       2.60120700       0.64028800
         C      -0.75086900       1.37782400      -2.43303700
         C      -0.05392100       2.51281000      -2.41769100
         H      -1.78964800       1.33942600      -2.09651100
         H      -0.30849400       0.43896500      -2.76734700
         H      -0.49177100       3.45043100      -2.06789100
         H       0.98633900       2.54913500      -2.74329400
      End
   End
```

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```
   PESScan
      ScanCoordinate
         nPoints 25
         Distance  1 11   3.36  1.538
         Distance  4 12   3.36  1.538
      End
   End

   Engine DFTB
      Model DFTB0
      ResourcesDir DFTB.org/mio-1-1
   EndEngine

EOF



echo
echo "====================================="
echo "Retinal trans -> 11-cis isomerization"
echo "====================================="
echo

AMS_JOBNAME=retinal_transcis $AMSBIN/ams << EOF

   Task PESScan

   System
      Atoms
         H      -2.10968473      -1.58238733       0.78224517
         C      -2.10306857      -0.54058322       0.46363503
         C      -0.89436995       0.04807217       0.25528247
         H      -0.85555481       1.05432693      -0.15803658
         C       0.38987539      -0.58661182       0.49038464
         C       1.53213446       0.09657801       0.14394773
         H       1.40518949       1.08783970      -0.29205231
         H       3.05232192      -1.34477492       0.72115301
         C       2.88311454      -0.36358433       0.28105432
         C       3.96024700       0.37378345      -0.12385974
         H       3.77965758       1.35231793      -0.56821856
         C       5.34627719      -0.04025647      -0.02249097
         C       6.32191717       0.80135945      -0.49190463
         H       6.00090638       1.74979100      -0.92101391
         C      -4.46825064      -0.90426552      -0.39585925
         C      -5.87277429      -0.25303564      -0.45007491
         C      -3.41139545       0.06493448       0.19516310
         C      -3.67932839       1.38221399       0.41656971
         C      -5.81598497       1.19032366      -0.92660753
         C      -5.00049358       2.01922634       0.05561242
         C      -4.58391145      -2.18782901       0.46346394
         C      -4.01729542      -1.30039402      -1.82272212
         C      -2.72429960       2.32303313       1.10290124
         C       0.40919453      -1.96244629       1.09501374
         C       5.64155973      -1.38034133       0.59419110
         C       7.76996060       0.56699126      -0.48750226
         O       8.57693167       1.36615612      -0.92976322
```

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```
         H      -6.51997817      -0.84904979      -1.10100203
         H      -6.32039371      -0.28079023       0.54871092
         H      -5.36159995       1.23817633      -1.92112092
         H      -6.82595442       1.60207678      -1.01946858
         H      -5.58216571       2.18390764       0.97424181
         H      -4.81292271       3.01993001      -0.35246294
         H      -4.74166770      -1.94289144       1.51126095
         H      -5.43008715      -2.78247632       0.12572479
         H      -3.69644845      -2.81116549       0.38705593
         H      -3.02900804      -1.75403268      -1.79820003
         H      -4.71056940      -2.01489741      -2.26202914
         H      -3.97070839      -0.42860260      -2.47090348
         H      -2.16469005       2.92261100       0.38111736
         H      -3.27791517       3.02297911       1.72885233
         H      -2.00470188       1.79865198       1.72726573
         H      -0.13689001      -1.97717074       2.03825359
         H      -0.07664772      -2.68134154       0.43362393
         H       1.41837401      -2.31391556       1.28591185
         H       5.15278730      -2.17622743       0.03222328
         H       6.70436647      -1.59729505       0.62729622
         H       5.25700064      -1.42489613       1.61313095
         H       8.12614442      -0.41441814      -0.04549414
      End
   End

   PESScan
      ScanCoordinate
         nPoints 25
         Dihedral  6 9 10 12  180  0
         Dihedral  8 9 10 11  180  0
      End
   End

   Engine DFTB
      Model DFTB0
      ResourcesDir DFTB.org/mio-1-1
   EndEngine

EOF
```

10.3.2 Example: Linear Transit periodic

Download LinearTransit_periodic.run

```
#! /bin/sh


AMS_JOBNAME=benzene_chain_fixlat $AMSBIN/ams << EOF

Task PESScan

System
    Atoms
        C -1.489965953299734 -1.196709452657141 0.0
        C 2.88853832859411 -1.196342899137159 0.0
```

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```
        H -0.9793010528075118 -2.156600187713776 0.0
        H 3.399964258112557 -2.155323474266199 0.0
        H -3.399964258111068 2.15532347426531 0.0
        H 0.9793010528058212 2.156600187714014 0.0
        H -0.9793010528078538 2.156600187713226 0.0
        H 3.399964258114027 2.155323474265703 0.0
        H -3.399964258114545 -2.155323474265097 0.0
        H 0.9793010528059179 -2.156600187714516 0.0
        C -3.620245510890842 0.0 0.0
        C 0.7584629375509923 0.0 0.0
        C -0.758462937550813 0.0 0.0
        C 3.620245510892222 0.0 0.0
        C -2.888538328594733 -1.196342899137046 0.0
        C 1.48996595330026 -1.196709452655725 0.0
        C -2.888538328594084 1.196342899137163 0.0
        C 1.489965953301639 1.196709452655903 0.0
        C -1.489965953301249 1.196709452657369 0.0
        C 2.888538328594885 1.196342899137957 0.0
    End
    Lattice
        8.758301940824319 0.0 0.0
    End
End

PESScan
    ScanCoordinate
        nPoints 11
        Dihedral  1 13 12 16  0 90
        Dihedral 19 13 12 18  0 90
    End
End

GeometryOptimization
    OptimizeLattice No
    Convergence
        Energy 1.0e-6
        Gradients 1.0e-4
    End
End

Engine DFTB
    Model DFTB0
    ResourcesDir DFTB.org/mio-1-1
    KSpace Quality=GammaOnly
EndEngine

EOF



AMS_JOBNAME=benzene_chain_latopt $AMSBIN/ams << EOF

Task PESScan

System
    Atoms
        C -1.489965953299734 -1.196709452657141 0.0
```

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```
        C 2.88853832859411 -1.196342899137159 0.0
        H -0.9793010528075118 -2.156600187713776 0.0
        H 3.399964258112557 -2.155323474266199 0.0
        H -3.399964258111068 2.15532347426531 0.0
        H 0.9793010528058212 2.156600187714014 0.0
        H -0.9793010528078538 2.156600187713226 0.0
        H 3.399964258114027 2.155323474265703 0.0
        H -3.399964258114545 -2.155323474265097 0.0
        H 0.9793010528059179 -2.156600187714516 0.0
        C -3.620245510890842 0.0 0.0
        C 0.7584629375509923 0.0 0.0
        C -0.758462937550813 0.0 0.0
        C 3.620245510892222 0.0 0.0
        C -2.888538328594733 -1.196342899137046 0.0
        C 1.48996595330026 -1.196709452655725 0.0
        C -2.888538328594084 1.196342899137163 0.0
        C 1.489965953301639 1.196709452655903 0.0
        C -1.489965953301249 1.196709452657369 0.0
        C 2.888538328594885 1.196342899137957 0.0
    End
    Lattice
        8.758301940824319 0.0 0.0
    End
End

PESScan
    ScanCoordinate
        nPoints 11
        Dihedral  1 13 12 16  0 90
        Dihedral 19 13 12 18  0 90
    End
End

GeometryOptimization
    OptimizeLattice Yes
    Convergence
        Energy 1.0e-6
        Gradients 1.0e-4
    End
End

Engine DFTB
    Model DFTB0
    ResourcesDir DFTB.org/mio-1-1
    KSpace Quality=GammaOnly
EndEngine

EOF
```

10.3.3 Example: PESScan ethane

Download PESScan.run

```
#!/bin/sh


echo "=============="
echo "Ethane torsion"
echo "=============="
echo

AMS_JOBNAME=ethane_torsion $AMSBIN/ams << EOF

   Task PESScan

   System
      Atoms
         C   0.0          0.0          0.76576
         C   0.0          0.0         -0.76576
         H  -0.88668938   0.51193036   1.16677
         H   0.88668938   0.51193036   1.16677
         H   0.0         -1.02386071   1.16677
         H   0.0          1.02386071  -1.16677
         H  -0.88668938  -0.51193036  -1.16677
         H   0.88668938  -0.51193036  -1.16677
      End
   End

   PESScan
      # First scan coordinate: C--C bond distance
      ScanCoordinate
         nPoints 5
         Distance  1 2  1.3 1.7
      End
      # Second scan coordinate: One of the H--C--C--H dihedral angles (others will␣
↪follow naturally)
      ScanCoordinate
         nPoints 21
         Dihedral  3 1 2 6  60.0 0.0
      End
   End

   GeometryOptimization
      Convergence Step=1.0e-3
   End

   Engine DFTB
      Model DFTB3
      ResourcesDir DFTB.org/3ob-3-1
      DispersionCorrection D3-BJ
   EndEngine

EOF


echo "=============="
echo "Ethene torsion"
```

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```
echo "=============="
echo

AMS_JOBNAME=ethene_torsion $AMSBIN/ams << EOF

   Task PESScan

   System
      Atoms
         C   0.0   0.0       0.66687
         C   0.0   0.0      -0.66687
         H   0.0   0.92974  -1.23912
         H   0.0   0.92974   1.23912
         H   0.0  -0.92974   1.23912
         H   0.0  -0.92974  -1.23912
      End
   End

   PESScan
      # First scan coordinate: C--C bond distance
      ScanCoordinate
         nPoints 5
         Distance  1 2  1.1 1.8
      End
      # Second scan coordinate: Two of the H--C--C--H dihedrals
      ScanCoordinate
         nPoints 21
         Dihedral  4 1 2 3  0.0 60.0
         Dihedral  5 1 2 6  0.0 60.0
      End
   End

   GeometryOptimization
      Convergence Step=1.0e-3
   End

   Engine DFTB
      Model DFTB3
      ResourcesDir DFTB.org/3ob-3-1
      DispersionCorrection D3-BJ
   EndEngine

EOF



# Below are more technical examples, demonstrating the PES scan gap filling.
# The QUASINANO2015 parameter set shows some discontinuities in the PES,
# which leads to problems with convergence. The first job leaves the
# non-converged steps as is while the second job instructs AMS to
# attempt a second optimization for non-converged point starting from
# a different initial geometry.

echo "=============================="
echo "Ethane gap filling test (1/2)"
echo "=============================="
echo
```

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```
AMS_JOBNAME=ethane_nofillgaps $AMSBIN/ams << EOF

   Task PESScan

   System
      Atoms
         C  -2.333834610464788   -2.268837915270455  -0.2417723425321957
         C  -0.8081611038872945  -2.334371994724881  -0.04271045326758349
         H  -0.2505615773096904  -1.473443563856088  -0.38077110593546
         H  -0.3249814761083244  -3.235478579439597  -0.3904810245975267
         H  -0.583247370537557   -2.349691649662279   1.013499336841977
         H  -2.817014238243758   -1.367731330555738   0.1059982287977475
         H  -2.891434137042391   -3.129766346139247   0.09628831013568076
         H  -2.558748343814525   -2.253518260333056  -1.297982132641757
      End
   End

   GeometryOptimization
      CoordinateType Cartesian
      Convergence Step=1.0e-3
   End

   PESScan
      FillUnconvergedGaps False
      CalcPropertiesAtPESPoints True
      ScanCoordinate
         nPoints 10
         Distance 1 2  1.4 1.7
      End
      ScanCoordinate
         nPoints 10
         Distance 7 1  1.0 1.2
         Dihedral 7 1 2 3  60.0 180.0
      End
   End

   Engine DFTB
      Model SCC-DFTB
      ResourcesDir QUASINANO2015
   EndEngine

EOF


echo "============================="
echo "Ethane gap filling test (2/2)"
echo "============================="
echo

AMS_JOBNAME=ethane_fillgaps $AMSBIN/ams << EOF

   Task PESScan

   System
      Atoms
         C  -2.333834610464788   -2.268837915270455  -0.2417723425321957
```

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```
         C  -0.8081611038872945  -2.334371994724881  -0.04271045326758349
         H  -0.2505615773096904  -1.473443563856088  -0.38077110593546
         H  -0.3249814761083244  -3.235478579439597  -0.3904810245975267
         H  -0.583247370537557   -2.349691649662279   1.013499336841977
         H  -2.817014238243758   -1.367731330555738   0.1059982287977475
         H  -2.891434137042391   -3.129766346139247   0.09628831013568076
         H  -2.558748343814525   -2.253518260333056  -1.297982132641757
      End
   End

   GeometryOptimization
      CoordinateType Cartesian
      Convergence Step=1.0e-3
   End

   PESScan
      FillUnconvergedGaps True
      CalcPropertiesAtPESPoints True
      ScanCoordinate
         nPoints 10
         Distance 1 2  1.4 1.7
      End
      ScanCoordinate
         nPoints 10
         Distance 7 1  1.0 1.2
         Dihedral 7 1 2 3  60.0 180.0
      End
   End

   Engine DFTB
      Model SCC-DFTB
      ResourcesDir QUASINANO2015
   EndEngine

EOF
```

10.3.4 Example: PES scan and transition state search for H2 on graphene

Download PESScan_and_TS_H2_on_Graphene.run

```
#! /bin/sh

# First we do a 2D PES scan varying the z-coordinate of the two hydrogen atoms
# In this example we will keep the graphene slab fixed. From a physical/chemical
# standpoint this is not a good approximation. The graphene slab is
# intentionally not perfectly symmetric.

AMS_JOBNAME=PESScan $AMSBIN/ams << EOF

   Task PESScan

   System
      Atoms
         H   0.0      1.53633037    1.1
         H   0.0     -0.11341359    1.1
```

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```
         C   0.001    1.42028166    0.0
         C   1.230    2.13042249    0.0
         C   1.230   -0.71014083    0.0
         C   2.460    0.00000000    0.0
         C   2.460    1.42028167    0.0
         C   0.000    0.00000000    0.0
      End
      Lattice
         3.69   -2.13042249   0.0
         0.00    4.26084499   0.0
      End
   End

   PESScan
      ScanCoordinate
         nPoints 10
         Coordinate 1 Z 1.1 2.0
      End
      ScanCoordinate
         nPoints 10
         Coordinate 2 Z 1.1 2.0
      End
   End

   GeometryOptimization
      Convergence Step=1.0e-3
   End

   Constraints
      # Fix the entire graphene slab.
      Atom 3
      Atom 4
      Atom 5
      Atom 6
      Atom 7
      Atom 8
   End

   Engine DFTB
      Model DFTB
      ResourcesDir DFTB.org/3ob-3-1
      DispersionCorrection D3-BJ
      KSpace
        Type Symmetric
        Symmetric KInteg=3
      End
   EndEngine

EOF


# A human looks at the PES scan and picks a reasonable starting point for the
# TS search. (Normally you would do that in AMSMovie by looking at the PES and
# then exporting the geometry into an xyz file.)

#           _           ____
#        ___))         [  | \
```

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```
#        ) //o          | | ]
#     _ (_    >         | | ]
#    (O)  \__<          | | ]
#    [/] /   \)        [__|/_
#    [\]|  ( \        __/___\______
#    [/]|   \ \__  ___|             |
#    [\]|    \___E/%%/|_____________|_
#    [/]|=====__   (___________________)

cat << EOF > initial_geometry_for_TS.xyz
8

H    0.4145668856457391      1.72927656037925      1.100000023839768     region=H2
H   -0.05533871972549955    -0.06805093626643093   1.500000013242627     region=H2
C    0.001                   1.42028166            0.0
C    1.230                   2.13042249            0.0
C    1.230                  -0.71014083            0.0
C    2.460                   0.00000000            0.0
C    2.460                   1.42028167            0.0
C    0.000                   0.00000000            0.0
VEC1 3.69 -2.13042249 0.0
VEC2 0.0   4.26084499 0.0
EOF


# Compute the partial initial Hessian to be used in the transition state
# search. (The Hessian will be computed only for the hydrogen atoms.)

AMS_JOBNAME=Hessian $AMSBIN/ams << EOF

   Task SinglePoint

   System
      # Load the geometry we just saved.
      GeometryFile initial_geometry_for_TS.xyz
   End

   Properties
      # Calculate the Hessian (implied when calculating normal modes) ...
      NormalModes True
      # ... but only the part related to the hydrogen atoms.
      SelectedRegionForHessian H2
   End

   Engine DFTB
      Model DFTB
      ResourcesDir DFTB.org/3ob-3-1
      DispersionCorrection D3-BJ
      KSpace
        Type Symmetric
        Symmetric KInteg=3
      End
   EndEngine

EOF

echo "Extract the frequencies from the kf file using amsreport:"
```

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```
$AMSBIN/amsreport Hessian.results/dftb.rkf -r "Vibrations%Frequencies[cm-1]##1"


# Do a transition state search using the initial Hessian just computed (the
# Graphene slab is constrained). Also compute the final Hessian for the
# hydrogen atoms to validate the TS.

AMS_JOBNAME=TS $AMSBIN/ams << EOF

   Task TransitionStateSearch

   System
      # Load the geometry we just saved.
      GeometryFile initial_geometry_for_TS.xyz
   End

   GeometryOptimization
      Quasi-Newton
         Step TrustRadius=0.05
      End
      Convergence Gradients=1.0e-4
      InitialHessian
          # Load previously calculated Hessian as initial Hessian for a
          # transition state search with the Quasi-Newton optimizer.
          Type FromFile
          File Hessian.results/dftb.rkf
      End
   End

   TransitionStateSearch
       # Follow the mode with the smallest frequency.
       ModeToFollow 1
       # (This is also the default, we wouldn't need to specify this.)
   End

   Constraints
      # Fix the entire graphene slab.
      Atom 3
      Atom 4
      Atom 5
      Atom 6
      Atom 7
      Atom 8
   End

   Properties
      NormalModes Yes
      SelectedRegionForHessian H2
   End

   Engine DFTB
       Model DFTB
       ResourcesDir DFTB.org/3ob-3-1
       DispersionCorrection D3-BJ
      KSpace
        Type Symmetric
        Symmetric KInteg=3
```

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```
      End
   EndEngine

EOF

echo "Extract energy from the rkf file using amsreport:"
$AMSBIN/amsreport TS.results/dftb.rkf -r "AMSResults%Energy"
```

10.3.5 Example: Transition state search Ethane

Download TS_ethane.run

```
#!/bin/sh

AMS_JOBNAME=0D $AMSBIN/ams << EOF

Task TransitionStateSearch

GeometryOptimization
   Convergence Energy=1.25e-6
End

Properties
   NormalModes true
End

System
   Atoms
      C       0.000000000000       0.000000000000       0.767685465031
      C       0.000000000000       0.000000000000      -0.767685465031
      H       0.964354016767       0.347635559279       1.177128271450
      H      -0.181115782790      -1.008972856410       1.177128271450
      H      -0.783238233981       0.661337297125       1.177128271450
      H      -0.500471876676       0.894626767091      -1.177128271450
      H      -0.524533568868      -0.880734742626      -1.177128271450
      H       1.025005445540      -0.013892024465      -1.177128271450
   End
End

Engine DFTB
   Model SCC-DFTB
   ResourcesDir DFTB.org/mio-1-1
EndEngine

EOF

# For periodic systems the rotation around C-C bond does not have to be lowest mode.
# Rotations of the molecule as the whole will likely have a smaller force constant.
# Since we do not want to search for a TS in molecular rotation we have to specify
# a reaction coordinate as precisely as possible..

AMS_JOBNAME=1D $AMSBIN/ams << EOF

Task TransitionStateSearch
```

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```
TransitionStateSearch
   ReactionCoordinate
      Dihedral  3 1 2 6    0.3
      Dihedral  3 1 2 8    0.3
      Dihedral  3 1 2 7    0.3
      Dihedral  5 1 2 6    0.3
      Dihedral  5 1 2 8    0.3
      Dihedral  5 1 2 7    0.3
      Dihedral  4 1 2 6    0.3
      Dihedral  4 1 2 8    0.3
      Dihedral  4 1 2 7    0.3
   End
End

GeometryOptimization
   Convergence Energy=1.25e-6 Gradients=1.e-5
End

Properties
   NormalModes true
End

System
   Atoms
      C       0.000000000000       0.000000000000       0.767685465031
      C       0.000000000000       0.000000000000      -0.767685465031
      H       0.964354016767       0.347635559279       1.177128271450
      H      -0.181115782790      -1.008972856410       1.177128271450
      H      -0.783238233981       0.661337297125       1.177128271450
      H      -0.500471876676       0.894626767091      -1.177128271450
      H      -0.524533568868      -0.880734742626      -1.177128271450
      H       1.025005445540      -0.013892024465      -1.177128271450
   End
   Lattice
      50.0  0.0  0.0
   End
End

Engine DFTB
   Model SCC-DFTB
   ResourcesDir DFTB.org/mio-1-1
EndEngine

EOF


AMS_JOBNAME=2D $AMSBIN/ams << EOF

Task TransitionStateSearch

TransitionStateSearch
   ReactionCoordinate
      Dihedral  3 1 2 6    0.3
      Dihedral  3 1 2 8    0.3
      Dihedral  3 1 2 7    0.3
      Dihedral  5 1 2 6    0.3
      Dihedral  5 1 2 8    0.3
```

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```
      Dihedral  5 1 2 7    0.3
      Dihedral  4 1 2 6    0.3
      Dihedral  4 1 2 8    0.3
      Dihedral  4 1 2 7    0.3
   End
End

GeometryOptimization
   Convergence Energy=1.25e-6 Gradients=1.e-5
End

Properties
   NormalModes true
End

System
   Atoms
      C       0.000000000000       0.000000000000       0.767685465031
      C       0.000000000000       0.000000000000      -0.767685465031
      H       0.964354016767       0.347635559279       1.177128271450
      H      -0.181115782790      -1.008972856410       1.177128271450
      H      -0.783238233981       0.661337297125       1.177128271450
      H      -0.500471876676       0.894626767091      -1.177128271450
      H      -0.524533568868      -0.880734742626      -1.177128271450
      H       1.025005445540      -0.013892024465      -1.177128271450
   End
   Lattice
      50.0  0.0  0.0
      0.0  50.0  0.0
   End
End

Engine DFTB
   Model SCC-DFTB
   ResourcesDir DFTB.org/mio-1-1
EndEngine

EOF


AMS_JOBNAME=3D $AMSBIN/ams << EOF

Task TransitionStateSearch

TransitionStateSearch
   ReactionCoordinate
      Dihedral  3 1 2 6    0.3
      Dihedral  3 1 2 8    0.3
      Dihedral  3 1 2 7    0.3
      Dihedral  5 1 2 6    0.3
      Dihedral  5 1 2 8    0.3
      Dihedral  5 1 2 7    0.3
      Dihedral  4 1 2 6    0.3
      Dihedral  4 1 2 8    0.3
      Dihedral  4 1 2 7    0.3
   End
End
```

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```
GeometryOptimization
   Convergence Energy=1.25e-6 Gradients=1.e-5
End

Properties
   NormalModes true
End

System
   Atoms
      C       0.000000000000       0.000000000000       0.767685465031
      C       0.000000000000       0.000000000000      -0.767685465031
      H       0.964354016767       0.347635559279       1.177128271450
      H      -0.181115782790      -1.008972856410       1.177128271450
      H      -0.783238233981       0.661337297125       1.177128271450
      H      -0.500471876676       0.894626767091      -1.177128271450
      H      -0.524533568868      -0.880734742626      -1.177128271450
      H       1.025005445540      -0.013892024465      -1.177128271450
   End
   Lattice
      50.0  0.0  0.0
      0.0  50.0  0.0
      0.0   0.0 50.0
   End
End

Engine DFTB
   Model SCC-DFTB
   ResourcesDir DFTB.org/mio-1-1
EndEngine

EOF
```

10.3.6 Example: TS H2O on frozen MgO

Download TS_H2O_on_frozen_MgO.run

```
#! /bin/sh


cat <<eor > H2O_on_MgO.xyz
39

O   0.0            0.0            0.0            region=H2O
H  -0.704320560    0.0           -0.66779884     region=H2O
H   0.704320560    0.0           -0.66779884     region=H2O
O   1.50158914     0.108856250  -2.19963815
O  -1.48731305     0.108246430  -2.19972248
Mg  0.00563782     1.59225904   -2.33893848
Mg  0.00352084    -1.44762418   -2.24965831
O   0.00696938     1.57832358   -4.42106808
O   0.00696938     4.55524313   -4.42106808
O   2.98388893    -1.39859597   -4.42106808
O   2.98388893     1.57832358   -4.42106808
```

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```
O   2.98388893    4.55524313   -4.42106808
Mg -2.97355121   -1.39556394   -2.31959606
Mg -2.97743483    1.58619377   -2.31874087
Mg -2.97337639    4.55937829   -2.31649087
Mg  0.00549444    4.55739475   -2.31753869
Mg  2.98277888   -1.39600311   -2.32043545
Mg  2.98920147    1.58770902   -2.31910664
Mg  2.98383523    4.55827076   -2.31621824
O  -1.49388075   -2.89172181   -2.22718875
O  -1.48165368    3.06816545   -2.20685378
O   1.50285846   -2.89006842   -2.22921666
O   1.49233399    3.06893483   -2.20786341
O   4.47002638   -2.88279517   -2.21228396
O   4.47076537    0.09231531   -2.20652142
O   4.47074422    3.07217257   -2.21022983
Mg -1.48149039   -2.88705574   -4.42106808
Mg -1.48149039    0.08986381   -4.42106808
Mg -1.48149039    3.06678335   -4.42106808
Mg  1.49542915   -2.88705574   -4.42106808
Mg  1.49542915    0.08986381   -4.42106808
Mg  1.49542915    3.06678335   -4.42106808
Mg  4.47234870   -2.88705574   -4.42106808
Mg  4.47234870    0.08986381   -4.42106808
Mg  4.47234870    3.06678335   -4.42106808
O  -2.96995017   -1.39859597   -4.42106808
O  -2.96995017    1.57832358   -4.42106808
O  -2.96995017    4.55524313   -4.42106808
O   0.00696938   -1.39859597   -4.42106808
VEC1  8.93075865       0.00000000       0.00000000
VEC2  0.00000000       8.93075865       0.00000000
eor



AMS_JOBNAME=hessian $AMSBIN/ams << eor

Task SinglePoint
System
    GeometryFile H2O_on_MgO.xyz
End
Properties
    NormalModes Yes
    SelectedRegionForHessian H2O
End

NumericalDifferentiation
    NuclearStepSize 0.0001
End

Engine DFTB
    Model SCC-DFTB
    ResourcesDir DFTB.org/3ob-3-1
    DispersionCorrection D3-BJ
    KSpace Quality=GammaOnly
EndEngine
eor
```

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```
AMS_JOBNAME=TS $AMSBIN/ams << eor

Task TransitionStateSearch

System
    GeometryFile H2O_on_MgO.xyz
End

Properties
    NormalModes Yes
    SelectedRegionForHessian H2O
End

GeometryOptimization
    Convergence Step=1.0e-3
    Quasi-Newton
       Step
           TrustRadius 0.015
       End
    End
    InitialHessian
        Type FromFile
        File hessian.results/dftb.rkf
    End
End

TransitionStateSearch
    ModeToFollow 1
End

Constraints
    Atom 4
    Atom 5
    Atom 6
    Atom 7
    Atom 8
    Atom 9
    Atom 10
    Atom 11
    Atom 12
    Atom 13
    Atom 14
    Atom 15
    Atom 16
    Atom 17
    Atom 18
    Atom 19
    Atom 20
    Atom 21
    Atom 22
    Atom 23
    Atom 24
    Atom 25
    Atom 26
    Atom 27
    Atom 28
```

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```
    Atom 29
    Atom 30
    Atom 31
    Atom 32
    Atom 33
    Atom 34
    Atom 35
    Atom 36
    Atom 37
    Atom 38
    Atom 39
End

Engine DFTB
    Model SCC-DFTB
    ResourcesDir DFTB.org/3ob-3-1
    DispersionCorrection D3-BJ
    KSpace Quality=GammaOnly
EndEngine

eor


echo "Extract energy from the rkf file using amsreport:"
$AMSBIN/amsreport TS.results/dftb.rkf -r "AMSResults%Energy"

echo "Extract frequencies from the rkf file using amsreport:"
$AMSBIN/amsreport TS.results/dftb.rkf -r "Vibrations%Frequencies[cm-1]##1"
```

10.3.7 Example: TS partial Hessian and constraints

Download TS_partial_Hessian.run

```
#! /bin/sh

cat <<eor > mol.xyz
36

H       0.766097657598      -2.768081018033      -2.876300126478    region=hess
H      -0.644603976315      -2.714699771693      -3.929852776492    region=hess
C      -0.314948403193      -2.901426268843      -2.908504973433    region=hess
H      -0.525208929148      -3.944769739904      -2.674640344590    region=hess
H      -1.659140560000      -2.541065820000      -1.240914090000
H       0.637739730000      -1.797283340000      -0.540602480000
H       0.603811710000      -0.541646840000      -1.760941100000
H      -1.694120490000      -1.284261220000      -2.461059940000
C      -1.020738570000      -1.956617890000      -1.915045680000
C      -0.035811270000      -1.127675680000      -1.089473150000
C      -0.737469990000      -0.190898040000      -0.106418940000
H      -1.376897440000      -0.775607050000       0.566750310000
H      -1.411731640000       0.479328280000      -0.654571120000
C       0.248194490000       0.638103820000       0.715570210000
H       0.887974040000       1.223068560000       0.044475600000
C      -0.460306390000       1.579379480000       1.701432460000
H       3.444573290000       6.004736970000       2.731567780000
```

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```
H       0.919641810000      -0.027959660000       1.269936690000
H      -1.069142800000       0.981241120000       2.389125900000
H      -1.159317960000       2.220389850000       1.149887980000
C       0.514968080000       2.419179460000       2.496433200000
C       0.820924370000       2.058868020000       3.798151210000
C       1.746750310000       2.796607360000       4.568985860000
C       2.373333170000       3.899456660000       4.033228060000
C       2.454935040000       5.835427930000       0.837034550000
C       1.524064120000       5.107109800000       0.061961810000
C       0.889322320000       4.002365640000       0.587927370000
C       1.153526110000       3.565291180000       1.917194200000
C       2.093121000000       4.309192450000       2.700422740000
C       2.730884060000       5.445174340000       2.128828880000
H       0.337576610000       1.188182970000       4.238172010000
H       1.961399330000       2.484594700000       5.588953990000
H       3.089298910000       4.469787090000       4.622399420000
H       2.948386600000       6.705375610000       0.408799030000
H       1.308349370000       5.424773150000      -0.956092870000
H       0.173208090000       3.458554860000      -0.024205760000
eor


AMS_JOBNAME=hessian $AMSBIN/ams << eor

Task SinglePoint

Properties
   Hessian True
End

System
   GeometryFile mol.xyz
End

Engine DFTB
   Model SCC-DFTB
   ResourcesDir DFTB.org/3ob-3-1
EndEngine
eor



AMS_JOBNAME=TS $AMSBIN/ams << eor

Task TransitionStateSearch

System
   GeometryFile mol.xyz
End

Properties
   NormalModes True
   SelectedRegionForHessian hess
End

Constraints
   Atom 5
```

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```
   Atom 6
   Atom 7
   Atom 8
   Atom 9
   Atom 10
   Atom 11
   Atom 12
   Atom 13
   Atom 14
   Atom 15
   Atom 16
   Atom 17
   Atom 18
   Atom 19
   Atom 20
   Atom 21
   Atom 22
   Atom 23
   Atom 24
   Atom 25
   Atom 26
   Atom 27
   Atom 28
   Atom 29
   Atom 30
   Atom 31
   Atom 32
   Atom 33
   Atom 34
   Atom 35
   Atom 36
End

GeometryOptimization
   CoordinateType Cartesian
   InitialHessian
      Type FromFile
      File hessian.results/dftb.rkf
   End
End

TransitionStateSearch
   ModeToFollow 1
End

Engine DFTB
   Model SCC-DFTB
   ResourcesDir DFTB.org/3ob-3-1
EndEngine
eor
```

10.4 Electronic structure of periodic systems

10.4.1 Example: Effective mass

Download SP_EffectiveMass.run

```
#!/bin/sh

$AMSBIN/ams << EOF

Task SinglePoint

System
    Atoms
        C 0.7332149300 0.0000000000 0.0000000000
        C 26.0557850700 3.5850000000 7.1055000000
        C 26.0557850700 0.0000000000 0.0000000000
        C 0.7332149300 3.5850000000 7.1055000000
        C 14.1277149300 3.5850000000 0.0000000000
        C 12.6612850700 0.0000000000 7.1055000000
        C 12.6612850700 3.5850000000 0.0000000000
        C 14.1277149300 0.0000000000 7.1055000000
        C 1.4235674600 6.1329312000 0.6983285400
        C 25.3654325400 4.6220688000 7.8038285400
        C 1.4235674600 1.0370688000 13.5126714600
        C 25.3654325400 2.5479312000 6.4071714600
        C 25.3654325400 1.0370688000 13.5126714600
        C 1.4235674600 2.5479312000 6.4071714600
        C 25.3654325400 6.1329312000 0.6983285400
        C 1.4235674600 4.6220688000 7.8038285400
        C 14.8180674600 2.5479312000 0.6983285400
        C 11.9709325400 1.0370688000 7.8038285400
        C 14.8180674600 4.6220688000 13.5126714600
        C 11.9709325400 6.1329312000 6.4071714600
        C 11.9709325400 4.6220688000 13.5126714600
        C 14.8180674600 6.1329312000 6.4071714600
        C 11.9709325400 2.5479312000 0.6983285400
        C 14.8180674600 1.0370688000 7.8038285400
        C 0.7174094200 5.0492574000 1.2441730500
        C 26.0715905800 5.7057426000 8.3496730500
        C 0.7174094200 2.1207426000 12.9668269500
        C 26.0715905800 1.4642574000 5.8613269500
        C 26.0715905800 2.1207426000 12.9668269500
        C 0.7174094200 1.4642574000 5.8613269500
        C 26.0715905800 5.0492574000 1.2441730500
        C 0.7174094200 5.7057426000 8.3496730500
        C 14.1119094200 1.4642574000 1.2441730500
        C 12.6770905800 2.1207426000 8.3496730500
        C 14.1119094200 5.7057426000 12.9668269500
        C 12.6770905800 5.0492574000 5.8613269500
        C 12.6770905800 5.7057426000 12.9668269500
        C 14.1119094200 5.0492574000 5.8613269500
        C 12.6770905800 1.4642574000 1.2441730500
        C 14.1119094200 2.1207426000 8.3496730500
        C 1.3906169900 3.9611382000 1.9059793200
        C 25.3983830100 6.7938618000 9.0114793200
        C 1.3906169900 3.2088618000 12.3050206800
```

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```
        C 25.3983830100 0.3761382000 5.1995206800
        C 25.3983830100 3.2088618000 12.3050206800
        C 1.3906169900 0.3761382000 5.1995206800
        C 25.3983830100 3.9611382000 1.9059793200
        C 1.3906169900 6.7938618000 9.0114793200
        C 14.7851169900 0.3761382000 1.9059793200
        C 12.0038830100 3.2088618000 9.0114793200
        C 14.7851169900 6.7938618000 12.3050206800
        C 12.0038830100 3.9611382000 5.1995206800
        C 12.0038830100 6.7938618000 12.3050206800
        C 14.7851169900 3.9611382000 5.1995206800
        C 12.0038830100 0.3761382000 1.9059793200
        C 14.7851169900 3.2088618000 9.0114793200
        C 0.7088369400 2.9444322000 2.4917567400
        C 26.0801630600 0.6405678000 9.5972567400
        C 0.7088369400 4.2255678000 11.7192432600
        C 26.0801630600 6.5294322000 4.6137432600
        C 26.0801630600 4.2255678000 11.7192432600
        C 0.7088369400 6.5294322000 4.6137432600
        C 26.0801630600 2.9444322000 2.4917567400
        C 0.7088369400 0.6405678000 9.5972567400
        C 14.1033369400 6.5294322000 2.4917567400
        C 12.6856630600 4.2255678000 9.5972567400
        C 14.1033369400 0.6405678000 11.7192432600
        C 12.6856630600 2.9444322000 4.6137432600
        C 12.6856630600 0.6405678000 11.7192432600
        C 14.1033369400 2.9444322000 4.6137432600
        C 12.6856630600 6.5294322000 2.4917567400
        C 14.1033369400 4.2255678000 9.5972567400
        C 2.8824964000 6.2057784000 1.0337081400
        C 23.9065036000 4.5492216000 8.1392081400
        C 2.8824964000 0.9642216000 13.1772918600
        C 23.9065036000 2.6207784000 6.0717918600
        C 23.9065036000 0.9642216000 13.1772918600
        C 2.8824964000 2.6207784000 6.0717918600
        C 23.9065036000 6.2057784000 1.0337081400
        C 2.8824964000 4.5492216000 8.1392081400
        C 16.2769964000 2.6207784000 1.0337081400
        C 10.5120036000 0.9642216000 8.1392081400
        C 16.2769964000 4.5492216000 13.1772918600
        C 10.5120036000 6.2057784000 6.0717918600
        C 10.5120036000 4.5492216000 13.1772918600
        C 16.2769964000 6.2057784000 6.0717918600
        C 10.5120036000 2.6207784000 1.0337081400
        C 16.2769964000 0.9642216000 8.1392081400
        C 3.8286838800 5.3906211000 0.4094189100
        C 22.9603161200 5.3643789000 7.5149189100
        C 3.8286838800 1.7793789000 13.8015810900
        C 22.9603161200 1.8056211000 6.6960810900
        C 22.9603161200 1.7793789000 13.8015810900
        C 3.8286838800 1.8056211000 6.6960810900
        C 22.9603161200 5.3906211000 0.4094189100
        C 3.8286838800 5.3643789000 7.5149189100
        C 17.2231838800 1.8056211000 0.4094189100
        C 9.5658161200 1.7793789000 7.5149189100
        C 17.2231838800 5.3643789000 13.8015810900
        C 9.5658161200 5.3906211000 6.6960810900
```

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```
        C 9.5658161200 5.3643789000 13.8015810900
        C 17.2231838800 5.3906211000 6.6960810900
        C 9.5658161200 1.8056211000 0.4094189100
        C 17.2231838800 1.7793789000 7.5149189100
        C 5.1432201100 5.3711187000 0.8496756900
        C 21.6457798900 5.3838813000 7.9551756900
        C 5.1432201100 1.7988813000 13.3613243100
        C 21.6457798900 1.7861187000 6.2558243100
        C 21.6457798900 1.7988813000 13.3613243100
        C 5.1432201100 1.7861187000 6.2558243100
        C 21.6457798900 5.3711187000 0.8496756900
        C 5.1432201100 5.3838813000 7.9551756900
        C 18.5377201100 1.7861187000 0.8496756900
        C 8.2512798900 1.7988813000 7.9551756900
        C 18.5377201100 5.3838813000 13.3613243100
        C 8.2512798900 5.3711187000 6.2558243100
        C 8.2512798900 5.3838813000 13.3613243100
        C 18.5377201100 5.3711187000 6.2558243100
        C 8.2512798900 1.7861187000 0.8496756900
        C 18.5377201100 1.7988813000 7.9551756900
        C 5.5413046500 6.1740870000 1.9110952800
        C 21.2476953500 4.5809130000 9.0165952800
        C 5.5413046500 0.9959130000 12.2999047200
        C 21.2476953500 2.5890870000 5.1944047200
        C 21.2476953500 0.9959130000 12.2999047200
        C 5.5413046500 2.5890870000 5.1944047200
        C 21.2476953500 6.1740870000 1.9110952800
        C 5.5413046500 4.5809130000 9.0165952800
        C 18.9358046500 2.5890870000 1.9110952800
        C 7.8531953500 0.9959130000 9.0165952800
        C 18.9358046500 4.5809130000 12.2999047200
        C 7.8531953500 6.1740870000 5.1944047200
        C 7.8531953500 4.5809130000 12.2999047200
        C 18.9358046500 6.1740870000 5.1944047200
        C 7.8531953500 2.5890870000 1.9110952800
        C 18.9358046500 0.9959130000 9.0165952800
        C 4.6127979100 6.9900330000 2.5376582700
        C 22.1762020900 3.7649670000 9.6431582700
        C 4.6127979100 0.1799670000 11.6733417300
        C 22.1762020900 3.4050330000 4.5678417300
        C 22.1762020900 0.1799670000 11.6733417300
        C 4.6127979100 3.4050330000 4.5678417300
        C 22.1762020900 6.9900330000 2.5376582700
        C 4.6127979100 3.7649670000 9.6431582700
        C 18.0072979100 3.4050330000 2.5376582700
        C 8.7817020900 0.1799670000 9.6431582700
        C 18.0072979100 3.7649670000 11.6733417300
        C 8.7817020900 6.9900330000 4.5678417300
        C 8.7817020900 3.7649670000 11.6733417300
        C 18.0072979100 6.9900330000 4.5678417300
        C 8.7817020900 3.4050330000 2.5376582700
        C 18.0072979100 0.1799670000 9.6431582700
        C 3.2955827800 7.0006446000 2.1055017600
        C 23.4934172200 3.7543554000 9.2110017600
        C 3.2955827800 0.1693554000 12.1054982400
        C 23.4934172200 3.4156446000 4.9999982400
        C 23.4934172200 0.1693554000 12.1054982400
```

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```
        C 3.2955827800 3.4156446000 4.9999982400
        C 23.4934172200 7.0006446000 2.1055017600
        C 3.2955827800 3.7543554000 9.2110017600
        C 16.6900827800 3.4156446000 2.1055017600
        C 10.0989172200 0.1693554000 9.2110017600
        C 16.6900827800 3.7543554000 12.1054982400
        C 10.0989172200 7.0006446000 4.9999982400
        C 10.0989172200 3.7543554000 12.1054982400
        C 16.6900827800 7.0006446000 4.9999982400
        C 10.0989172200 3.4156446000 2.1055017600
        C 16.6900827800 0.1693554000 9.2110017600
        H 2.3654687000 3.9650100000 1.9284327000
        H 24.4235313000 6.7899900000 9.0339327000
        H 2.3654687000 3.2049900000 12.2825673000
        H 24.4235313000 0.3800100000 5.1770673000
        H 24.4235313000 3.2049900000 12.2825673000
        H 2.3654687000 0.3800100000 5.1770673000
        H 24.4235313000 3.9650100000 1.9284327000
        H 2.3654687000 6.7899900000 9.0339327000
        H 15.7599687000 0.3800100000 1.9284327000
        H 11.0290313000 3.2049900000 9.0339327000
        H 15.7599687000 6.7899900000 12.2825673000
        H 11.0290313000 3.9650100000 5.1770673000
        H 11.0290313000 6.7899900000 12.2825673000
        H 15.7599687000 3.9650100000 5.1770673000
        H 11.0290313000 0.3800100000 1.9284327000
        H 15.7599687000 3.2049900000 9.0339327000
        H 1.1733582000 2.2298700000 2.9345715000
        H 25.6156418000 1.3551300000 10.0400715000
        H 1.1733582000 4.9401300000 11.2764285000
        H 25.6156418000 5.8148700000 4.1709285000
        H 25.6156418000 4.9401300000 11.2764285000
        H 1.1733582000 5.8148700000 4.1709285000
        H 25.6156418000 2.2298700000 2.9345715000
        H 1.1733582000 1.3551300000 10.0400715000
        H 14.5678582000 5.8148700000 2.9345715000
        H 12.2211418000 4.9401300000 10.0400715000
        H 14.5678582000 1.3551300000 11.2764285000
        H 12.2211418000 2.2298700000 4.1709285000
        H 12.2211418000 1.3551300000 11.2764285000
        H 14.5678582000 2.2298700000 4.1709285000
        H 12.2211418000 5.8148700000 2.9345715000
        H 14.5678582000 4.9401300000 10.0400715000
        H 3.5575792000 4.8254100000 13.8471984000
        H 23.2314208000 5.9295900000 6.7416984000
        H 3.5575792000 2.3445900000 0.3638016000
        H 23.2314208000 1.2404100000 7.4693016000
        H 23.2314208000 2.3445900000 0.3638016000
        H 3.5575792000 1.2404100000 7.4693016000
        H 23.2314208000 4.8254100000 13.8471984000
        H 3.5575792000 5.9295900000 6.7416984000
        H 16.9520792000 1.2404100000 13.8471984000
        H 9.8369208000 2.3445900000 6.7416984000
        H 16.9520792000 5.9295900000 0.3638016000
        H 9.8369208000 4.8254100000 7.4693016000
        H 9.8369208000 5.9295900000 0.3638016000
        H 16.9520792000 4.8254100000 7.4693016000
```

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```
        H 9.8369208000 1.2404100000 13.8471984000
        H 16.9520792000 2.3445900000 6.7416984000
        H 5.8051763000 4.7895600000 0.3964869000
        H 20.9838237000 5.9654400000 7.5019869000
        H 5.8051763000 2.3804400000 13.8145131000
        H 20.9838237000 1.2045600000 6.7090131000
        H 20.9838237000 2.3804400000 13.8145131000
        H 5.8051763000 1.2045600000 6.7090131000
        H 20.9838237000 4.7895600000 0.3964869000
        H 5.8051763000 5.9654400000 7.5019869000
        H 19.1996763000 1.2045600000 0.3964869000
        H 7.5893237000 2.3804400000 7.5019869000
        H 19.1996763000 5.9654400000 13.8145131000
        H 7.5893237000 4.7895600000 6.7090131000
        H 7.5893237000 5.9654400000 13.8145131000
        H 19.1996763000 4.7895600000 6.7090131000
        H 7.5893237000 1.2045600000 0.3964869000
        H 19.1996763000 2.3804400000 7.5019869000
        H 6.4641857000 6.1662000000 2.1970206000
        H 20.3248143000 4.5888000000 9.3025206000
        H 6.4641857000 1.0038000000 12.0139794000
        H 20.3248143000 2.5812000000 4.9084794000
        H 20.3248143000 1.0038000000 12.0139794000
        H 6.4641857000 2.5812000000 4.9084794000
        H 20.3248143000 6.1662000000 2.1970206000
        H 6.4641857000 4.5888000000 9.3025206000
        H 19.8586857000 2.5812000000 2.1970206000
        H 6.9303143000 1.0038000000 9.3025206000
        H 19.8586857000 4.5888000000 12.0139794000
        H 6.9303143000 6.1662000000 4.9084794000
        H 6.9303143000 4.5888000000 12.0139794000
        H 19.8586857000 6.1662000000 4.9084794000
        H 6.9303143000 2.5812000000 2.1970206000
        H 19.8586857000 1.0038000000 9.3025206000
        H 4.8889925000 0.3871800000 3.2841621000
        H 21.9000075000 3.1978200000 10.3896621000
        H 4.8889925000 6.7828200000 10.9268379000
        H 21.9000075000 3.9721800000 3.8213379000
        H 21.9000075000 6.7828200000 10.9268379000
        H 4.8889925000 3.9721800000 3.8213379000
        H 21.9000075000 0.3871800000 3.2841621000
        H 4.8889925000 3.1978200000 10.3896621000
        H 18.2834925000 3.9721800000 3.2841621000
        H 8.5055075000 6.7828200000 10.3896621000
        H 18.2834925000 3.1978200000 10.9268379000
        H 8.5055075000 0.3871800000 3.8213379000
        H 8.5055075000 3.1978200000 10.9268379000
        H 18.2834925000 0.3871800000 3.8213379000
        H 8.5055075000 3.9721800000 3.2841621000
        H 18.2834925000 6.7828200000 10.3896621000
        H 2.6199642000 0.3871800000 2.5636644000
        H 24.1690358000 3.1978200000 9.6691644000
        H 2.6199642000 6.7828200000 11.6473356000
        H 24.1690358000 3.9721800000 4.5418356000
        H 24.1690358000 6.7828200000 11.6473356000
        H 2.6199642000 3.9721800000 4.5418356000
        H 24.1690358000 0.3871800000 2.5636644000
```

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```
        H 2.6199642000 3.1978200000 9.6691644000
        H 16.0144642000 3.9721800000 2.5636644000
        H 10.7745358000 6.7828200000 9.6691644000
        H 16.0144642000 3.1978200000 11.6473356000
        H 10.7745358000 0.3871800000 4.5418356000
        H 10.7745358000 3.1978200000 11.6473356000
        H 16.0144642000 0.3871800000 4.5418356000
        H 10.7745358000 3.9721800000 2.5636644000
        H 16.0144642000 6.7828200000 9.6691644000
    End
    Lattice
        26.789 0.0 0.0
        0.0 7.17 0.0
        0.0 0.0 14.211
    End
End

Engine DFTB
    Model SCC-DFTB
    ResourcesDir DFTB.org/3ob-3-1
    Periodic
        EffectiveMass
            Enabled Yes
            KPointCoord 0.0 0.0 0.0
        End
        BandStructure
            Automatic No
            DeltaK 0.01
        End
        BZPath
            Path
                0.5  0.0   0.0
                0.0  0.0   0.0
                0.0  0.5   0.0
                0.0  0.0   0.0
                0.0  0.0   0.5
            End
        End
    End
EndEngine

EOF
```

10.5 Excited States

10.5.1 Example: Fullerene excitations

Download SP_LR-TDDFTB_fullerene.run

```
#!/bin/sh

AMS_JOBNAME=SOTonly $AMSBIN/ams << eor
```

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```
Task SinglePoint

System
    Atoms
              C    -0.72604297     0.99931275     3.33713795
              C    -1.17476257    -0.38170316     3.33713793
              C    -1.42973769     1.96786514     2.59722371
              C    -2.31336391    -0.75165747     2.59722338
              C    -2.31336503    -1.98687660     1.83381747
              C     0.00000000    -1.23521836     3.33713791
              C     0.00000000    -2.43241456     2.59722318
              C    -1.17476306    -2.81412029     1.83381769
              C     0.70369481     2.96717937     1.83381781
              C     1.42973769     1.96786514     2.59722371
              C    -0.70369481     2.96717937     1.83381781
              C     0.72604297     0.99931275     3.33713795
              C     1.17476257    -0.38170316     3.33713793
              C     2.60450100     1.58616203     1.83381755
              C     3.03940953     0.24765522     1.83381790
              C     2.31336391    -0.75165747     2.59722338
              C    -0.72604313     3.43172901    -0.59859929
              C     0.72604313     3.43172901    -0.59859929
              C    -1.42973797     3.20308436     0.59859932
              C     1.42973797     3.20308436     0.59859932
              C     2.60450023     2.34956878     0.59859923
              C     1.17476306     2.81412029    -1.83381769
              C     2.31336503     1.98687660    -1.83381747
              C     3.03940785     1.75097015    -0.59859921
              C    -3.03940785     1.75097015    -0.59859921
              C    -2.31336503     1.98687660    -1.83381747
              C    -2.60450023     2.34956878     0.59859923
              C    -1.17476306     2.81412029    -1.83381769
              C     0.00000000     2.43241456    -2.59722318
              C    -2.31336391     0.75165747    -2.59722338
              C    -1.17476257     0.38170316    -3.33713793
              C     0.00000000     1.23521836    -3.33713791
              C    -3.03940953     0.24765522     1.83381790
              C    -3.48812825    -0.36995429     0.59859935
              C    -2.60450100     1.58616203     1.83381755
              C    -3.48812825     0.36995429    -0.59859935
              C    -3.03940953    -0.24765522    -1.83381790
              C    -3.03940785    -1.75097015     0.59859921
              C    -2.60450023    -2.34956878    -0.59859923
              C    -2.60450100    -1.58616203    -1.83381755
              C     0.72604297    -0.99931275    -3.33713795
              C    -0.72604297    -0.99931275    -3.33713795
              C    -1.42973769    -1.96786514    -2.59722371
              C     1.42973769    -1.96786514    -2.59722371
              C     3.03940953    -0.24765522    -1.83381790
              C     2.31336391     0.75165747    -2.59722338
              C     1.17476257     0.38170316    -3.33713793
              C     2.60450100    -1.58616203    -1.83381755
              C     3.03940785    -1.75097015     0.59859921
              C     3.48812825    -0.36995429     0.59859935
              C     3.48812825     0.36995429    -0.59859935
              C     2.60450023    -2.34956878    -0.59859923
              C     0.72604313    -3.43172901     0.59859929
```

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```
            C     1.17476306    -2.81412029     1.83381769
            C     2.31336503    -1.98687660     1.83381747
            C     1.42973797    -3.20308436    -0.59859932
            C    -0.70369481    -2.96717937    -1.83381781
            C    -1.42973797    -3.20308436    -0.59859932
            C    -0.72604313    -3.43172901     0.59859929
            C     0.70369481    -2.96717937    -1.83381781
    End
End

Engine DFTB
   Model SCC-DFTB
   ResourcesDir DFTB.org/mio-1-1
   Properties
       Excitations
           SingleOrbTrans
               printlowest 166
           End
       End
   End
EndEngine

eor


AMS_JOBNAME=fullTDDFTB $AMSBIN/ams << eor

Task SinglePoint

System
    Atoms
            C    -0.72604297     0.99931275     3.33713795
            C    -1.17476257    -0.38170316     3.33713793
            C    -1.42973769     1.96786514     2.59722371
            C    -2.31336391    -0.75165747     2.59722338
            C    -2.31336503    -1.98687660     1.83381747
            C     0.00000000    -1.23521836     3.33713791
            C     0.00000000    -2.43241456     2.59722318
            C    -1.17476306    -2.81412029     1.83381769
            C     0.70369481     2.96717937     1.83381781
            C     1.42973769     1.96786514     2.59722371
            C    -0.70369481     2.96717937     1.83381781
            C     0.72604297     0.99931275     3.33713795
            C     1.17476257    -0.38170316     3.33713793
            C     2.60450100     1.58616203     1.83381755
            C     3.03940953     0.24765522     1.83381790
            C     2.31336391    -0.75165747     2.59722338
            C    -0.72604313     3.43172901    -0.59859929
            C     0.72604313     3.43172901    -0.59859929
            C    -1.42973797     3.20308436     0.59859932
            C     1.42973797     3.20308436     0.59859932
            C     2.60450023     2.34956878     0.59859923
            C     1.17476306     2.81412029    -1.83381769
            C     2.31336503     1.98687660    -1.83381747
            C     3.03940785     1.75097015    -0.59859921
            C    -3.03940785     1.75097015    -0.59859921
            C    -2.31336503     1.98687660    -1.83381747
```

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```
           C    -2.60450023     2.34956878     0.59859923
           C    -1.17476306     2.81412029    -1.83381769
           C     0.00000000     2.43241456    -2.59722318
           C    -2.31336391     0.75165747    -2.59722338
           C    -1.17476257     0.38170316    -3.33713793
           C     0.00000000     1.23521836    -3.33713791
           C    -3.03940953     0.24765522     1.83381790
           C    -3.48812825    -0.36995429     0.59859935
           C    -2.60450100     1.58616203     1.83381755
           C    -3.48812825     0.36995429    -0.59859935
           C    -3.03940953    -0.24765522    -1.83381790
           C    -3.03940785    -1.75097015     0.59859921
           C    -2.60450023    -2.34956878    -0.59859923
           C    -2.60450100    -1.58616203    -1.83381755
           C     0.72604297    -0.99931275    -3.33713795
           C    -0.72604297    -0.99931275    -3.33713795
           C    -1.42973769    -1.96786514    -2.59722371
           C     1.42973769    -1.96786514    -2.59722371
           C     3.03940953    -0.24765522    -1.83381790
           C     2.31336391     0.75165747    -2.59722338
           C     1.17476257     0.38170316    -3.33713793
           C     2.60450100    -1.58616203    -1.83381755
           C     3.03940785    -1.75097015     0.59859921
           C     3.48812825    -0.36995429     0.59859935
           C     3.48812825     0.36995429    -0.59859935
           C     2.60450023    -2.34956878    -0.59859923
           C     0.72604313    -3.43172901     0.59859929
           C     1.17476306    -2.81412029     1.83381769
           C     2.31336503    -1.98687660     1.83381747
           C     1.42973797    -3.20308436    -0.59859932
           C    -0.70369481    -2.96717937    -1.83381781
           C    -1.42973797    -3.20308436    -0.59859932
           C    -0.72604313    -3.43172901     0.59859929
           C     0.70369481    -2.96717937    -1.83381781
    End
End

Engine DFTB
   Model SCC-DFTB
   ResourcesDir DFTB.org/mio-1-1
   Properties
       Excitations
           TDDFTB
               calc singlet
               lowest 166
               print evcontribs
           End
       End
   End
EndEngine

eor
```

10.5.2 Example: Excitations Ir(ppy)3

Download SP_LR-TDDFTB_irppy3.run

```
#!/bin/sh

AMS_JOBNAME=SOTFilter $AMSBIN/ams << eor

Task SinglePoint

System
    Atoms
       Ir        0.04420       -0.00850       -0.05250
        N       -0.03840       -0.02260        2.09450
        C        1.19280       -0.03830        2.70820
        C        1.26670       -0.06050        4.11790
        H        2.23540       -0.06690        4.60410
        C        0.09850       -0.08170        4.88230
        H        0.15460       -0.10000        5.96680
        C       -1.15030       -0.08660        4.23240
        H       -2.08120       -0.11360        4.78810
        C       -1.17170       -0.06000        2.83740
        H       -2.10440       -0.06910        2.28650
        C        2.33160       -0.05220        1.78990
        C        2.01060       -0.06450        0.39570
        C        3.09340       -0.07380       -0.51520
        H        2.88840       -0.08880       -1.58140
        C        4.42260       -0.07790       -0.07030
        C        4.71950       -0.06800        1.30830
        H        5.75200       -0.06940        1.64760
        C        3.67310       -0.05370        2.23400
        H        3.90660       -0.04300        3.29620
        H        5.23270       -0.08580       -0.79660
        C        0.28050        0.12200       -2.02430
        C        0.41650        1.50790       -2.52520
        C        0.60550        1.72820       -3.93050
        H        0.72650        2.73720       -4.31530
        C        0.63750        0.65370       -4.80680
        H        0.78420        0.83230       -5.87040
        C        0.48640       -0.68860       -4.33810
        H        0.51890       -1.51460       -5.04390
        C        0.30700       -0.92910       -2.96920
        H        0.20840       -1.95190       -2.61810
        C        0.32730        2.53850       -1.55870
        N        0.15930        2.07950       -0.21100
        C        0.16220        2.99060        0.79600
        H        0.07210        2.58960        1.80040
        C        0.26440        4.36230        0.58890
        C        0.38740        4.85520       -0.76210
        H        0.46050        5.92190       -0.95130
        C        0.42240        3.94780       -1.80030
        H        0.52760        4.29590       -2.82360
        H        0.25450        5.03830        1.43730
        N       -2.08080       -0.05260       -0.33870
        C       -2.62190       -1.31760       -0.38820
        C       -4.00890       -1.46660       -0.61030
        H       -4.44160       -2.45950       -0.65200
        C       -4.81680       -0.34140       -0.78650
```

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```
        H       -5.88260        -0.45700        -0.96200
        C       -4.23730         0.94110        -0.74160
        H       -4.82890         1.83860        -0.88430
        C       -2.86380         1.04010        -0.51650
        H       -2.35710         1.99710        -0.48110
        C       -1.65980        -2.40740        -0.20580
        C       -0.29620        -2.01350        -0.02460
        C        0.64840        -3.04760         0.17060
        H        1.69450        -2.79030         0.31090
        C        0.26950        -4.39840         0.17140
        C       -1.07890        -4.76580        -0.01610
        H       -1.36750        -5.81370        -0.01700
        C       -2.04030        -3.76920        -0.20280
        H       -3.07920        -4.05800        -0.34770
        H        1.02320        -5.17010         0.31590
    End
End

Engine DFTB
   Model SCC-DFTB
   ResourcesDir QUASINANO2013.1
   Properties
       Excitations
           SingleOrbTrans
               Filter
                   dEMin 0.15
                   dEMax 1.0
                   OSMin 0.01
               End
               PrintLowest 200
           End
           TDDFTB
               Calc singlet
               Lowest 200
               Print evcontribs
           End
       End
   End
EndEngine

eor



AMS_JOBNAME=upto $AMSBIN/ams << eor

Task SinglePoint

System
    Atoms
       Ir        0.04420        -0.00850        -0.05250
        N       -0.03840        -0.02260         2.09450
        C        1.19280        -0.03830         2.70820
        C        1.26670        -0.06050         4.11790
        H        2.23540        -0.06690         4.60410
        C        0.09850        -0.08170         4.88230
        H        0.15460        -0.10000         5.96680
```

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```
        C       -1.15030        -0.08660         4.23240
        H       -2.08120        -0.11360         4.78810
        C       -1.17170        -0.06000         2.83740
        H       -2.10440        -0.06910         2.28650
        C        2.33160        -0.05220         1.78990
        C        2.01060        -0.06450         0.39570
        C        3.09340        -0.07380        -0.51520
        H        2.88840        -0.08880        -1.58140
        C        4.42260        -0.07790        -0.07030
        C        4.71950        -0.06800         1.30830
        H        5.75200        -0.06940         1.64760
        C        3.67310        -0.05370         2.23400
        H        3.90660        -0.04300         3.29620
        H        5.23270        -0.08580        -0.79660
        C        0.28050         0.12200        -2.02430
        C        0.41650         1.50790        -2.52520
        C        0.60550         1.72820        -3.93050
        H        0.72650         2.73720        -4.31530
        C        0.63750         0.65370        -4.80680
        H        0.78420         0.83230        -5.87040
        C        0.48640        -0.68860        -4.33810
        H        0.51890        -1.51460        -5.04390
        C        0.30700        -0.92910        -2.96920
        H        0.20840        -1.95190        -2.61810
        C        0.32730         2.53850        -1.55870
        N        0.15930         2.07950        -0.21100
        C        0.16220         2.99060         0.79600
        H        0.07210         2.58960         1.80040
        C        0.26440         4.36230         0.58890
        C        0.38740         4.85520        -0.76210
        H        0.46050         5.92190        -0.95130
        C        0.42240         3.94780        -1.80030
        H        0.52760         4.29590        -2.82360
        H        0.25450         5.03830         1.43730
        N       -2.08080        -0.05260        -0.33870
        C       -2.62190        -1.31760        -0.38820
        C       -4.00890        -1.46660        -0.61030
        H       -4.44160        -2.45950        -0.65200
        C       -4.81680        -0.34140        -0.78650
        H       -5.88260        -0.45700        -0.96200
        C       -4.23730         0.94110        -0.74160
        H       -4.82890         1.83860        -0.88430
        C       -2.86380         1.04010        -0.51650
        H       -2.35710         1.99710        -0.48110
        C       -1.65980        -2.40740        -0.20580
        C       -0.29620        -2.01350        -0.02460
        C        0.64840        -3.04760         0.17060
        H        1.69450        -2.79030         0.31090
        C        0.26950        -4.39840         0.17140
        C       -1.07890        -4.76580        -0.01610
        H       -1.36750        -5.81370        -0.01700
        C       -2.04030        -3.76920        -0.20280
        H       -3.07920        -4.05800        -0.34770
        H        1.02320        -5.17010         0.31590
    End
End
```

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```
Engine DFTB
   Model SCC-DFTB
   ResourcesDir QUASINANO2013.1
   Properties
       Excitations
           SingleOrbTrans
               printlowest 200
           End
           TDDFTB
               Calc singlet
               UpTo 7.0 [eV]
               Print evcontribs
           End
       End
   End
EndEngine

eor
```

10.5.3 Example: Excitations Davidson algorithm

Download SP_LR-TDDFTB_Davidson.run

```
#!/bin/sh


# =======
# Benzene
# =======

AMS_JOBNAME=benzene $AMSBIN/ams << eor

Task SinglePoint

System
    Atoms
      C     1.20938551     0.69823911     0.00000000
      C    -1.20938551    -0.69823911     0.00000000
      C     0.00000000     1.39647931     0.00000000
      C     1.20938551    -0.69823911     0.00000000
      C     0.00000000    -1.37647931     0.00000000
      C    -1.20938551     0.69823911     0.00000000
      H     2.18068291     1.24747033     0.00000000
      H     2.16068291    -1.24747033     0.00000000
      H     0.00000000    -2.49494279     0.00000000
      H    -2.14068291    -1.24747033     0.00000000
      H    -2.16068291     1.24747033     0.00000000
      H     0.00000000     2.47494279     0.00000000
    End
End

Engine DFTB
   Model SCC-DFTB
   ResourcesDir DFTB.org/mio-1-1
   Properties
```

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```
        Excitations
            SingleOrbTrans
                printlowest 20
            End
            TDDFTB
                calc singlet
                lowest 14
                diagonalization davidson
                print evcontribs
            End
        End
    End
EndEngine

eor


# =========
# Butadiene
# =========

AMS_JOBNAME=butadiene $AMSBIN/ams << eor

Task SinglePoint

System
    Atoms
      C     0.00466252    -0.00028952    -0.00104529
      H    -0.49779025     0.97930953    -0.00159217
      C     1.45987721     0.00047513    -0.00103479
      C    -0.72357617    -1.12728993    -0.00048806
      H     1.96233457    -0.97912057    -0.00242387
      C     2.18814037     1.12751916     0.00036000
      H     1.71167857     2.11236793     0.00203718
      H     3.28068998     1.10035883     0.00074531
      H    -1.81612590    -1.10012490    -0.00008198
      H    -0.24711388    -2.11214067     0.00035465
    End
End

Engine DFTB
   Model SCC-DFTB
   ResourcesDir DFTB.org/mio-1-1
   Properties
       Excitations
           SingleOrbTrans
               printlowest 20
           End
           TDDFTB
               calc triplet
               lowest 13
               diagonalization davidson
               print evcontribs
           End
       End
   End
EndEngine
```

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(continued from previous page)

```
eor


# ============
# Cyclopropene
# ============

AMS_JOBNAME=cyclopropene $AMSBIN/ams << eor

Task SinglePoint

System
    Atoms
      C     0.57102290    -2.27031483     0.21362813
      C     0.48029660    -0.79657680    -0.01804280
      C     1.71237550    -1.60993397     0.21483841
      H     0.05089823    -3.22311984     0.31173291
      H     0.09953799    -0.14003315     0.78693532
      H     0.26136156    -0.41625182    -1.03364050
      H     2.79743635    -1.63396435     0.31513170
    End
End

Engine DFTB
   Model SCC-DFTB
   ResourcesDir DFTB.org/mio-1-1
   Properties
       Excitations
           SingleOrbTrans
               printlowest 20
           End
           TDDFTB
               calc singlet
               lowest 12
               diagonalization davidson
               print evcontribs
           End
       End
   End
EndEngine

eor


# ========
# Ethylene
# ========

AMS_JOBNAME=ethylene $AMSBIN/ams << eor

Task SinglePoint

System
    Atoms
      C     0.00000000     0.00000000     0.66358767
      C     0.00000000     0.00000000    -0.66358767
```

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```
      H     0.00000000     0.93162477    -1.23681998
      H     0.00000000     0.93162477     1.23681998
      H     0.00000000    -0.93162477     1.23681998
      H     0.00000000    -0.93162477    -1.23681998
    End
End

Engine DFTB
   Model SCC-DFTB
   ResourcesDir DFTB.org/mio-1-1
   Properties
       Excitations
           SingleOrbTrans
               printlowest 20
           End
           TDDFTB
               calc triplet
               lowest 14
               diagonalization davidson
               print evcontribs
           End
       End
   End
EndEngine

eor



# ============
# Formaldehyde
# ============

AMS_JOBNAME=formaldehyde $AMSBIN/ams << eor

Task SinglePoint

System
    Atoms
      C     0.00000000     0.00000000    -0.01786493
      O     0.00000000     0.00000000    -1.20109680
      H     0.00000000    -0.95460929     0.60948087
      H     0.00000000     0.95460929     0.60948087
    End
End

Engine DFTB
   Model SCC-DFTB
   ResourcesDir DFTB.org/mio-1-1
   Properties
       Excitations
           SingleOrbTrans
               printlowest 20
           End
           TDDFTB
               calc singlet
               lowest 9
```

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```
                diagonalization davidson
                print evcontribs
            End
        End
    End
EndEngine

eor


# =======
# Glyoxal
# =======

AMS_JOBNAME=glyoxal $AMSBIN/ams << eor

Task SinglePoint

System
    Atoms
      O      1.72385877      0.13122797      0.00000000
      O     -1.72385877     -0.13122797      0.00000000
      C      0.64697620     -0.39816537      0.00000000
      C     -0.64697620      0.39816537      0.00000000
      H      0.53384841     -1.53815588      0.00000000
      H     -0.53384841      1.53815588      0.00000000
    End
End

Engine DFTB
   Model SCC-DFTB
   ResourcesDir DFTB.org/mio-1-1
   Properties
       Excitations
           SingleOrbTrans
               printlowest 20
           End
           TDDFTB
               calc triplet
               lowest 15
               diagonalization davidson
               print evcontribs
           End
       End
   End
EndEngine

eor


# ======
# Ketene
# ======

AMS_JOBNAME=ketene $AMSBIN/ams << eor

Task SinglePoint
```

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(continued from previous page)

```
System
    Atoms
      C     0.00000000     0.00000000     0.54640785
      C     0.00000000     0.00000000    -0.78272675
      O     0.00000000     0.00000000    -1.93849838
      H     0.00000000    -0.94519170     1.08740863
      H     0.00000000     0.94519170     1.08740863
    End
End

Engine DFTB
   Model SCC-DFTB
   ResourcesDir DFTB.org/mio-1-1
   Properties
       Excitations
           SingleOrbTrans
               printlowest 20
           End
           TDDFTB
               calc singlet
               lowest 12
               diagonalization davidson
               print evcontribs
           End
       End
   End
EndEngine

eor


# =======
# Propene
# =======

AMS_JOBNAME=propene $AMSBIN/ams << eor

Task SinglePoint

System
    Atoms
      C     0.00000000    -0.18063145     1.36950456
      C     0.00000000     0.50453710     0.22489796
      C     0.00000000    -0.12822183    -1.11902990
      H     0.00000000     1.60588976     0.24796806
      H     0.00000000     0.32869011     2.33647979
      H     0.00000000    -1.27447627     1.38113901
      H     0.00000000    -1.22278585    -1.05105048
      H     0.88416595     0.18349923    -1.69495452
      H    -0.88416595     0.18349923    -1.69495452
    End
End

Engine DFTB
   Model SCC-DFTB
   ResourcesDir DFTB.org/mio-1-1
```

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```
   Properties
       Excitations
           SingleOrbTrans
               printlowest 20
           End
           TDDFTB
               calc triplet
               lowest 13
               diagonalization davidson
               print evcontribs
           End
       End
   End
EndEngine

eor


# ========
# Propynal
# ========

AMS_JOBNAME=propynal $AMSBIN/ams << eor

Task SinglePoint

System
    Atoms
      C      0.00000000     0.27956244    -1.52026344
      C      0.00000000     0.12195280    -0.32047659
      C      0.00000000    -0.19208888     1.11108555
      O      0.00000000     0.63096241     1.98042927
      H      0.00000000    -1.31675676     1.32754962
      H      0.00000000     0.47636799    -2.57832442
    End
End

Engine DFTB
   Model SCC-DFTB
   ResourcesDir DFTB.org/mio-1-1
   Properties
       Excitations
           SingleOrbTrans
               printlowest 20
           End
           TDDFTB
               calc singlet
               lowest 10
               diagonalization davidson
               print evcontribs
           End
       End
   End
EndEngine

eor
```

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```
# ========
# Pyridine
# ========

AMS_JOBNAME=pyridine $AMSBIN/ams << eor

Task SinglePoint

System
    Atoms
      N     0.00000000     0.00000000    -1.60262045
      C     0.00000000     0.00000000     1.19107401
      C     0.00000000     1.15158459    -0.91948133
      C     0.00000000    -1.15158459    -0.91948133
      C     0.00000000    -1.19927371     0.47941227
      C     0.00000000     1.19927371     0.47941227
      H     0.00000000     2.16322205     1.00470037
      H     0.00000000     2.09200426    -1.50384439
      H     0.00000000     0.00000000     2.28997262
      H     0.00000000    -2.16322205     1.00470037
      H     0.00000000    -2.09200426    -1.50384439
    End
End

Engine DFTB
   Model SCC-DFTB
   ResourcesDir DFTB.org/mio-1-1
   Properties
       Excitations
           SingleOrbTrans
               printlowest 20
           End
           TDDFTB
               calc triplet
               lowest 15
               diagonalization davidson
               print evcontribs
           End
       End
   End
EndEngine

eor
```

10.5.4 Example: Excitations transition charges on the fly

Download SP_LR-TDDFTB_Davidson_onthefly.run

```
#!/bin/sh


# =======
# Benzene
# =======
```

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```
AMS_JOBNAME=benzene $AMSBIN/ams << eor

Task SinglePoint

System
    Atoms
      C     1.20938551     0.69823911     0.00000000
      C    -1.20938551    -0.69823911     0.00000000
      C     0.00000000     1.39647931     0.00000000
      C     1.20938551    -0.69823911     0.00000000
      C     0.00000000    -1.37647931     0.00000000
      C    -1.20938551     0.69823911     0.00000000
      H     2.18068291     1.24747033     0.00000000
      H     2.16068291    -1.24747033     0.00000000
      H     0.00000000    -2.49494279     0.00000000
      H    -2.14068291    -1.24747033     0.00000000
      H    -2.16068291     1.24747033     0.00000000
      H     0.00000000     2.47494279     0.00000000
    End
End

Engine DFTB
   Model SCC-DFTB
   ResourcesDir DFTB.org/mio-1-1
   Properties
       Excitations
           SingleOrbTrans
               printlowest 20
           End
           TDDFTB
               calc singlet
               lowest 14
               diagonalization davidson
               DavidsonConfig
                   ATCharges onTheFly
               End
               print evcontribs
           End
       End
   End
EndEngine

eor


# =========
# Butadiene
# =========

AMS_JOBNAME=butadiene $AMSBIN/ams << eor

Task SinglePoint

System
    Atoms
      C     0.00466252    -0.00028952    -0.00104529
```

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(continued from previous page)

```
      H    -0.49779025     0.97930953    -0.00159217
      C     1.45987721     0.00047513    -0.00103479
      C    -0.72357617    -1.12728993    -0.00048806
      H     1.96233457    -0.97912057    -0.00242387
      C     2.18814037     1.12751916     0.00036000
      H     1.71167857     2.11236793     0.00203718
      H     3.28068998     1.10035883     0.00074531
      H    -1.81612590    -1.10012490    -0.00008198
      H    -0.24711388    -2.11214067     0.00035465
    End
End

Engine DFTB
   Model SCC-DFTB
   ResourcesDir DFTB.org/mio-1-1
   Properties
       Excitations
           SingleOrbTrans
               printlowest 20
           End
           TDDFTB
               calc triplet
               lowest 13
               diagonalization davidson
               DavidsonConfig
                   ATCharges onTheFly
               End
               print evcontribs
           End
       End
   End
EndEngine

eor


# ============
# Cyclopropene
# ============

AMS_JOBNAME=cyclopropene $AMSBIN/ams << eor

Task SinglePoint

System
    Atoms
      C     0.57102290    -2.27031483     0.21362813
      C     0.48029660    -0.79657680    -0.01804280
      C     1.71237550    -1.60993397     0.21483841
      H     0.05089823    -3.22311984     0.31173291
      H     0.09953799    -0.14003315     0.78693532
      H     0.26136156    -0.41625182    -1.03364050
      H     2.79743635    -1.63396435     0.31513170
    End
End

Engine DFTB
```

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(continued from previous page)

```
   Model SCC-DFTB
   ResourcesDir DFTB.org/mio-1-1
   Properties
       Excitations
           SingleOrbTrans
               printlowest 20
           End
           TDDFTB
               calc singlet
               lowest 12
               diagonalization davidson
               DavidsonConfig
                   ATCharges onTheFly
               End
               print evcontribs
           End
       End
   End
EndEngine

eor


# ========
# Ethylene
# ========

AMS_JOBNAME=ethylene $AMSBIN/ams << eor

Task SinglePoint

System
    Atoms
      C      0.00000000      0.00000000      0.66358767
      C      0.00000000      0.00000000     -0.66358767
      H      0.00000000      0.93162477     -1.23681998
      H      0.00000000      0.93162477      1.23681998
      H      0.00000000     -0.93162477      1.23681998
      H      0.00000000     -0.93162477     -1.23681998
    End
End

Engine DFTB
   Model SCC-DFTB
   ResourcesDir DFTB.org/mio-1-1
   Properties
       Excitations
           SingleOrbTrans
               printlowest 20
           End
           TDDFTB
               calc triplet
               lowest 14
               diagonalization davidson
               DavidsonConfig
                   ATCharges onTheFly
               End
```

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```
                print evcontribs
            End
        End
    End
EndEngine

eor



# ============
# Formaldehyde
# ============

AMS_JOBNAME=formaldehyde $AMSBIN/ams << eor

Task SinglePoint

System
    Atoms
      C     0.00000000     0.00000000    -0.01786493
      O     0.00000000     0.00000000    -1.20109680
      H     0.00000000    -0.95460929     0.60948087
      H     0.00000000     0.95460929     0.60948087
    End
End

Engine DFTB
   Model SCC-DFTB
   ResourcesDir DFTB.org/mio-1-1
   Properties
       Excitations
           SingleOrbTrans
               printlowest 20
           End
           TDDFTB
               calc singlet
               lowest 9
               diagonalization davidson
               DavidsonConfig
                   ATCharges onTheFly
               End
               print evcontribs
           End
       End
   End
EndEngine

eor


# =======
# Glyoxal
# =======

AMS_JOBNAME=glyoxal $AMSBIN/ams << eor
```

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(continued from previous page)

```
Task SinglePoint

System
    Atoms
      O     1.72385877     0.13122797     0.00000000
      O    -1.72385877    -0.13122797     0.00000000
      C     0.64697620    -0.39816537     0.00000000
      C    -0.64697620     0.39816537     0.00000000
      H     0.53384841    -1.53815588     0.00000000
      H    -0.53384841     1.53815588     0.00000000
    End
End

Engine DFTB
   Model SCC-DFTB
   ResourcesDir DFTB.org/mio-1-1
   Properties
       Excitations
           SingleOrbTrans
               printlowest 20
           End
           TDDFTB
               calc triplet
               lowest 15
               diagonalization davidson
               DavidsonConfig
                   ATCharges onTheFly
               End
               print evcontribs
           End
       End
   End
EndEngine

eor


# ======
# Ketene
# ======

AMS_JOBNAME=ketene $AMSBIN/ams << eor

Task SinglePoint

System
    Atoms
      C     0.00000000     0.00000000     0.54640785
      C     0.00000000     0.00000000    -0.78272675
      O     0.00000000     0.00000000    -1.93849838
      H     0.00000000    -0.94519170     1.08740863
      H     0.00000000     0.94519170     1.08740863
    End
End

Engine DFTB
   Model SCC-DFTB
```

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```
   ResourcesDir DFTB.org/mio-1-1
   Properties
       Excitations
           SingleOrbTrans
               printlowest 20
           End
           TDDFTB
               calc singlet
               lowest 12
               diagonalization davidson
               DavidsonConfig
                   ATCharges onTheFly
               End
               print evcontribs
           End
       End
   End
EndEngine

eor


# =======
# Propene
# =======

AMS_JOBNAME=propene $AMSBIN/ams << eor

Task SinglePoint

System
    Atoms
      C      0.00000000    -0.18063145     1.36950456
      C      0.00000000     0.50453710     0.22489796
      C      0.00000000    -0.12822183    -1.11902990
      H      0.00000000     1.60588976     0.24796806
      H      0.00000000     0.32869011     2.33647979
      H      0.00000000    -1.27447627     1.38113901
      H      0.00000000    -1.22278585    -1.05105048
      H      0.88416595     0.18349923    -1.69495452
      H     -0.88416595     0.18349923    -1.69495452
    End
End

Engine DFTB
   Model SCC-DFTB
   ResourcesDir DFTB.org/mio-1-1
   Properties
       Excitations
           SingleOrbTrans
               printlowest 20
           End
           TDDFTB
               calc triplet
               lowest 13
               diagonalization davidson
               DavidsonConfig
```

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(continued from previous page)

```
                    ATCharges onTheFly
                End
                print evcontribs
            End
        End
    End
EndEngine

eor


# ========
# Propynal
# ========

AMS_JOBNAME=propynal $AMSBIN/ams << eor

Task SinglePoint

System
    Atoms
      C     0.00000000     0.27956244    -1.52026344
      C     0.00000000     0.12195280    -0.32047659
      C     0.00000000    -0.19208888     1.11108555
      O     0.00000000     0.63096241     1.98042927
      H     0.00000000    -1.31675676     1.32754962
      H     0.00000000     0.47636799    -2.57832442
    End
End

Engine DFTB
   Model SCC-DFTB
   ResourcesDir DFTB.org/mio-1-1
   Properties
       Excitations
           SingleOrbTrans
               printlowest 20
           End
           TDDFTB
               calc singlet
               lowest 10
               diagonalization davidson
               DavidsonConfig
                   ATCharges onTheFly
               End
               print evcontribs
           End
       End
   End
EndEngine

eor


# ========
# Pyridine
# ========
```

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```
AMS_JOBNAME=pyridine $AMSBIN/ams << eor

Task SinglePoint

System
    Atoms
      N     0.00000000     0.00000000    -1.60262045
      C     0.00000000     0.00000000     1.19107401
      C     0.00000000     1.15158459    -0.91948133
      C     0.00000000    -1.15158459    -0.91948133
      C     0.00000000    -1.19927371     0.47941227
      C     0.00000000     1.19927371     0.47941227
      H     0.00000000     2.16322205     1.00470037
      H     0.00000000     2.09200426    -1.50384439
      H     0.00000000     0.00000000     2.28997262
      H     0.00000000    -2.16322205     1.00470037
      H     0.00000000    -2.09200426    -1.50384439
    End
End

Engine DFTB
   Model SCC-DFTB
   ResourcesDir DFTB.org/mio-1-1
   Properties
       Excitations
           SingleOrbTrans
               printlowest 20
           End
           TDDFTB
               calc triplet
               lowest 15
               diagonalization davidson
               DavidsonConfig
                   ATCharges onTheFly
               End
               print evcontribs
           End
       End
   End
EndEngine

eor
```

10.5.5 Example: Excitations exact diagonalization

Download SP_LR-TDDFTB_exact.run

```
#!/bin/sh


# =======
# Benzene
# =======
```

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```
AMS_JOBNAME=benzene $AMSBIN/ams << eor

Task SinglePoint

System
    Atoms
      C     1.20938551     0.69823911     0.00000000
      C    -1.20938551    -0.69823911     0.00000000
      C     0.00000000     1.39647931     0.00000000
      C     1.20938551    -0.69823911     0.00000000
      C     0.00000000    -1.37647931     0.00000000
      C    -1.20938551     0.69823911     0.00000000
      H     2.18068291     1.24747033     0.00000000
      H     2.16068291    -1.24747033     0.00000000
      H     0.00000000    -2.49494279     0.00000000
      H    -2.14068291    -1.24747033     0.00000000
      H    -2.16068291     1.24747033     0.00000000
      H     0.00000000     2.47494279     0.00000000
    End
End

Engine DFTB
   Model SCC-DFTB
   ResourcesDir DFTB.org/mio-1-1
   Properties
       Excitations
           SingleOrbTrans
               printlowest 100000
           End
           TDDFTB
               calc singlet
               lowest 100000
               diagonalization exact
               print evcontribs
           End
       End
   End
EndEngine

eor


# =========
# Butadiene
# =========

AMS_JOBNAME=butadiene $AMSBIN/ams << eor

Task SinglePoint

System
    Atoms
      C     0.00466252    -0.00028952    -0.00104529
      H    -0.49779025     0.97930953    -0.00159217
      C     1.45987721     0.00047513    -0.00103479
      C    -0.72357617    -1.12728993    -0.00048806
      H     1.96233457    -0.97912057    -0.00242387
```

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```
      C     2.18814037     1.12751916     0.00036000
      H     1.71167857     2.11236793     0.00203718
      H     3.28068998     1.10035883     0.00074531
      H    -1.81612590    -1.10012490    -0.00008198
      H    -0.24711388    -2.11214067     0.00035465
    End
End

Engine DFTB
   Model SCC-DFTB
   ResourcesDir DFTB.org/mio-1-1
   Properties
       Excitations
           SingleOrbTrans
               printlowest 100000
           End
           TDDFTB
               calc triplet
               lowest 100000
               diagonalization exact
               print evcontribs
           End
       End
   End
EndEngine

eor


# ============
# Cyclopropene
# ============

AMS_JOBNAME=cyclopropene $AMSBIN/ams << eor

Task SinglePoint

System
    Atoms
      C     0.57102290    -2.27031483     0.21362813
      C     0.48029660    -0.79657680    -0.01804280
      C     1.71237550    -1.60993397     0.21483841
      H     0.05089823    -3.22311984     0.31173291
      H     0.09953799    -0.14003315     0.78693532
      H     0.26136156    -0.41625182    -1.03364050
      H     2.79743635    -1.63396435     0.31513170
    End
End

Engine DFTB
   Model SCC-DFTB
   ResourcesDir DFTB.org/mio-1-1
   Properties
       Excitations
           SingleOrbTrans
               printlowest 100000
           End
```

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```
            TDDFTB
                calc singlet
                lowest 100000
                diagonalization exact
                print evcontribs
            End
        End
    End
EndEngine

eor


# ========
# Ethylene
# ========

AMS_JOBNAME=ethylene $AMSBIN/ams << eor

Task SinglePoint

System
    Atoms
      C     0.00000000     0.00000000     0.66358767
      C     0.00000000     0.00000000    -0.66358767
      H     0.00000000     0.93162477    -1.23681998
      H     0.00000000     0.93162477     1.23681998
      H     0.00000000    -0.93162477     1.23681998
      H     0.00000000    -0.93162477    -1.23681998
    End
End

Engine DFTB
   Model SCC-DFTB
   ResourcesDir DFTB.org/mio-1-1
   Properties
       Excitations
           SingleOrbTrans
               printlowest 100000
           End
           TDDFTB
               calc triplet
               lowest 100000
               diagonalization exact
               print evcontribs
           End
       End
   End
EndEngine

eor



# ============
# Formaldehyde
# ============
```

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```
AMS_JOBNAME=formaldehyde $AMSBIN/ams << eor

Task SinglePoint

System
    Atoms
      C     0.00000000     0.00000000    -0.01786493
      O     0.00000000     0.00000000    -1.20109680
      H     0.00000000    -0.95460929     0.60948087
      H     0.00000000     0.95460929     0.60948087
    End
End

Engine DFTB
   Model SCC-DFTB
   ResourcesDir DFTB.org/mio-1-1
   Properties
       Excitations
           SingleOrbTrans
               printlowest 100000
           End
           TDDFTB
               calc singlet
               lowest 100000
               diagonalization exact
               print evcontribs
           End
       End
   End
EndEngine

eor


# =======
# Glyoxal
# =======

AMS_JOBNAME=glyoxal $AMSBIN/ams << eor

Task SinglePoint

System
    Atoms
      O     1.72385877     0.13122797     0.00000000
      O    -1.72385877    -0.13122797     0.00000000
      C     0.64697620    -0.39816537     0.00000000
      C    -0.64697620     0.39816537     0.00000000
      H     0.53384841    -1.53815588     0.00000000
      H    -0.53384841     1.53815588     0.00000000
    End
End

Engine DFTB
   Model SCC-DFTB
   ResourcesDir DFTB.org/mio-1-1
```

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```
   Properties
       Excitations
           SingleOrbTrans
               printlowest 100000
           End
           TDDFTB
               calc triplet
               lowest 100000
               diagonalization exact
               print evcontribs
           End
       End
   End
EndEngine

eor


# ======
# Ketene
# ======

AMS_JOBNAME=ketene $AMSBIN/ams << eor

Task SinglePoint

System
    Atoms
      C      0.00000000     0.00000000     0.54640785
      C      0.00000000     0.00000000    -0.78272675
      O      0.00000000     0.00000000    -1.93849838
      H      0.00000000    -0.94519170     1.08740863
      H      0.00000000     0.94519170     1.08740863
    End
End

Engine DFTB
   Model SCC-DFTB
   ResourcesDir DFTB.org/mio-1-1
   Properties
       Excitations
           SingleOrbTrans
               printlowest 100000
           End
           TDDFTB
               calc singlet
               lowest 100000
               diagonalization exact
               print evcontribs
           End
       End
   End
EndEngine

eor
```

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```
# =======
# Propene
# =======

AMS_JOBNAME=propene $AMSBIN/ams << eor

Task SinglePoint

System
    Atoms
      C     0.00000000    -0.18063145     1.36950456
      C     0.00000000     0.50453710     0.22489796
      C     0.00000000    -0.12822183    -1.11902990
      H     0.00000000     1.60588976     0.24796806
      H     0.00000000     0.32869011     2.33647979
      H     0.00000000    -1.27447627     1.38113901
      H     0.00000000    -1.22278585    -1.05105048
      H     0.88416595     0.18349923    -1.69495452
      H    -0.88416595     0.18349923    -1.69495452
    End
End

Engine DFTB
   Model SCC-DFTB
   ResourcesDir DFTB.org/mio-1-1
   Properties
       Excitations
           SingleOrbTrans
               printlowest 100000
           End
           TDDFTB
               calc triplet
               lowest 100000
               diagonalization exact
               print evcontribs
           End
       End
   End
EndEngine

eor


# ========
# Propynal
# ========

AMS_JOBNAME=propynal $AMSBIN/ams << eor

Task SinglePoint

System
    Atoms
      C     0.00000000     0.27956244    -1.52026344
      C     0.00000000     0.12195280    -0.32047659
      C     0.00000000    -0.19208888     1.11108555
      O     0.00000000     0.63096241     1.98042927
```

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```
      H     0.00000000    -1.31675676     1.32754962
      H     0.00000000     0.47636799    -2.57832442
    End
End

Engine DFTB
   Model SCC-DFTB
   ResourcesDir DFTB.org/mio-1-1
   Properties
       Excitations
           SingleOrbTrans
               printlowest 100000
           End
           TDDFTB
               calc singlet
               lowest 100000
               diagonalization exact
               print evcontribs
           End
       End
   End
EndEngine

eor


# ========
# Pyridine
# ========

AMS_JOBNAME=pyridine $AMSBIN/ams << eor

Task SinglePoint

System
    Atoms
      N     0.00000000     0.00000000    -1.60262045
      C     0.00000000     0.00000000     1.19107401
      C     0.00000000     1.15158459    -0.91948133
      C     0.00000000    -1.15158459    -0.91948133
      C     0.00000000    -1.19927371     0.47941227
      C     0.00000000     1.19927371     0.47941227
      H     0.00000000     2.16322205     1.00470037
      H     0.00000000     2.09200426    -1.50384439
      H     0.00000000     0.00000000     2.28997262
      H     0.00000000    -2.16322205     1.00470037
      H     0.00000000    -2.09200426    -1.50384439
    End
End

Engine DFTB
   Model SCC-DFTB
   ResourcesDir DFTB.org/mio-1-1
   Properties
       Excitations
           SingleOrbTrans
               printlowest 100000
```

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```
            End
            TDDFTB
                calc triplet
                lowest 100000
                diagonalization exact
                print evcontribs
            End
        End
    End
EndEngine

eor
```

10.5.6 Example: Excited state gradients: plams

Download SP_LR-TDDFTB_gradients.run

```
#!/bin/sh

cp $AMSHOME/examples/dftb/SP_LR-TDDFTB_gradients/SP_LR-TDDFTB_gradients.plms .
cp -r $AMSHOME/examples/dftb/SP_LR-TDDFTB_gradients/molecules .
cp -r $AMSHOME/examples/dftb/SP_LR-TDDFTB_gradients/numgrad_precalc .

export NSCM=1
$AMSBIN/plams SP_LR-TDDFTB_gradients.plms
```

Download SP_LR-TDDFTB_gradients.plms

```
import numpy as np
import os.path


# our test molecules and their excitations for which we want to calculate the␣
↪gradients
tests = [
    ("acetamide", "singlet", 2, False),
    ("acetone", "singlet", 5, False),
    ("adenine", "singlet", 2, False),
    ("benzene", "singlet", 1, False),
    ("benzoquinone", "singlet", 1, False),
    ("butadiene", "singlet", 1, False),
    ("carbonmonoxide", "singlet", 8, False),
    ("cyclopentadiene", "singlet", 1, False),
    ("cyclopropene", "singlet", 1, False),
    ("cytosine", "singlet", 2, False),
    ("ethene", "singlet", 2, False),
    ("formaldehyde", "singlet", 4, False),
    ("formamide", "singlet", 2, False),
    ("furan", "singlet", 1, False),
    ("hexatriene", "singlet", 1, False),
    ("imidazole", "singlet", 2, False),
    ("naphthalene", "singlet", 1, False),
    ("nitrogen", "singlet", 8, False),
    ("norbornadiene", "singlet", 1, False),
    ("octatetraene", "singlet", 1, False),
```

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```
    ("propanamide", "singlet", 2, False),
    ("pyrazine", "singlet", 3, False),
    ("pyridazine", "singlet", 4, False),
    ("pyridine", "singlet", 3, False),
    ("pyrimidine", "singlet", 6, False),
    ("pyrrole", "singlet", 3, False),
    ("tetrazine", "singlet", 6, False),
    ("thymine", "singlet", 3, False),
    ("triazine", "singlet", 6, False),
    ("uracil", "singlet", 3, False),
    ("betacarotene", "singlet", 1, False),
    ("acetamide", "triplet", 3, False),
    ("acetone", "triplet", 1, False),
    ("adenine", "triplet", 4, False),
    ("benzene", "triplet", 1, False),
    ("benzoquinone", "triplet", 4, False),
    ("butadiene", "triplet", 1, False),
    ("carbonmonoxide", "triplet", 3, False),
    ("cyclopentadiene", "triplet", 2, False),
    ("cyclopropene", "triplet", 1, False),
    ("cytosine", "triplet", 3, False),
    ("ethene", "triplet", 1, False),
    ("formaldehyde", "triplet", 7, False),
    ("formamide", "triplet", 10, False),
    ("furan", "triplet", 2, False),
    ("hexatriene", "triplet", 2, False),
    ("imidazole", "triplet", 1, False),
    ("naphthalene", "triplet", 9, False),
    ("nitrogen", "triplet", 1, False),
    ("norbornadiene", "triplet", 2, False),
    ("octatetraene", "triplet", 1, False),
    ("propanamide", "triplet", 1, False),
    ("pyrazine", "triplet", 4, False),
    ("pyridazine", "triplet", 1, False),
    ("pyridine", "triplet", 5, False),
    ("pyrimidine", "triplet", 1, False),
    ("pyrrole", "triplet", 2, False),
    ("tetrazine", "triplet", 6, False),
    ("thymine", "triplet", 4, False),
    ("triazine", "triplet", 5, False),
    ("uracil", "triplet", 2, False),
    ("betacarotene", "triplet", 1, False),
    ("acetamide", "singlet", 2, True),
    ("acetone", "singlet", 5, True),
    ("adenine", "singlet", 2, True),
    ("benzene", "singlet", 1, True),
    ("benzoquinone", "singlet", 1, True),
    ("butadiene", "singlet", 1, True),
    ("carbonmonoxide", "singlet", 8, True),
    ("cyclopentadiene", "singlet", 1, True),
    ("cyclopropene", "singlet", 1, True),
    ("cytosine", "singlet", 2, True),
    ("ethene", "singlet", 2, True),
    ("formaldehyde", "singlet", 4, True),
    ("formamide", "singlet", 2, True),
    ("furan", "singlet", 1, True),
    ("hexatriene", "singlet", 1, True),
```

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```
    ("imidazole", "singlet", 2, True),
    ("naphthalene", "singlet", 1, True),
    ("nitrogen", "singlet", 8, True),
    ("norbornadiene", "singlet", 1, True),
    ("octatetraene", "singlet", 1, True),
    ("propanamide", "singlet", 2, True),
    ("pyrazine", "singlet", 3, True),
    ("pyridazine", "singlet", 4, True),
    ("pyridine", "singlet", 3, True),
    ("pyrimidine", "singlet", 6, True),
    ("pyrrole", "singlet", 3, True),
    ("tetrazine", "singlet", 6, True),
    ("thymine", "singlet", 3, True),
    ("triazine", "singlet", 6, True),
    ("uracil", "singlet", 3, True),
    ("betacarotene", "singlet", 1, True),
    ("acetamide", "triplet", 3, True),
    ("acetone", "triplet", 1, True),
    ("adenine", "triplet", 4, True),
    ("benzene", "triplet", 1, True),
    ("benzoquinone", "triplet", 4, True),
    ("butadiene", "triplet", 1, True),
    ("carbonmonoxide", "triplet", 3, True),
    ("cyclopentadiene", "triplet", 2, True),
    ("cyclopropene", "triplet", 1, True),
    ("cytosine", "triplet", 3, True),
    ("ethene", "triplet", 1, True),
    ("formaldehyde", "triplet", 7, True),
    ("formamide", "triplet", 10, True),
    ("furan", "triplet", 2, True),
    ("hexatriene", "triplet", 2, True),
    ("imidazole", "triplet", 1, True),
    ("naphthalene", "triplet", 9, True),
    ("nitrogen", "triplet", 1, True),
    ("norbornadiene", "triplet", 2, True),
    ("octatetraene", "triplet", 1, True),
    ("propanamide", "triplet", 1, True),
    ("pyrazine", "triplet", 4, True),
    ("pyridazine", "triplet", 1, True),
    ("pyridine", "triplet", 5, True),
    ("pyrimidine", "triplet", 1, True),
    ("pyrrole", "triplet", 2, True),
    ("tetrazine", "triplet", 6, True),
    ("thymine", "triplet", 4, True),
    ("triazine", "triplet", 5, True),
    ("uracil", "triplet", 2, True),
    ("betacarotene", "triplet", 1, True),
]


# numpy setup
# np.set_printoptions(precision=8, suppress=True)
np.set_printoptions(formatter={"float": " {: 0.8f} ".format})

# plams set up
config.log.stdout = 0
```

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```
# common input for all tests
comin = Settings()
comin.input.ams.task = "SinglePoint"
comin.input.ams.properties.gradients = True
comin.input.DFTB.model = "SCC-DFTB"
comin.input.DFTB.resourcesdir = "DFTB.org/mio-1-1"
comin.input.DFTB.properties.excitations.tddftb["print"] = "evcontribs"

failedtests = []
for test in tests:
    molname = test[0]
    multi = test[1]
    excit = test[2]
    ldep = test[3]
    if multi == "singlet":
        kfsec = "SS"
    else:
        kfsec = "ST"
    if ldep:
        ldpf = "ldep"
    else:
        ldpf = "noldep"

    print("\nTESTING: " + molname + " " + multi + " " + str(excit) + " " + ldpf)
    teststr = molname + "_" + multi + "_" + str(excit) + "_" + ldpf

    comin_thistest = comin.copy()
    comin_thistest.input.DFTB.properties.excitations.tddftb.calc = multi
    comin_thistest.input.DFTB.properties.excitations.tddftb.lowest = excit
    if ldep:
        comin_thistest.input.DFTB.scc.orbitaldependent = "yes"
    mol = Molecule(filename="./molecules/" + molname + ".xyz")

    # numerical gradient
    if os.path.isfile("./numgrad_precalc/" + teststr + ".npy"):
        print("Precalculated numerical gradient found -> reading from file")
        numgrad = np.load("./numgrad_precalc/" + teststr + ".npy")
    else:
        print("Precalculated numerical gradient not found -> calculating")
        numgradjob = AMSNumGradJob(name=teststr + "_numgrad", molecule=mol, npoints=3,
↪ step=0.001)
        numgradjob.settings.child = comin_thistest
        numgradresults = numgradjob.run()

        def exenergy(results):
            if excit == 1:
                return results.readrkf("Excitations " + kfsec + " A", "excenergies",␣
↪file="dftb")
            else:
                return results.readrkf("Excitations " + kfsec + " A", "excenergies",␣
↪file="dftb")[excit - 1]

        numgrad = np.empty([len(mol), 3])
        for n in range(1, len(mol) + 1):
            numgrad[n - 1, 0] = numgradresults.get_gradient(n, "x", func=exenergy)
            numgrad[n - 1, 1] = numgradresults.get_gradient(n, "y", func=exenergy)
            numgrad[n - 1, 2] = numgradresults.get_gradient(n, "z", func=exenergy)
```

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```
        numgrad = Units.conversion_ratio("bohr", "angstrom") * numgrad

        # write numerical gradient to file
        print("Saving numerical gradient to file")
        np.save("./numgrad_precalc/" + teststr + ".npy", numgrad)
    print("Numerical gradient =")
    print(numgrad)

    # analytical gradient
    job = AMSJob(name=teststr + "_anagrad", molecule=mol, settings=comin_thistest)
    job.settings.input.DFTB.properties.excitations.tddftbgradients.excitation = excit
    results = job.run()
    anagrad = np.array(results.readrkf("Excitations " + kfsec + " A", "gradient " +␣
↪str(excit), file="dftb")).reshape(
        (-1, 3)
    )
    print("Analytical gradient =")
    print(anagrad)

    # print the difference between analytical and numerical gradients
    diff = numgrad - anagrad
    print("Deviation =")
    print(diff)

    # check if the difference is small enough
    passed = np.allclose(numgrad, anagrad, atol=1e-4)
    if passed:
        print("TEST FINISHED: PASSED!")
    else:
        print("TEST FINISHED: FAILED!")
        failedtests.append(test)

print("\nTESTS PASSED: " + str(len(tests) - len(failedtests)) + "/" + str(len(tests)))
for test in failedtests:
    molname = test[0]
    multi = test[1]
    excit = test[2]
    ldep = test[3]
    if ldep:
        ldpf = "ldep"
    else:
        ldpf = "noldep"
    print("FAILED: " + molname + " " + multi + " " + str(excit) + " " + ldpf)
```

10.5.7 Example: Excitations SOT filter

Download SP_LR-TDDFTB_grimmefilter.run

```
#!/bin/sh

AMS_JOBNAME=noPertCorr $AMSBIN/ams << eor

Task SinglePoint

System
```

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```
    Atoms
        Ir       0.04420       -0.00850       -0.05250
         N      -0.03840       -0.02260        2.09450
         C       1.19280       -0.03830        2.70820
         C       1.26670       -0.06050        4.11790
         H       2.23540       -0.06690        4.60410
         C       0.09850       -0.08170        4.88230
         H       0.15460       -0.10000        5.96680
         C      -1.15030       -0.08660        4.23240
         H      -2.08120       -0.11360        4.78810
         C      -1.17170       -0.06000        2.83740
         H      -2.10440       -0.06910        2.28650
         C       2.33160       -0.05220        1.78990
         C       2.01060       -0.06450        0.39570
         C       3.09340       -0.07380       -0.51520
         H       2.88840       -0.08880       -1.58140
         C       4.42260       -0.07790       -0.07030
         C       4.71950       -0.06800        1.30830
         H       5.75200       -0.06940        1.64760
         C       3.67310       -0.05370        2.23400
         H       3.90660       -0.04300        3.29620
         H       5.23270       -0.08580       -0.79660
         C       0.28050        0.12200       -2.02430
         C       0.41650        1.50790       -2.52520
         C       0.60550        1.72820       -3.93050
         H       0.72650        2.73720       -4.31530
         C       0.63750        0.65370       -4.80680
         H       0.78420        0.83230       -5.87040
         C       0.48640       -0.68860       -4.33810
         H       0.51890       -1.51460       -5.04390
         C       0.30700       -0.92910       -2.96920
         H       0.20840       -1.95190       -2.61810
         C       0.32730        2.53850       -1.55870
         N       0.15930        2.07950       -0.21100
         C       0.16220        2.99060        0.79600
         H       0.07210        2.58960        1.80040
         C       0.26440        4.36230        0.58890
         C       0.38740        4.85520       -0.76210
         H       0.46050        5.92190       -0.95130
         C       0.42240        3.94780       -1.80030
         H       0.52760        4.29590       -2.82360
         H       0.25450        5.03830        1.43730
         N      -2.08080       -0.05260       -0.33870
         C      -2.62190       -1.31760       -0.38820
         C      -4.00890       -1.46660       -0.61030
         H      -4.44160       -2.45950       -0.65200
         C      -4.81680       -0.34140       -0.78650
         H      -5.88260       -0.45700       -0.96200
         C      -4.23730        0.94110       -0.74160
         H      -4.82890        1.83860       -0.88430
         C      -2.86380        1.04010       -0.51650
         H      -2.35710        1.99710       -0.48110
         C      -1.65980       -2.40740       -0.20580
         C      -0.29620       -2.01350       -0.02460
         C       0.64840       -3.04760        0.17060
         H       1.69450       -2.79030        0.31090
         C       0.26950       -4.39840        0.17140
```

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```
         C      -1.07890      -4.76580      -0.01610
         H      -1.36750      -5.81370      -0.01700
         C      -2.04030      -3.76920      -0.20280
         H      -3.07920      -4.05800      -0.34770
         H       1.02320      -5.17010       0.31590
    End
End

Engine DFTB
   Model SCC-DFTB
   ResourcesDir QUASINANO2013.1
   Properties
       Excitations
           SingleOrbTrans
               Filter
                   primRange 0.3
                   minPertCont 1.0e-5
                   usePertCorr false
               End
               PrintLowest 200
           End
           TDDFTB
               Calc singlet
               Print evcontribs
           End
       End
   End
EndEngine

eor


AMS_JOBNAME=pertCorr $AMSBIN/ams << eor

Task SinglePoint

System
    Atoms
        Ir       0.04420      -0.00850      -0.05250
         N      -0.03840      -0.02260       2.09450
         C       1.19280      -0.03830       2.70820
         C       1.26670      -0.06050       4.11790
         H       2.23540      -0.06690       4.60410
         C       0.09850      -0.08170       4.88230
         H       0.15460      -0.10000       5.96680
         C      -1.15030      -0.08660       4.23240
         H      -2.08120      -0.11360       4.78810
         C      -1.17170      -0.06000       2.83740
         H      -2.10440      -0.06910       2.28650
         C       2.33160      -0.05220       1.78990
         C       2.01060      -0.06450       0.39570
         C       3.09340      -0.07380      -0.51520
         H       2.88840      -0.08880      -1.58140
         C       4.42260      -0.07790      -0.07030
         C       4.71950      -0.06800       1.30830
         H       5.75200      -0.06940       1.64760
         C       3.67310      -0.05370       2.23400
```

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```
         H       3.90660      -0.04300       3.29620
         H       5.23270      -0.08580      -0.79660
         C       0.28050       0.12200      -2.02430
         C       0.41650       1.50790      -2.52520
         C       0.60550       1.72820      -3.93050
         H       0.72650       2.73720      -4.31530
         C       0.63750       0.65370      -4.80680
         H       0.78420       0.83230      -5.87040
         C       0.48640      -0.68860      -4.33810
         H       0.51890      -1.51460      -5.04390
         C       0.30700      -0.92910      -2.96920
         H       0.20840      -1.95190      -2.61810
         C       0.32730       2.53850      -1.55870
         N       0.15930       2.07950      -0.21100
         C       0.16220       2.99060       0.79600
         H       0.07210       2.58960       1.80040
         C       0.26440       4.36230       0.58890
         C       0.38740       4.85520      -0.76210
         H       0.46050       5.92190      -0.95130
         C       0.42240       3.94780      -1.80030
         H       0.52760       4.29590      -2.82360
         H       0.25450       5.03830       1.43730
         N      -2.08080      -0.05260      -0.33870
         C      -2.62190      -1.31760      -0.38820
         C      -4.00890      -1.46660      -0.61030
         H      -4.44160      -2.45950      -0.65200
         C      -4.81680      -0.34140      -0.78650
         H      -5.88260      -0.45700      -0.96200
         C      -4.23730       0.94110      -0.74160
         H      -4.82890       1.83860      -0.88430
         C      -2.86380       1.04010      -0.51650
         H      -2.35710       1.99710      -0.48110
         C      -1.65980      -2.40740      -0.20580
         C      -0.29620      -2.01350      -0.02460
         C       0.64840      -3.04760       0.17060
         H       1.69450      -2.79030       0.31090
         C       0.26950      -4.39840       0.17140
         C      -1.07890      -4.76580      -0.01610
         H      -1.36750      -5.81370      -0.01700
         C      -2.04030      -3.76920      -0.20280
         H      -3.07920      -4.05800      -0.34770
         H       1.02320      -5.17010       0.31590
    End
End

Engine DFTB
   Model SCC-DFTB
   ResourcesDir QUASINANO2013.1
   Properties
       Excitations
           SingleOrbTrans
               Filter
                   primRange 0.3
                   minPertCont 1.0e-5
                   usePertCorr true
               End
               PrintLowest 200
```

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```
            End
            TDDFTB
                Calc singlet
                Print evcontribs
            End
        End
    End
EndEngine

eor
```

10.5.8 Example: Orbital dependent DFTB: Excitations

Download SP_LR-TDDFTB_ldep.run

```
#!/bin/sh

echo 'SINGLET-SINGLET (atomic)'

AMS_JOBNAME=SS_atomic $AMSBIN/ams << eor

Task SinglePoint

System
    Atoms
        C       0.81279382      -0.19089242      -7.80488100
        H       5.07095595       1.79589101      -2.49503084
        O      -4.34169576       0.18496986       6.16216037
        H       0.65114558      -2.34332052       3.04942157
        H      -3.72094001      -0.30746453      10.65629162
        C      -5.57421344      -4.70045219       5.73919974
        O      -1.36633817       0.16493071       6.55850374
        H      -1.46686146      -1.86573607      -2.18086178
        C      -3.01691915       1.21584087       8.51312360
        H       0.85684819       0.38891329      -5.92035442
        H      -0.85768102      -0.39560272       5.91987385
        C       4.58793450       0.45500454      -7.38543703
        C      -3.96886809       0.03106136       8.54450871
        H      -3.33250841       1.95291681       9.26711187
        C       3.92209138      -0.59739278      -2.62315330
        C       1.59592218      -0.78493633      -8.81907146
        C       5.37967772       1.61610989      -7.38157700
        H      -3.06208979       1.69077468       7.52509148
        H       3.33153483      -1.95208262      -9.27107004
        H      -5.94850232      -1.45420297       5.29308601
        H      -1.63880964       1.21218459      -4.01748238
        C       5.59481994       2.26846676      -8.60056436
        C      -5.08388814      -3.39466282       5.62101538
        C       1.05877651      -0.90567994     -10.10253961
        H      -6.26086371      -5.15389973      -0.52026711
        C      -3.69329118      -0.44136733       1.61892397
        O      -2.12246826       0.96951335       0.48734843
        H      -3.36468025      -5.09261646       1.88651583
        H       3.06148271      -1.69152499      -7.52879231
        H       3.17373326      -1.41052238      -2.65483607
```

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```
N       -4.93118484       0.57668964       3.42288416
C        5.02671217       1.78315021      -9.77819438
C       -2.76322583      -0.21060941       0.58045389
C        1.61310315       4.08163625      -4.15853296
H        1.65781749      -1.38443872     -10.88135435
H        5.20362845       2.30053217     -10.72284683
N        0.98411405      -0.08507509       1.63291837
C       -0.11811043       0.25869794      -2.77564955
H       -6.45048439      -5.05126436       1.93188479
H        1.59815263       3.20254199      -3.50183331
H        1.34234482      -0.41208751       6.12452565
H        1.63737674      -1.21173256       4.01945340
C        4.20911444       0.65414989      -9.74493762
H        6.57696147       4.84639419      -6.15450696
C       -0.21818699      -0.42562635     -10.40106016
C        5.70951738       4.20198950       0.53163316
H        3.72582808       0.30473367     -10.65974126
H        1.30002230       4.95753032      -3.56997865
C       -5.38332193       1.10327004       5.76258524
O        2.11876506      -0.96761719      -0.48368602
H        3.36747987       5.09257434      -1.88669707
C        3.96955931      -0.03154911      -8.54709739
H       -5.45202800       1.91756888       6.50354887
H       -0.05604443      -0.66172821      -3.38565283
C       -1.29259172       1.02692065      -7.03188178
C        4.92598760       4.02834229      -0.78640963
H        5.41810069       4.00816916      -2.92592937
H        0.62681991       0.54013154      11.40524357
N        4.92387904      -0.57709179      -3.42327889
H       -6.67262735      -3.28997925       1.88188980
C       -5.01964339       1.65230714       4.39464527
N       -0.98529210       0.08880229      -1.62845425
C        0.96153143      -0.19336875       9.39922574
H       -2.32333946       1.12272724      -7.40204855
H        0.89745958       0.50420958      -2.43123110
C       -2.52759360      -1.24514953      -0.37160649
C       -4.16508398      -2.69707260       0.74479053
H        1.95792265      -0.58228753       9.62376812
H       -4.08676441       2.24629054       4.46107261
H        6.43082358       3.38289578       0.66634506
H        5.82384519      -2.33703188      -4.09740481
H       -5.83676722       2.33355915       4.09698464
C       -3.92859324       0.59805505       2.62379415
C        0.46851796      -0.32472735       8.09496128
C       -0.81292062       0.18985987       7.80374992
C       -4.37031926      -1.67149537       1.67363244
C       -1.61111027      -4.08066448       4.15769794
H       -3.18127053       1.41209360       2.65618469
C       -1.59618119       0.78622700       8.81666658
C       -3.22571504      -2.45726125      -0.26496047
C       -0.03721842      -2.64149792       5.57203231
H        6.45378047       5.04688468      -1.93244382
C       -1.05947475       0.90972314      10.10003828
H       -0.62806832      -0.53344921     -11.40625539
H        6.26468464       5.15196874       0.51871132
H       -1.59669820      -3.20085654       3.50197697
H       -1.65873209       1.39040088      10.87751570
```

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```
C       0.76170014      -2.41223156       6.70387740
C      -0.96223359       0.19573796      -9.39859424
H      -6.57418468      -4.84847602       6.15445239
C       0.21729712       0.43018409      10.40014258
H      -3.02101125      -3.22412477      -1.01674298
H      -1.33836424       0.41028647      -6.12174251
H      -1.95871363       0.58505816      -9.62203947
C       0.99557164      -3.48608765       7.57009940
C       2.52728814       1.24669288       0.37476371
H      -1.29763246      -4.95571538       3.56810592
C       5.91215643       2.21280288      -6.08973566
C      -0.46874333       0.32431833      -8.09425711
C       3.22697000       2.45791773       0.26752851
H       6.19838453       3.17876306      -8.61634613
H       1.60525462      -3.32686188       8.46233319
H       5.04370683       4.21405615       1.40646415
H       3.02419610       3.22494895       1.01966091
C       0.03796998       2.64154211      -5.57021148
C       1.29391356      -1.02858260       7.03463312
H      -6.94337647      -2.55729410       6.25033158
C       0.44422052      -4.74079106       7.31190581
C      -0.76019298       2.41089752      -6.70235581
O      -0.30854601      -1.55602015       4.72689111
C      -5.70709602      -4.20307659      -0.53194180
C       3.92154498       5.18836628      -0.94315623
C      -0.99252733       3.48334068      -7.57075461
H       5.94851729       1.45248334      -5.29512213
O      -3.23388160      -1.97990720       4.89463888
H       0.63641924      -5.57147390       7.99331049
H      -1.60151250       3.32281756      -8.46323999
C       5.37718603      -1.10386498      -5.76265521
C       3.68958071       0.44168957      -1.61727297
H      -4.45119723      -6.15159749       0.95621376
C      -0.44029160       4.73806913      -7.31466302
H      -3.79047474      -1.23510905       5.24022747
H      -6.42953925      -3.38488638      -0.66602236
C       2.76065892       0.21188975      -0.57755797
H      -0.63125189       5.56756528      -7.99785314
C      -0.37619636      -4.92848081       6.20030574
H       2.32363204      -1.12532089       7.40739960
H      -6.19333565      -3.18218232       8.61380622
C       0.37977422       4.92707746      -6.20301510
C      -0.62330686       1.41385499      -3.63375315
H       5.44526365      -1.91794390      -6.50389777
H      -0.84603671      -5.89907747       6.02769899
H       0.85074323       5.89743958      -6.03213250
H       6.94435956       2.55526827      -6.25170134
H       4.45511515       6.15074627      -0.95680824
H      -5.07444981      -1.79709374       2.49486194
C       0.64209808       3.88039463      -5.31002856
C      -0.64007530      -3.88038447       5.30939434
H      -5.41692966      -4.01081395       2.92588066
H      -0.65579031       2.34681310      -3.04768782
C       3.79761163       3.20232022      -5.07690932
C      -3.91857929      -5.18868521       0.94289180
C      -5.91142065      -2.21425858       6.08792264
C      -3.79656900      -3.20281743       5.07502995
```

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```
        C       3.02092796       4.30891399      -4.66697576
        C       4.16519226       2.69671733      -0.74350579
        H      -6.35193486       0.57780531       5.72398567
        C      -4.58861684      -0.45480589       7.38332328
        C       3.55447069       5.59373051      -4.79121698
        C       5.00971521      -1.65242908      -4.39564865
        C       4.36776079       1.67112262      -1.67288393
        H       6.34696806      -0.58066583      -5.72209568
        H       2.95800170       6.44665309      -4.45743689
        C      -3.01881386      -4.30896131       4.66601867
        C      -5.37863287      -1.61713107       7.37944408
        H      -3.19524634      -5.21394510       0.11518976
        C       4.82895730       5.79998572      -5.32277400
        C       5.92123014       4.08538851      -1.95322332
        C      -5.91969598      -4.08879523       1.95306303
        C      -5.59119031      -2.27093964       8.59813012
        H       5.23641015       6.80821376      -5.40846166
        C      -3.55114085      -5.59417826       4.79140898
        C      -4.92424440      -4.02961195       0.78653208
        C      -1.60888032      -1.03118918      -1.46946159
        C       5.57678188       4.69894843      -5.73953640
        O       0.30792351       1.55817533      -4.72234841
        H      -5.04089930      -4.21310846      -1.40650801
        H       3.19829313       5.21450999      -0.11539003
        H      -2.95396593      -6.44685493       4.45827526
        C       0.62107613      -1.41110213       3.63669716
        O       3.23393255       1.97982570      -4.89735589
        C       1.60923028       1.03399767       1.47346350
        O       4.33848133      -0.18282864      -6.16375879
        C      -5.02194271      -1.78615195       9.77540439
        H       4.07470090      -2.24285276      -4.46378030
        H       1.46939706       1.86861800       2.18521111
        H       3.78928004       1.23433567      -5.24433158
        C      -4.82536099      -5.80111641       5.32332451
        C       5.08519491       3.39352371      -5.62257098
        C       0.11730322      -0.25386051       2.78062472
        H       6.67266617       3.28517127      -1.88201051
        H      -5.19673746      -2.30474679      10.71978984
        C       3.01657412      -1.21552394      -8.51632426
        H       0.05797623       0.66601530       3.39171136
        O       1.36660360      -0.16880782      -6.55959668
        H      -5.23189059      -6.80964319       5.40983229
        C      -4.20556541      -0.65628284       9.74197413
        H      -0.89911822      -0.49654458       2.43669069
        H      -1.52529996       0.88966309      -0.35559018
        H       1.52209394      -0.88701370       0.35943608
    End
End

Engine DFTB
   Model SCC-DFTB
   ResourcesDir DFTB.org/mio-1-1
   SCC
      OrbitalDependent false
   End
   Properties
       Excitations
```

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```
            SingleOrbTrans
                Filter
                    OSMin 0.0001
                End
                PrintLowest 50
            End
            TDDFTB
                Calc singlet
                Lowest 20
                Print evcontribs
            End
        End
    End
EndEngine

eor


echo 'SINGLET-SINGLET (l-dependent)'

AMS_JOBNAME=SS_ldep $AMSBIN/ams << eor

Task SinglePoint

System
    Atoms
        C       0.81279382      -0.19089242      -7.80488100
        H       5.07095595       1.79589101      -2.49503084
        O      -4.34169576       0.18496986       6.16216037
        H       0.65114558      -2.34332052       3.04942157
        H      -3.72094001      -0.30746453      10.65629162
        C      -5.57421344      -4.70045219       5.73919974
        O      -1.36633817       0.16493071       6.55850374
        H      -1.46686146      -1.86573607      -2.18086178
        C      -3.01691915       1.21584087       8.51312360
        H       0.85684819       0.38891329      -5.92035442
        H      -0.85768102      -0.39560272       5.91987385
        C       4.58793450       0.45500454      -7.38543703
        C      -3.96886809       0.03106136       8.54450871
        H      -3.33250841       1.95291681       9.26711187
        C       3.92209138      -0.59739278      -2.62315330
        C       1.59592218      -0.78493633      -8.81907146
        C       5.37967772       1.61610989      -7.38157700
        H      -3.06208979       1.69077468       7.52509148
        H       3.33153483      -1.95208262      -9.27107004
        H      -5.94850232      -1.45420297       5.29308601
        H      -1.63880964       1.21218459      -4.01748238
        C       5.59481994       2.26846676      -8.60056436
        C      -5.08388814      -3.39466282       5.62101538
        C       1.05877651      -0.90567994     -10.10253961
        H      -6.26086371      -5.15389973      -0.52026711
        C      -3.69329118      -0.44136733       1.61892397
        O      -2.12246826       0.96951335       0.48734843
        H      -3.36468025      -5.09261646       1.88651583
        H       3.06148271      -1.69152499      -7.52879231
        H       3.17373326      -1.41052238      -2.65483607
        N      -4.93118484       0.57668964       3.42288416
```

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```
C       5.02671217       1.78315021      -9.77819438
C      -2.76322583      -0.21060941       0.58045389
C       1.61310315       4.08163625      -4.15853296
H       1.65781749      -1.38443872     -10.88135435
H       5.20362845       2.30053217     -10.72284683
N       0.98411405      -0.08507509       1.63291837
C      -0.11811043       0.25869794      -2.77564955
H      -6.45048439      -5.05126436       1.93188479
H       1.59815263       3.20254199      -3.50183331
H       1.34234482      -0.41208751       6.12452565
H       1.63737674      -1.21173256       4.01945340
C       4.20911444       0.65414989      -9.74493762
H       6.57696147       4.84639419      -6.15450696
C      -0.21818699      -0.42562635     -10.40106016
C       5.70951738       4.20198950       0.53163316
H       3.72582808       0.30473367     -10.65974126
H       1.30002230       4.95753032      -3.56997865
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       Excitations
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        H       1.46939706       1.86861800       2.18521111
        H       3.78928004       1.23433567      -5.24433158
        C      -4.82536099      -5.80111641       5.32332451
        C       5.08519491       3.39352371      -5.62257098
        C       0.11730322      -0.25386051       2.78062472
        H       6.67266617       3.28517127      -1.88201051
        H      -5.19673746      -2.30474679      10.71978984
        C       3.01657412      -1.21552394      -8.51632426
        H       0.05797623       0.66601530       3.39171136
        O       1.36660360      -0.16880782      -6.55959668
        H      -5.23189059      -6.80964319       5.40983229
        C      -4.20556541      -0.65628284       9.74197413
        H      -0.89911822      -0.49654458       2.43669069
        H      -1.52529996       0.88966309      -0.35559018
        H       1.52209394      -0.88701370       0.35943608
    End
End

Engine DFTB
   Model SCC-DFTB
   ResourcesDir DFTB.org/mio-1-1
   SCC
      orbitaldependent false
   End
   Properties
       Excitations
           SingleOrbTrans
               Filter
```

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```
                    OSMin 0.0001
                End
                PrintLowest 50
            End
            TDDFTB
                Calc triplet
                Lowest 20
                Print evcontribs
            End
        End
    End
EndEngine

eor


echo 'SINGLET-TRIPLET (l-dependent)'

AMS_JOBNAME=ST_ldep $AMSBIN/ams << eor

Task SinglePoint

System
    Atoms
        C       0.81279382      -0.19089242      -7.80488100
        H       5.07095595       1.79589101      -2.49503084
        O      -4.34169576       0.18496986       6.16216037
        H       0.65114558      -2.34332052       3.04942157
        H      -3.72094001      -0.30746453      10.65629162
        C      -5.57421344      -4.70045219       5.73919974
        O      -1.36633817       0.16493071       6.55850374
        H      -1.46686146      -1.86573607      -2.18086178
        C      -3.01691915       1.21584087       8.51312360
        H       0.85684819       0.38891329      -5.92035442
        H      -0.85768102      -0.39560272       5.91987385
        C       4.58793450       0.45500454      -7.38543703
        C      -3.96886809       0.03106136       8.54450871
        H      -3.33250841       1.95291681       9.26711187
        C       3.92209138      -0.59739278      -2.62315330
        C       1.59592218      -0.78493633      -8.81907146
        C       5.37967772       1.61610989      -7.38157700
        H      -3.06208979       1.69077468       7.52509148
        H       3.33153483      -1.95208262      -9.27107004
        H      -5.94850232      -1.45420297       5.29308601
        H      -1.63880964       1.21218459      -4.01748238
        C       5.59481994       2.26846676      -8.60056436
        C      -5.08388814      -3.39466282       5.62101538
        C       1.05877651      -0.90567994     -10.10253961
        H      -6.26086371      -5.15389973      -0.52026711
        C      -3.69329118      -0.44136733       1.61892397
        O      -2.12246826       0.96951335       0.48734843
        H      -3.36468025      -5.09261646       1.88651583
        H       3.06148271      -1.69152499      -7.52879231
        H       3.17373326      -1.41052238      -2.65483607
        N      -4.93118484       0.57668964       3.42288416
        C       5.02671217       1.78315021      -9.77819438
        C      -2.76322583      -0.21060941       0.58045389
```

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```
        C      1.61310315      4.08163625     -4.15853296
        H      1.65781749     -1.38443872    -10.88135435
        H      5.20362845      2.30053217    -10.72284683
        N      0.98411405     -0.08507509      1.63291837
        C     -0.11811043      0.25869794     -2.77564955
        H     -6.45048439     -5.05126436      1.93188479
        H      1.59815263      3.20254199     -3.50183331
        H      1.34234482     -0.41208751      6.12452565
        H      1.63737674     -1.21173256      4.01945340
        C      4.20911444      0.65414989     -9.74493762
        H      6.57696147      4.84639419     -6.15450696
        C     -0.21818699     -0.42562635    -10.40106016
        C      5.70951738      4.20198950      0.53163316
        H      3.72582808      0.30473367    -10.65974126
        H      1.30002230      4.95753032     -3.56997865
        C     -5.38332193      1.10327004      5.76258524
        O      2.11876506     -0.96761719     -0.48368602
        H      3.36747987      5.09257434     -1.88669707
        C      3.96955931     -0.03154911     -8.54709739
        H     -5.45202800      1.91756888      6.50354887
        H     -0.05604443     -0.66172821     -3.38565283
        C     -1.29259172      1.02692065     -7.03188178
        C      4.92598760      4.02834229     -0.78640963
        H      5.41810069      4.00816916     -2.92592937
        H      0.62681991      0.54013154     11.40524357
        N      4.92387904     -0.57709179     -3.42327889
        H     -6.67262735     -3.28997925      1.88188980
        C     -5.01964339      1.65230714      4.39464527
        N     -0.98529210      0.08880229     -1.62845425
        C      0.96153143     -0.19336875      9.39922574
        H     -2.32333946      1.12272724     -7.40204855
        H      0.89745958      0.50420958     -2.43123110
        C     -2.52759360     -1.24514953     -0.37160649
        C     -4.16508398     -2.69707260      0.74479053
        H      1.95792265     -0.58228753      9.62376812
        H     -4.08676441      2.24629054      4.46107261
        H      6.43082358      3.38289578      0.66634506
        H      5.82384519     -2.33703188     -4.09740481
        H     -5.83676722      2.33355915      4.09698464
        C     -3.92859324      0.59805505      2.62379415
        C      0.46851796     -0.32472735      8.09496128
        C     -0.81292062      0.18985987      7.80374992
        C     -4.37031926     -1.67149537      1.67363244
        C     -1.61111027     -4.08066448      4.15769794
        H     -3.18127053      1.41209360      2.65618469
        C     -1.59618119      0.78622700      8.81666658
        C     -3.22571504     -2.45726125     -0.26496047
        C     -0.03721842     -2.64149792      5.57203231
        H      6.45378047      5.04688468     -1.93244382
        C     -1.05947475      0.90972314     10.10003828
        H     -0.62806832     -0.53344921    -11.40625539
        H      6.26468464      5.15196874      0.51871132
        H     -1.59669820     -3.20085654      3.50197697
        H     -1.65873209      1.39040088     10.87751570
        C      0.76170014     -2.41223156      6.70387740
        C     -0.96223359      0.19573796     -9.39859424
        H     -6.57418468     -4.84847602      6.15445239
```

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```
        C      0.21729712      0.43018409     10.40014258
        H     -3.02101125     -3.22412477     -1.01674298
        H     -1.33836424      0.41028647     -6.12174251
        H     -1.95871363      0.58505816     -9.62203947
        C      0.99557164     -3.48608765      7.57009940
        C      2.52728814      1.24669288      0.37476371
        H     -1.29763246     -4.95571538      3.56810592
        C      5.91215643      2.21280288     -6.08973566
        C     -0.46874333      0.32431833     -8.09425711
        C      3.22697000      2.45791773      0.26752851
        H      6.19838453      3.17876306     -8.61634613
        H      1.60525462     -3.32686188      8.46233319
        H      5.04370683      4.21405615      1.40646415
        H      3.02419610      3.22494895      1.01966091
        C      0.03796998      2.64154211     -5.57021148
        C      1.29391356     -1.02858260      7.03463312
        H     -6.94337647     -2.55729410      6.25033158
        C      0.44422052     -4.74079106      7.31190581
        C     -0.76019298      2.41089752     -6.70235581
        O     -0.30854601     -1.55602015      4.72689111
        C     -5.70709602     -4.20307659     -0.53194180
        C      3.92154498      5.18836628     -0.94315623
        C     -0.99252733      3.48334068     -7.57075461
        H      5.94851729      1.45248334     -5.29512213
        O     -3.23388160     -1.97990720      4.89463888
        H      0.63641924     -5.57147390      7.99331049
        H     -1.60151250      3.32281756     -8.46323999
        C      5.37718603     -1.10386498     -5.76265521
        C      3.68958071      0.44168957     -1.61727297
        H     -4.45119723     -6.15159749      0.95621376
        C     -0.44029160      4.73806913     -7.31466302
        H     -3.79047474     -1.23510905      5.24022747
        H     -6.42953925     -3.38488638     -0.66602236
        C      2.76065892      0.21188975     -0.57755797
        H     -0.63125189      5.56756528     -7.99785314
        C     -0.37619636     -4.92848081      6.20030574
        H      2.32363204     -1.12532089      7.40739960
        H     -6.19333565     -3.18218232      8.61380622
        C      0.37977422      4.92707746     -6.20301510
        C     -0.62330686      1.41385499     -3.63375315
        H      5.44526365     -1.91794390     -6.50389777
        H     -0.84603671     -5.89907747      6.02769899
        H      0.85074323      5.89743958     -6.03213250
        H      6.94435956      2.55526827     -6.25170134
        H      4.45511515      6.15074627     -0.95680824
        H     -5.07444981     -1.79709374      2.49486194
        C      0.64209808      3.88039463     -5.31002856
        C     -0.64007530     -3.88038447      5.30939434
        H     -5.41692966     -4.01081395      2.92588066
        H     -0.65579031      2.34681310     -3.04768782
        C      3.79761163      3.20232022     -5.07690932
        C     -3.91857929     -5.18868521      0.94289180
        C     -5.91142065     -2.21425858      6.08792264
        C     -3.79656900     -3.20281743      5.07502995
        C      3.02092796      4.30891399     -4.66697576
        C      4.16519226      2.69671733     -0.74350579
        H     -6.35193486      0.57780531      5.72398567
```

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```
        C      -4.58861684      -0.45480589       7.38332328
        C       3.55447069       5.59373051      -4.79121698
        C       5.00971521      -1.65242908      -4.39564865
        C       4.36776079       1.67112262      -1.67288393
        H       6.34696806      -0.58066583      -5.72209568
        H       2.95800170       6.44665309      -4.45743689
        C      -3.01881386      -4.30896131       4.66601867
        C      -5.37863287      -1.61713107       7.37944408
        H      -3.19524634      -5.21394510       0.11518976
        C       4.82895730       5.79998572      -5.32277400
        C       5.92123014       4.08538851      -1.95322332
        C      -5.91969598      -4.08879523       1.95306303
        C      -5.59119031      -2.27093964       8.59813012
        H       5.23641015       6.80821376      -5.40846166
        C      -3.55114085      -5.59417826       4.79140898
        C      -4.92424440      -4.02961195       0.78653208
        C      -1.60888032      -1.03118918      -1.46946159
        C       5.57678188       4.69894843      -5.73953640
        O       0.30792351       1.55817533      -4.72234841
        H      -5.04089930      -4.21310846      -1.40650801
        H       3.19829313       5.21450999      -0.11539003
        H      -2.95396593      -6.44685493       4.45827526
        C       0.62107613      -1.41110213       3.63669716
        O       3.23393255       1.97982570      -4.89735589
        C       1.60923028       1.03399767       1.47346350
        O       4.33848133      -0.18282864      -6.16375879
        C      -5.02194271      -1.78615195       9.77540439
        H       4.07470090      -2.24285276      -4.46378030
        H       1.46939706       1.86861800       2.18521111
        H       3.78928004       1.23433567      -5.24433158
        C      -4.82536099      -5.80111641       5.32332451
        C       5.08519491       3.39352371      -5.62257098
        C       0.11730322      -0.25386051       2.78062472
        H       6.67266617       3.28517127      -1.88201051
        H      -5.19673746      -2.30474679      10.71978984
        C       3.01657412      -1.21552394      -8.51632426
        H       0.05797623       0.66601530       3.39171136
        O       1.36660360      -0.16880782      -6.55959668
        H      -5.23189059      -6.80964319       5.40983229
        C      -4.20556541      -0.65628284       9.74197413
        H      -0.89911822      -0.49654458       2.43669069
        H      -1.52529996       0.88966309      -0.35559018
        H       1.52209394      -0.88701370       0.35943608
    End
End

Engine DFTB
   Model SCC-DFTB
   ResourcesDir DFTB.org/mio-1-1
   SCC
      OrbitalDependent true
   End
   Properties
       Excitations
           SingleOrbTrans
               Filter
                   OSMin 0.0001
```

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```
                End
                PrintLowest 50
            End
            TDDFTB
                Calc triplet
                Lowest 20
                Print evcontribs
            End
        End
    End
EndEngine

eor
```

10.5.9 Example: Excitations benchmark

Download SP_LR-TDDFTB_tbe.run

```
#! /bin/sh

echo Singlet Excitations
for f in $AMSHOME/examples/dftb/SP_LR-TDDFTB_tbe/molecules/*.xyz
do
cat <<eor > in
Task SinglePoint
System
    Atoms
eor
cat $f >> in
cat <<eor >> in
    End
End
Engine DFTB
   Model SCC-DFTB
   ResourcesDir DFTB.org/mio-1-1
   Properties
       Excitations
           TDDFTB
               calc singlet
               print evcontribs
           End
       End
   End
EndEngine
eor
g=`basename $f .xyz`
echo $g
AMS_JOBNAME=${g}_SS $AMSBIN/ams <in > $g.SS.out 2>&1
grep Excitation $g.SS.out
done
echo Ready


echo Triplet Excitations
for f in $AMSHOME/examples/dftb/SP_LR-TDDFTB_tbe/molecules/*.xyz
```

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```
do
cat <<eor > in
System
    Atoms
eor
cat $f >> in
cat <<eor >> in
    End
End
Task SinglePoint
Engine DFTB
   Model SCC-DFTB
   ResourcesDir DFTB.org/mio-1-1
   Properties
       Excitations
           TDDFTB
               calc triplet
               print evcontribs
           End
       End
   End
EndEngine
eor
g=`basename $f .xyz`
echo $g
AMS_JOBNAME=${g}_ST $AMSBIN/ams <in > $g.ST.out 2>&1
grep Excitation $g.ST.out
done
echo Ready
```

10.5.10 Example: Test parallelization

Download SP_LR-TDDFTB_betacarotene.run

```
#!/bin/sh

# this test runs betacarotene in serial and in parallel
# to check if the results are the same ...

inputfile=$AMSHOME/examples/dftb/SP_LR-TDDFTB_betacarotene/inputfile

AMS_JOBNAME=NSCM1 NSCM=1 $AMSBIN/ams < $inputfile
AMS_JOBNAME=NSCM2 NSCM=2 $AMSBIN/ams < $inputfile
AMS_JOBNAME=NSCM4 NSCM=4 $AMSBIN/ams < $inputfile
```

Download inputfile

```
Task SinglePoint

Properties
   Gradients true
End

System
    Atoms
```

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```
        C      -1.67096000       1.41980000      -1.15887000
        C      -0.38686000       2.25210000      -1.41391000
        C      -1.74087000       0.49471000      -0.15347000
        C      -2.78739000       1.72912000      -2.05465000
        C       0.64868000       2.05301000      -0.28395000
        C       0.23104000       1.84552000      -2.77135000
        C      -0.70560000       3.76543000      -1.46182000
        C      -0.54745000       0.11313000       0.69574000
        C      -3.00351000      -0.21803000       0.26657000
        C      -3.76926000       0.89738000      -2.51350000
        C       0.78914000       0.59489000       0.13981000
        C      -4.86625000       1.29159000      -3.36539000
        C      -5.83916000       0.35729000      -3.66241000
        C      -4.93554000       2.71910000      -3.84917000
        C      -7.05227000       0.56749000      -4.37867000
        C      -8.05019000      -0.37384000      -4.49171000
        C      -9.34557000      -0.15733000      -5.06205000
        C     -10.30909000      -1.14399000      -4.91514000
        C      -9.64286000       1.17054000      -5.71730000
        C     -11.69180000      -1.05048000      -5.21459000
        C     -12.61955000      -2.01468000      -4.87148000
        C     -14.02165000      -1.83518000      -4.98190000
        C     -15.01934000      -2.67078000      -4.50243000
        C     -16.37196000      -2.20132000      -4.51598000
        C     -14.71829000      -4.01459000      -3.88235000
        C     -17.44392000      -2.81539000      -3.90884000
        C     -18.74098000      -2.23505000      -3.81068000
        C     -19.81891000      -2.70482000      -3.08600000
        C     -21.01079000      -1.89278000      -3.01886000
        C     -19.77834000      -4.00300000      -2.31809000
        C     -22.11699000      -2.17469000      -2.26831000
        C     -23.34229000      -1.38813000      -2.11260000
        C     -24.62364000      -2.22792000      -1.86832000
        C     -23.37421000      -0.02091000      -2.14864000
        C     -25.81771000      -1.33236000      -1.46707000
        C     -24.97031000      -3.02505000      -3.14664000
        C     -24.41619000      -3.23491000      -0.71197000
        C     -24.66206000       0.77221000      -2.09033000
        C     -22.15090000       0.86196000      -2.20093000
        C     -25.91751000      -0.06612000      -2.31089000
        H      -2.80910000       2.75370000      -2.43250000
        H       1.61418000       2.46808000      -0.61595000
        H       0.33480000       2.64516000       0.59383000
        H      -0.50118000       1.95999000      -3.58430000
        H       1.10267000       2.47962000      -3.00160000
        H       0.55846000       0.79551000      -2.76878000
        H      -1.27083000       4.08204000      -0.57268000
        H       0.23706000       4.33391000      -1.48690000
        H      -1.27659000       4.05053000      -2.35573000
        H      -0.69913000       0.51646000       1.71643000
        H      -0.54631000      -0.98424000       0.82135000
        H      -3.05490000      -1.23815000      -0.15105000
        H      -3.01240000      -0.33500000       1.36235000
        H      -3.91214000       0.31400000      -0.03789000
        H      -3.75416000      -0.15646000      -2.22797000
        H       1.07957000      -0.02480000      -0.72369000
        H       1.58320000       0.48035000       0.89321000
```

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```
      H      -5.69282000      -0.64720000      -3.25046000
      H      -4.00625000       2.99962000      -4.36844000
      H      -5.76674000       2.88684000      -4.54145000
      H      -5.05424000       3.41602000      -3.00441000
      H      -7.22923000       1.55534000      -4.80743000
      H      -7.87841000      -1.35648000      -4.03966000
      H      -9.98472000      -2.07170000      -4.43134000
      H      -8.86494000       1.42343000      -6.45273000
      H     -10.60514000       1.16993000      -6.23979000
      H      -9.66280000       1.98327000      -4.97344000
      H     -12.06891000      -0.12920000      -5.66646000
      H     -12.24343000      -2.93190000      -4.41065000
      H     -14.35090000      -0.88585000      -5.41809000
      H     -16.54169000      -1.22776000      -4.98799000
      H     -15.37918000      -4.79019000      -4.29660000
      H     -13.68496000      -4.33124000      -4.05827000
      H     -14.88466000      -3.99412000      -2.79324000
      H     -17.27327000      -3.77423000      -3.41639000
      H     -18.87740000      -1.27545000      -4.32124000
      H     -20.99304000      -0.98523000      -3.62576000
      H     -19.85755000      -3.82238000      -1.23433000
      H     -20.62535000      -4.64779000      -2.59868000
      H     -18.85754000      -4.56711000      -2.49752000
      H     -22.10976000      -3.13142000      -1.74142000
      H     -26.74148000      -1.93003000      -1.53138000
      H     -25.70276000      -1.04055000      -0.40816000
      H     -24.12173000      -3.65146000      -3.45913000
      H     -25.83556000      -3.68339000      -2.96560000
      H     -25.21348000      -2.35763000      -3.98638000
      H     -24.03490000      -2.73308000       0.18974000
      H     -25.38111000      -3.70177000      -0.46026000
      H     -23.72534000      -4.04703000      -0.97564000
      H     -24.71649000       1.28228000      -1.10831000
      H     -24.60164000       1.58888000      -2.83152000
      H     -21.95198000       1.22417000      -3.22414000
      H     -22.31941000       1.76042000      -1.58543000
      H     -21.24680000       0.35543000      -1.84399000
      H     -26.00957000      -0.32720000      -3.37736000
      H     -26.81690000       0.51083000      -2.04725000
    End
End

Engine DFTB
   Model SCC-DFTB
   ResourcesDir DFTB.org/mio-1-1
   Properties
       Excitations
           SingleOrbTrans
               PrintLowest 50
           End
           TDDFTB
               Calc singlet
               Lowest 20
               Print evcontribs
           End
           TDDFTBGradients
               Excitation 1
```

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```
            End
        End
    End
EndEngine
```

10.6 Vibrations, IR spectra, Normal Modes, VCD

10.6.1 Example: GO and frequencies aspirin

Download GOFREQ_aspirin_SCC.run

```
#!/bin/sh

$AMSBIN/ams << eor

Task GeometryOptimization

GeometryOptimization
   Convergence Step=1.0e-3
End

Properties
   NormalModes true
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

Engine DFTB
   Model SCC-DFTB
```

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```
   ResourcesDir Dresden
   DispersionCorrection Auto
EndEngine

eor
```

10.6.2 Example: Normal modes (frequencies) for aspirin

Download FREQ_aspirin_SCC.run

```
#!/bin/sh

$AMSBIN/ams << eor

Task SinglePoint

Properties
   NormalModes True
End

System
    Atoms [Bohr]
      C     0.10101850     0.08267677     0.12682447
      C     2.73114989     0.06204296     0.11077263
      C     4.06439820     2.33164310    -0.06363346
      C     2.75114112     4.60824084    -0.20693134
      C     0.10560321     4.61925499    -0.15860918
      C    -1.28409307     2.34805008    -0.03252711
      O    -1.20792113     7.03183985    -0.40850190
      C    -4.13965656     2.14765157     0.02233364
      O    -5.54836431     4.25852921    -0.97228229
      C    -1.20247915     8.69980548     1.91027321
      C    -0.35706426     7.45382767     4.35689712
      H    -0.93489190    -1.72586813     0.25196453
      H     3.75849578    -1.74924086     0.22698872
      H     6.15018038     2.32888238    -0.09570448
      H     3.79180159     6.41027432    -0.34559245
      O    -5.25833423     0.30011724     0.82528893
      H    -4.29660486     5.51580277    -1.46089257
      O    -1.91824073    10.83838092     1.66234642
      H    -0.92159688     8.64229425     5.99197100
      H     1.73372033     7.23956114     4.42010264
      H    -1.20899026     5.55080173     4.61014609
    End
End

Engine DFTB
   Model SCC-DFTB
   ResourcesDir Dresden
   Repulsion
       forcePolynomial true
   End
   DispersionCorrection Auto
EndEngine
```

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```
eor
```

10.6.3 Example: Frequencies H2O

Download FREQ_H2O.run

```
#! /bin/sh

$AMSBIN/ams << eor

Task SinglePoint

Properties
   NormalModes true
End

System
  Atoms [Bohr]
     O     0.00000000     0.14614781     0.00000000
     H    -1.41662694    -1.01221540     0.00000000
     H     1.41662694    -1.01221540     0.00000000
  End
End

Engine DFTB
   Model SCC-DFTB
   ResourcesDir Dresden
   Repulsion
       forcePolynomial true
   End
   DispersionCorrection Auto
EndEngine

eor
```

10.6.4 Example: Frequencies OH-

Download FREQ_OHminus.run

```
#! /bin/sh

$AMSBIN/ams << eor

Task SinglePoint

Properties
   NormalModes true
End

System
  Atoms [Bohr]
    O     0.00000000     0.00000000     10.07360092
    H     0.00000000     0.00000000     11.92639908
```

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```
  End
  Charge -1
End

Engine DFTB
   Model SCC-DFTB
   ResourcesDir Dresden
   Repulsion
       forcePolynomial true
   End
EndEngine

eor
```

10.6.5 Example: Frequencies H2 slab

Download constraints.run

```
#! /bin/sh


AMS_JOBNAME=nosym $AMSBIN/ams << eor

Task SinglePoint

Properties
   NormalModes true
End

System
  Atoms
     H -0.4 0 0.1
     H 0.4 0 -0.1
  End

  Lattice
       2.645886  0        0
       0         2.645886  0
  End
End

Engine DFTB
   Model SCC-DFTB
   ResourcesDir Dresden
   useSymmetry no
   Repulsion
       forcePolynomial true
   End
   KSpace
       Type Symmetric
       Symmetric KInteg=3
   End
EndEngine

eor
```

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```
AMS_JOBNAME=sym $AMSBIN/ams << eor

Task SinglePoint

Properties
   NormalModes true
End

System
  Atoms
     H -0.4 0 0.1
     H 0.4 0 -0.1
  End

  Lattice
       2.645886  0        0
       0         2.645886  0
  End
End

Engine DFTB
   Model SCC-DFTB
   ResourcesDir Dresden
   Repulsion
       forcePolynomial true
   End
   KSpace
       Type Symmetric
       Symmetric KInteg=3
   End
EndEngine

eor
```

10.6.6 Example: GO and frequencies C60

Download GOFREQ_C60.run

```
#!/bin/sh

$AMSBIN/ams << EOF

Task GeometryOptimization

Properties
   NormalModes True
End

System
   Atoms
        C   2.30706389   1.98586694   1.83102349
        C   2.30706389   0.74961050   2.59507199
        C   1.17574975   2.80781478   1.83102349
```

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```
        C   1.17574975   0.38202425   3.33024448
        C   0.72665331  -1.00015247   3.33024448
        C   3.03371719  -0.25054198   1.83102349
        C   2.60159365  -1.58048151   1.83102349
        C   1.42584390  -1.96250576   2.59507199
        C   1.42584390   3.19876221  -0.59476704
        C   2.60159365   2.34453001  -0.59476704
        C   0.72665331   3.42594300   0.59476704
        C   3.03371719   1.74976297   0.59476704
        C   3.48281364   0.36758625   0.59476704
        C   2.60159365   1.58048151  -1.83102349
        C   3.03371719   0.25054198  -1.83102349
        C   3.48281364  -0.36758625  -0.59476704
        C  -1.42584390   3.19876221  -0.59476704
        C  -0.69919059   2.96265823  -1.83102349
        C  -0.72665331   3.42594300   0.59476704
        C   0.69919059   2.96265823  -1.83102349
        C   1.42584390   1.96250576  -2.59507199
        C  -1.42584390   1.96250576  -2.59507199
        C  -0.72665331   1.00015247  -3.33024448
        C   0.72665331   1.00015247  -3.33024448
        C  -2.30706389   1.98586694   1.83102349
        C  -3.03371719   1.74976297   0.59476704
        C  -1.17574975   2.80781478   1.83102349
        C  -2.60159365   2.34453001  -0.59476704
        C  -2.60159365   1.58048151  -1.83102349
        C  -3.48281364   0.36758625   0.59476704
        C  -3.48281364  -0.36758625  -0.59476704
        C  -3.03371719   0.25054198  -1.83102349
        C  -0.00000000   1.23625645   3.33024448
        C  -1.17574975   0.38202425   3.33024448
        C  -0.00000000   2.42579053   2.59507199
        C  -2.30706389   0.74961050   2.59507199
        C  -3.03371719  -0.25054198   1.83102349
        C  -0.72665331  -1.00015247   3.33024448
        C  -1.42584390  -1.96250576   2.59507199
        C  -2.60159365  -1.58048151   1.83102349
        C  -2.30706389  -1.98586694  -1.83102349
        C  -3.03371719  -1.74976297  -0.59476704
        C  -2.60159365  -2.34453001   0.59476704
        C  -1.17574975  -2.80781478  -1.83102349
        C  -0.00000000  -1.23625645  -3.33024448
        C  -1.17574975  -0.38202425  -3.33024448
        C  -2.30706389  -0.74961050  -2.59507199
        C  -0.00000000  -2.42579053  -2.59507199
        C   2.30706389  -1.98586694  -1.83102349
        C   2.30706389  -0.74961050  -2.59507199
        C   1.17574975  -0.38202425  -3.33024448
        C   1.17574975  -2.80781478  -1.83102349
        C   1.42584390  -3.19876221   0.59476704
        C   2.60159365  -2.34453001   0.59476704
        C   3.03371719  -1.74976297  -0.59476704
        C   0.72665331  -3.42594300  -0.59476704
        C  -1.42584390  -3.19876221   0.59476704
        C  -0.69919059  -2.96265823   1.83102349
        C   0.69919059  -2.96265823   1.83102349
        C  -0.72665331  -3.42594300  -0.59476704
```

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```
   End
End

Engine DFTB
   Model DFTB3
   ResourcesDir DFTB.org/3ob-3-1
   DispersionCorrection D3-BJ
EndEngine
EOF
```

10.6.7 Example: Excited states frequencies

Download FREQ_LR-TDDFTB_benzene.run

```
#!/bin/sh

# This test calculates frequencies of the lowest singlet excitation
# of benzene. This was also done in Niehaus paper on excited state
# gradients, see:
#      D. Heringer et al. J. Comput. Chem. 28:2589-2601, 2007

$AMSBIN/ams << eor

Task SinglePoint

Properties
   NormalModes true
End

System
    Atoms
        H     0.00000000     2.52578099     0.00000000
        H     0.00000000    -2.52578099     0.00000000
        H     2.18739047     1.26289148     0.00000000
        H    -2.18739047    -1.26289148     0.00000000
        H    -2.18739047     1.26289148     0.00000000
        H     2.18739047    -1.26289148     0.00000000
        C     0.00000000     1.42809579     0.00000000
        C     0.00000000    -1.42809579     0.00000000
        C     1.23676731     0.71404770     0.00000000
        C    -1.23676731    -0.71404770     0.00000000
        C    -1.23676731     0.71404770     0.00000000
        C     1.23676731    -0.71404770     0.00000000
    End
End

Engine DFTB
   Model SCC-DFTB
   ResourcesDir DFTB.org/mio-1-1
   Properties
       Excitations
           TDDFTB
               Calc singlet
               Lowest 1
               Diagonalization exact
```

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```
            End
            TDDFTBGradients
                Excitation 1
            End
        End
    End
EndEngine

eor
```

10.6.8 Example: Vibration resolved electronic spectrum: plams

Download GOFREQ_LR-TDDFTB_anthracene_S0S1fcf.run

```
#!/bin/sh

cp $TEST_DIRECTORY/GOFREQ_LR-TDDFTB_anthracene_S0S1fcf.plms .
cp $TEST_DIRECTORY/anthracene.xyz .

$AMSBIN/plams GOFREQ_LR-TDDFTB_anthracene_S0S1fcf.plms
```

Download GOFREQ_LR-TDDFTB_anthracene_S0S1fcf.plms

```
import sys
import numpy as np

config.log.stdout = 0

# This test calculates the vibrational fine structure of the S_0 -> S_1 transition in␣
↪anthracene.

molfile = "anthracene.xyz"
excit = 1

# Common settings for all DFTB calculations:
comin = Settings()
comin.input.DFTB.resourcesdir = "DFTB.org/3ob-freq-1-2"
comin.input.DFTB.model = "DFTB3"


# ========= auxilliary functions␣
↪==================================================================
def get_total_energy(results):
    nprop = results.readrkf("Properties", "nEntries", file="dftb")
    for i in range(1, nprop + 1):
        if results.readrkf("Properties", "Subtype(%i)" % i, file="dftb").strip() ==
↪"DFTB Final Energy":
            return results.readrkf("Properties", "Value(%i)" % i, file="dftb")
    return None


def get_zero_point_energy(results):
    freqs = results.readrkf("Vibrations", "Frequencies[cm-1]", file="dftb")
    if isinstance(freqs, list):
        return Units.convert(0.5 * sum(freqs), "cm^-1", "Hartree")
```

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```
    else:
        return Units.convert(0.5 * freqs, "cm^-1", "Hartree")


def extract_spectrum(fcf_results):
    return np.array(fcf_results.readkf("Fcf", "spectrum")).reshape(2, -1).transpose()


# ========= STEP 1: Ground state␣
↪==================================================================

# Optimize ground state geometry:
gs_mol_unoptimized = Molecule(filename=molfile)
gs_go = AMSJob(name="gs_go", molecule=gs_mol_unoptimized, settings=comin)
gs_go.settings.input.ams.Task = "GeometryOptimization"
gs_go.settings.input.ams.GeometryOptimization.convergence = "Gradients=1.0e-5"
gs_go_results = gs_go.run()
if not gs_go.check():
    print("ERROR: Ground state optimization crashed")
    sys.exit(1)
if gs_go_results.grep_output("Optimization Did Not Converge"):
    print("ERROR: Ground state optimization did not converge")
    sys.exit(1)
gs_mol_optimized = gs_go_results.get_molecule("Molecule")

# Calculate frequencies and normal modes of the ground state:
gs_freq = AMSJob(name="gs_freq", molecule=gs_mol_optimized, settings=comin)
gs_freq.settings.input.ams.Task = "SinglePoint"
gs_freq.settings.input.ams.properties.NormalModes = "true"
gs_freq.settings.input.ams.NumericalDifferentiation.Parallel.nCoresPerGroup = 1
gs_freq_results = gs_freq.run()
if not gs_freq.check():
    print("ERROR: Ground state frequency calculation crashed")
    sys.exit(1)

# Calculate vertical excitations:
gs_excit = AMSJob(name="gs_excit", molecule=gs_mol_optimized, settings=comin)
gs_excit.settings.input.ams.Task = "SinglePoint"
gs_excit.settings.input.DFTB.properties.excitations.tddftb.calc = "singlet"
gs_excit.settings.input.DFTB.properties.excitations.tddftb.lowest = excit + 9
gs_excit.settings.input.DFTB.properties.excitations.tddftb["print"] = "evcontribs"
gs_excit_results = gs_excit.run()
if not gs_excit.check():
    print("ERROR: Ground state excitations calculation crashed")
    sys.exit(1)

# Print ground state energies:
print("Energies in the ground state equilibrium geometry:")
E_DFTB_RGS = get_total_energy(gs_excit_results)
E_ZPE_RGS = get_zero_point_energy(gs_freq_results)
Delta_RGS = gs_excit_results.readrkf("Excitations SS A", "excenergies", file="dftb
↪")[excit - 1]
E_GS = E_DFTB_RGS + E_ZPE_RGS
print("  E_DFTB(R_GS) = %f eV" % (Units.convert(E_DFTB_RGS, "Hartree", "eV")))
print("   E_ZPE(R_GS) = %f eV" % (Units.convert(E_ZPE_RGS, "Hartree", "eV")))
print("         E_GS  = %f eV" % (Units.convert(E_GS, "Hartree", "eV")))
```

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```
# ========= STEP 2: Excited state␣
↪===============================================================

# Optimize the excited state geometry:
ex_go = AMSJob(name="ex_go", molecule=gs_mol_optimized, settings=comin)
ex_go.settings.input.ams.Task = "GeometryOptimization"
ex_go.settings.input.ams.GeometryOptimization.convergence = "Gradients=1.0e-5"
ex_go.settings.input.DFTB.properties.excitations.tddftb.calc = "singlet"
ex_go.settings.input.DFTB.properties.excitations.tddftb.lowest = excit
ex_go.settings.input.DFTB.properties.excitations.tddftb["print"] = "evcontribs"
ex_go.settings.input.DFTB.properties.excitations.tddftbgradients.excitation = excit
ex_go.settings.input.DFTB.properties.excitations.tddftbgradients.eigenfollow = "true"
ex_go.settings.input.ams.log.info = "TDDFTBExcitationFollowerModule"
ex_go_results = ex_go.run()
if not ex_go.check():
    print("ERROR: Excited state optimization crashed")
    sys.exit(1)
if ex_go_results.grep_output("Optimization Did Not Converge"):
    print("ERROR: Excited state optimization did not converge")
    sys.exit(1)
ex_mol_optimized = ex_go_results.get_molecule("Molecule")

# Check if the potential energy surface was switched during the optimization:
# (This happens if the optimizer goes through a conical intersection.)
PES_switches = ex_go_results.grep_file("ams.log", "TD-DFTB Eigenfollower switching␣
↪PES:")
if PES_switches:
    newexcit = int(PES_switches[-1].split()[-1])
    print("PES switched during EXGO!!! %i -> %i" % (excit, newexcit))
else:
    newexcit = excit

# Calculate frequencies and normal modes of the excited state:
ex_freq = AMSJob(name="ex_freq", molecule=ex_mol_optimized, settings=comin)
ex_freq.settings.input.ams.Task = "SinglePoint"
ex_freq.settings.input.ams.properties.NormalModes = "true"
ex_freq.settings.input.ams.NumericalDifferentiation.Parallel.nCoresPerGroup = 1
ex_freq.settings.input.DFTB.properties.excitations.tddftb.calc = "singlet"
ex_freq.settings.input.DFTB.properties.excitations.tddftb.lowest = newexcit
ex_freq.settings.input.DFTB.properties.excitations.tddftb["print"] = "evcontribs"
ex_freq.settings.input.DFTB.properties.excitations.tddftbgradients.excitation =␣
↪newexcit
ex_freq_results = ex_freq.run()
if not ex_freq.check():
    print("ERROR: Excited state frequency calculation crashed")
    sys.exit(1)

# Calculate vertical excitations in excited state geometry:
ex_excit = AMSJob(name="ex_excit", molecule=ex_mol_optimized, settings=comin)
ex_excit.settings.input.ams.Task = "SinglePoint"
ex_excit.settings.input.DFTB.properties.excitations.tddftb.calc = "singlet"
ex_excit.settings.input.DFTB.properties.excitations.tddftb.lowest = newexcit + 9
ex_excit.settings.input.DFTB.properties.excitations.tddftb["print"] = "evcontribs"
ex_excit_results = ex_excit.run()
if not ex_excit.check():
    print("ERROR: Excited state geometry excitations calculation crashed")
```

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```
    sys.exit(1)

# Print excited state energies:
print("Energies in the excited state equilibrium geometry:")
E_DFTB_REX = get_total_energy(ex_excit_results)
E_ZPE_REX = get_zero_point_energy(ex_freq_results)
Delta_REX = ex_excit_results.readrkf("Excitations SS A", "excenergies", file="dftb
↪")[excit - 1]
E_EX = E_DFTB_REX + E_ZPE_REX + Delta_REX
print("  E_DFTB(R_EX) = %f eV" % (Units.convert(E_DFTB_REX, "Hartree", "eV")))
print("   E_ZPE(R_EX) = %f eV" % (Units.convert(E_ZPE_REX, "Hartree", "eV")))
print("   Delta(R_EX) = %f eV" % (Units.convert(Delta_REX, "Hartree", "eV")))
print("         E_EX  = %f eV" % (Units.convert(E_EX, "Hartree", "eV")))

# Print excitation energies:
print("Excitation energies:")
print("   Delta(R_GS) = %f eV" % (Units.convert(Delta_RGS, "Hartree", "eV")))
print("         E_0-0 = %f eV" % (Units.convert(E_EX - E_GS, "Hartree", "eV")))
print("          Diff = %f eV" % (Units.convert(Delta_RGS - (E_EX - E_GS), "Hartree",
↪"eV")))


# ========= STEP 3: Vibrational fine structure with the FCF program␣
↪===============================

# Settings for the FCF program
fcfin = Settings()
fcfin.input.spectrum.spcmin = "0.0"
fcfin.input.spectrum.spcmax = "5000.0"
fcfin.input.spectrum.spclen = "501"
fcfin.input.spectrum.lineshape = "Stick"
fcfin.input.numericalquality = "Basic"
fcfin.input.translate = True
fcfin.input.rotate = True

# Calculate vibrational fine structure
fcf = FCFJob(
    name="fcf",
    settings=fcfin,
    inputjob1=gs_freq_results.rkfpath(file="dftb"),
    inputjob2=ex_freq_results.rkfpath(file="dftb"),
)
fcf_results = fcf.run()
if not fcf.check():
    print("ERROR: FCF calculation failed")
    sys.exit(1)

# Extract and print the spectrum:
spectrum = extract_spectrum(fcf_results)
np.set_printoptions(formatter={"float": " {: 0.8f} ".format}, threshold=1e6)
print("Vibrational fine structure:")
print("Energy [cm^-1]    Intensity")
print(spectrum)
```

10.6.9 Example: Vibrational circular dichroism

Download FREQ_HNDT_VCD.run

```
#! /bin/sh

$AMSBIN/ams << eor

Task SinglePoint

Properties
   VCD true
End

System
    Atoms
        N  0.0              0.0              0.0
        H  0.0              0.0              1.02445577
        H -8.95690087e-01  4.13994999e-01 -2.75059085e-01   mass=2.01410178
        H -5.58123764e-02 -9.84657022e-01 -2.74917481e-01   mass=3.01604927
    End
End

Engine DFTB
   Model SCC-DFTB
   ResourcesDir DFTB.org/3ob-3-1
EndEngine
eor
```

10.7 Phonons

10.7.1 Example: Phonons graphene

Download Phonons_Graphene.run

```
#!/bin/sh

AMS_JOBNAME=graphene $AMSBIN/ams << EOF

   Task GeometryOptimization

   GeometryOptimization
!       CoordinateType Cartesian
      OptimizeLattice True
      Convergence Gradients=1.0e-5
      Method Quasi-Newton
   End

   Properties
      Phonons True
   End

   NumericalPhonons
     SuperCell
       2 0
```

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```
       0 2
     End
   End

   System
      Atoms
         C       0.000000000    -0.000000000     0.00000
         C       0.000000000    -1.420281662     0.00000
      End

      Lattice
         1.230000000    -2.130422493     0.000000000
         1.230000000     2.130422493     0.000000000
      End
   End

   Engine DFTB
      ResourcesDir Dresden
      Model DFTB0
      KSpace
        Type Symmetric
        Symmetric KInteg=9
      End
      Technical AnalyticalStressTensor=False # Not yet supported with symmetric k-
↪space grid ...
   EndEngine

EOF

echo ""
echo "Begin TOC of result file"

$AMSBIN/dmpkf -n 1 graphene.results/dftb.rkf --toc

echo "End TOC of result file"
```

10.7.2 Example: Phonons with isotopes

Download Phonons_Isotopes.run

```
#! /bin/sh


# ====================================
# Phonons with default nuclear masses:
# ====================================

AMS_JOBNAME=defmasses $AMSBIN/ams << EOF

   Task SinglePoint

   Properties
      Phonons True
   End

```

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```
   NumericalPhonons
      StepSize 0.01
      SuperCell
         4
      End
   End

   System
      Atoms
          C  -2.42906152   -0.3445528299    -0.1353492062
          C  -1.146891508  -1.134644249      0.1353492061
          H  -2.429062041   0.004468895147  -1.185797304
          H  -2.429062011   0.5753101439     0.4803683017
          H  -1.146891017  -2.054507222     -0.4803683019
          H  -1.146890987  -1.483665974      1.185797304
      End

      Lattice
          2.564338467 0.0 0.0
      End
   End

   Engine DFTB
      ResourcesDir QUASINANO2015
      Model DFTB0
      KSpace
        Type Symmetric
        Symmetric KInteg=9
      End
   EndEngine

EOF

echo ""
echo "Begin TOC of result file"
$AMSBIN/dmpkf -n 1 defmasses.results/dftb.rkf --toc
echo "End TOC of result file"


# =================================
# Phonons with two deuterium atoms:
# =================================

AMS_JOBNAME=usermasses $AMSBIN/ams << EOF

   Task SinglePoint

   Properties
      Phonons true
   End

   NumericalPhonons
      StepSize 0.01
      SuperCell
         4
      End
   End
```

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```
   System
       Atoms
           C   -2.42906152   -0.3445528299    -0.1353492062
           C   -1.146891508  -1.134644249      0.1353492061
           H   -2.429062041   0.004468895147  -1.185797304
           H   -2.429062011   0.5753101439     0.4803683017
           H   -1.146891017  -2.054507222     -0.4803683019    mass=2.014
           H   -1.146890987  -1.483665974      1.185797304     mass=2.014
       End
       Lattice
           2.564338467 0.0 0.0
       End
   End

   Engine DFTB
      ResourcesDir QUASINANO2015
      Model DFTB0
      KSpace
        Type Symmetric
        Symmetric KInteg=9
      End
   EndEngine

EOF

echo ""
echo "Begin TOC of result file"
$AMSBIN/dmpkf -n 1 usermasses.results/dftb.rkf --toc
echo "End TOC of result file"
```

10.7.3 Example: Diamond under pressure

Download Diamond_under_pressure.run

```
#! /bin/sh

# Calculate the phonon dispersion curves for diamond under pressure.

# Loop over pressure values (in GPa):
for P in -40 0 40 160 ; do
AMS_JOBNAME=pressure_$P $AMSBIN/ams << EOF

   Task GeometryOptimization

   System
       Atoms
           C -0.44625 -0.44625 -0.44625
           C  0.44625  0.44625  0.44625
       End
       Lattice
           0.0    1.785  1.785
           1.785  0.0    1.785
           1.785  1.785  0.0
       End
```

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```
   End

   GeometryOptimization
       OptimizeLattice Yes
       Convergence Gradients=1e-5 StressEnergyPerAtom=1E-5
       Method Quasi-Newton
   End

   EngineAddons
       Pressure $P
   End

   Properties
       # Request the calculation of phonons at the optimized geometry.
       Phonons Yes
   End

   NumericalPhonons
       SuperCell
           2 0 0
           0 2 0
           0 0 2
       End
   End

   Engine DFTB
       Model SCC-DFTB
       ResourcesDir DFTB.org/mio-1-1
       KSpace
           Type Symmetric
           Symmetric KInteg=5
       End
       Technical AnalyticalStressTensor=False
   EndEngine

EOF
done
```

10.8 Stress tensor, Elasticity

10.8.1 Example: Stress tensor

Download SP_stresstensor.run

```
#! /bin/sh

$AMSBIN/ams << EOF

Task SinglePoint

Properties
   StressTensor True
End
```

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```
System
   Atoms
      Cl       -3.27413732      17.07951309      11.46590854
      Cl        4.99858729       7.77406309       8.27058240
      Cl        7.93893730       1.53138691       1.69175208
      Cl       -0.33378731      10.83683691       4.88707823
      Cl       -2.62283362      13.61069415      10.36587591
      Cl        4.34728360       4.30524415       9.37061503
      Cl        7.28763360       5.00020585       2.79178471
      Cl        0.31751639      14.30565585       3.78704560
      O        4.45061833      13.97932690      12.65765874
      O       -2.72616836       4.67387690       7.07883220
      O        0.21418165       4.63157310       0.50000189
      O        7.39096834      13.93702310       6.07882842
      O       -1.67998789      17.02694622       9.23434128
      O        3.40443787       7.72149622      10.50214966
      O        6.34478788       1.58395378       3.92331935
      O        1.26036211      10.88940378       2.65551097
      N        4.96185602      15.23311375      10.79425410
      N       -3.23740605       5.92766375       8.94223683
      N       -0.29705604       3.37778625       2.36340652
      N        7.90220603      12.68323625       4.21542379
      N       -3.32221694      15.80795330       8.17067339
      N        5.04666692       6.50250330      11.56581755
      N        7.98701692       2.80294670       4.98698724
      N       -0.38186693      12.10839670       1.59184307
      C       -0.32679732      16.36453927       1.01679137
      C        7.93194732       7.05908927       5.56203894
      C        4.99159731       2.24636073      12.14086925
      C       -3.26714733      11.55181073       7.59562168
      C       -5.39328055      16.22890128      13.03400342
      C        7.11773052       6.92345128       6.70248752
      C       10.05808053       2.38199872       0.12365721
      C       -2.45293054      11.68744872       6.45517311
      C       -4.37216311      17.17136634      12.83355801
      C        6.09661309       7.86591634       6.90293293
      C        9.03696309       1.43953366       0.32410262
      C       -1.43181310      10.74498366       6.25472770
      C        1.70248570      18.21192289       0.58266919
      C        5.90266429       8.90647289       5.99616113
      C        2.96231428       0.39897711      12.57499144
      C       -1.23786431       9.70442711       7.16149950
      C        0.87902994      18.33819101       1.69886377
      C        6.72612005       9.03274101       4.87996654
      C        3.78577004       0.27270899      11.45879685
      C       -2.06132007       9.57815899       8.27769408
      C       -0.14633860      17.41192898       1.91683916
      C        7.75148859       8.10647898       4.66199116
      C        4.81113858       1.19897102      11.24082147
      C       -3.08668861      10.50442102       8.49566947
      C        4.84986903      15.05148082      12.15509818
      C       -3.12541905       5.74603082       7.58139276
      C       -0.18506905       3.55941918       1.00256245
      C        7.79021904      12.86486918       5.57626787
      C        4.61440419      14.34187564       9.75195839
      C       -2.88995421       5.03642564       9.98453255
```

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```
      C        0.05039580        4.26902436        3.40570224
      C        7.55475420       13.57447436        3.17312807
      C        4.58247005       14.85208549        8.44730031
      C       -2.85802008        5.54663549       11.28919063
      C        0.08232993        3.75881451        4.71036032
      C        7.52282006       13.06426451        1.86846999
      C        4.26779809       13.98303068        7.35568214
      C       -2.54334812        4.67758068       12.38080880
      C        0.39700189        4.62786932        5.80197849
      C        7.20814810       13.93331932        0.77685183
      C        3.93887163       12.61428732        7.61726689
      C       -2.21442166        3.30883732       12.11922405
      C        0.72592835        5.99661268        5.54039374
      C        6.87922164       15.30206268        1.03843657
      C        3.97815795       12.13796146        8.95803769
      C       -2.25370797        2.83251146       10.77845325
      C        0.68664204        6.47293854        4.19962293
      C        6.91850795       15.77838854        2.37920738
      C        4.32359175       12.97028648       10.00045258
      C       -2.59914177        3.66483648        9.73603836
      C        0.34120824        5.64061352        3.15720804
      C        7.26394176       14.94606352        3.42162227
      C        4.28942782       14.42981754        6.00353018
      C        3.31572217        5.12436754        0.57530013
      C        0.37537216        4.18108246        7.15413044
      C        1.34907781       13.48653246       12.58236050
      C        3.97615998       13.57242106        4.97038766
      C        3.62899001        4.26697106        1.60844266
      C        0.68864001        5.03847894        8.18727297
      C        1.03580997       14.34392894       11.54921797
      C        3.59007048       12.23546834        5.23347477
      C        4.01507951        2.93001834        1.34535554
      C        1.07472951        6.37543166        7.92418585
      C        0.64972047       15.68088166       11.81230509
      C        3.57942798       11.76653922        6.53102913
      C        4.02572201        2.46108922        0.04780119
      C        1.08537200        6.84436078        6.62663150
      C        0.63907797       16.14981078       13.10985944
      C        4.86328541       16.31909827        8.22021245
      C       -3.13883544        7.01364827       11.51627848
      C       -0.19848543        2.29180173        4.93744817
      C        7.80363542       11.59725173        1.64138214
      C        6.18319075       16.77307697        8.13696214
      C       -4.45874078        7.46762697       11.59952880
      C       -1.51839077        1.83782303        5.02069849
      C        9.12354076       11.14327303        1.55813182
      C        6.47127249       18.15826947        7.97988541
      C       -4.74682251        8.85281947       11.75660552
      C       -1.80647250        0.45263053        5.17777521
      C        9.41162249        9.75808053        1.40105510
      C        5.44012509        0.45783580        7.89557438
      C       -3.71567511        9.76328580       11.84091656
      C       -0.77532511       18.15306420        5.26208625
      C        8.38047510        8.84761420        1.31674406
      C        4.08231117        0.04352873        8.00806247
      C       -2.35786119        9.34897873       11.72842846
      C        0.58248881       18.56737127        5.14959815
```

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```
      C       7.02266118       9.26192127       1.42923216
      C       3.78975298      17.26601588       8.19945668
      C      -2.06530301       7.96056588      11.53703426
      C       0.87504700       1.34488412       4.95820394
      C       6.73010299      10.65033412       1.62062637
      C       3.00807658       0.97597001       7.97874488
      C      -1.28362661      10.28142001      11.75774606
      C       1.65672340      17.63492999       5.17891575
      C       5.94842659       8.32947999       1.39991457
      C       1.70966983       0.56324775       8.18980271
      C       0.01478015       9.86869775      11.54668822
      C       2.95513015      18.04765225       4.96785791
      C       4.65001984       8.74220225       1.61097240
      C       1.42279470      17.81036064       8.43407994
      C       0.30165527       8.50491064      11.30241100
      C       3.24200528       0.80053936       4.72358069
      C       4.36314471      10.10598936       1.85524962
      C       2.43725297      16.87568784       8.42024007
      C      -0.71280299       7.57023784      11.31625087
      C       2.22754702       1.73521216       4.73742056
      C       5.37760297      11.04066216       1.84140975
      C      -2.04299433      15.99564634       8.63316111
      C       3.76744431       6.69019634      11.10332983
      C       6.70779432       2.61525366       4.52449952
      C       0.89735568      11.92070366       2.05433080
      C      -1.12611526      14.81026883       8.42855071
      C       2.85056524       5.50481883      11.30794023
      C       5.79091525       3.80063117       4.72910992
      C       1.81423474      13.10608117       1.84972040
      C      -1.31692395      13.65173092       9.18657854
      C       3.04137392       4.34628092      10.54991240
      C       5.98172393       4.95916908       3.97108209
      C       1.62342606      14.26461908       2.60774822
      C      -0.49426876      12.53961138       9.04070240
      C       2.21871874       3.23416138      10.69578854
      C       5.15906874       6.07128862       4.11695822
      C       2.44608125      15.37673862       2.46187209
      C       0.53399491      12.57081639       8.09897786
      C       1.19045507       3.26536639      11.63751308
      C       4.13080508       6.04008361       5.05868276
      C       3.47434492      15.34553361       1.52014755
      C       0.73688489      13.71338210       7.32038359
      C       0.98756508       4.40793210      12.41610735
      C       3.92791509       4.89751790       5.83727704
      C       3.67723490      14.20296790       0.74155328
      C      -0.08592033      14.82957584       7.48853697
      C       1.81037030       5.52412584      12.24795396
      C       4.75072031       3.78132416       5.66912365
      C       2.85442968      13.08677416       0.90970666
      H      -0.66793224      11.65797166       9.64782399
      H       2.39238221       2.35252166      10.08866695
      H       5.33273222       6.95292834       3.50983664
      H       2.27241777      16.25837834       3.06899367
      H       1.17814887      11.70517867       7.97107323
      H       0.54630111       2.39972867      11.76541770
      H       3.48665112       6.90572133       5.18658739
      H       4.11849887      16.21117133       1.39224292
```

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```
H      1.53950361     13.73602312      6.58864369
H      0.18494637      4.43057312     13.14784725
H      3.12529637      4.87487688      6.56901694
H      4.47985362     14.18032688      0.00981338
H      0.06852126     15.71812944      6.87985591
H      1.65592872      6.41267944     12.85663502
H      4.59627872      2.89277056      6.27780471
H      3.00887127     12.19822056      0.30102560
H      7.02940811     14.91917221      7.69138939
H     -5.30495813      5.61372221     12.04510154
H     -2.36460812      3.69172779      5.46627123
H      9.96975812     12.99717779      1.11255908
H     -3.04038236     18.48242810      7.92213380
H      4.76483234      9.17697810     11.81435714
H      7.70518235      0.12847190      5.23552682
H     -0.10003236      9.43392190      1.34330349
H      5.65921598      1.51552308      7.75866896
H     -3.93476601     10.82097308     11.97782198
H     -0.99441600     17.09537692      5.39899166
H      8.59956599      7.78992692      1.17983865
H      3.22612999      2.02510401      7.78838638
H     -1.50168002     11.33055401     11.94810456
H      1.43866999     16.58579599      5.36927424
H      6.16648000      7.28034599      1.20955607
H      0.89760454      1.28608561      8.17042888
H      0.82684544     10.59153561     11.56606205
H      3.76719545     17.32481439      4.98723174
H      3.83795454      8.01936439      1.59159857
H      0.39661775     17.50551993      8.63189857
H      1.32783222      8.20006993     11.10459237
H      4.26818223      1.10538007      4.52576205
H      3.33696776     10.41083007      2.05306826
H      2.21434665     15.82482508      8.59390958
H     -0.48989667      6.51937508     11.14258136
H      2.45045334      2.78607492      4.56375105
H      5.15469666     12.09152492      2.01507926
H      4.57639152     15.45809159      5.79414173
H      3.02875847      6.15264159      0.78468859
H      0.08840846      3.15280841      7.36351890
H      1.63604151     12.45825841     12.37297204
H      4.02539579     13.92259271      3.94280751
H      3.57975421      4.61714271      2.63602280
H      0.63940420      4.68830729      9.21485311
H      1.08504578     13.99375729     10.52163782
H      3.30607699     11.58512640      4.40995342
H      4.29907301      2.27967640      2.16887690
H      1.35872300      7.02577360      8.74770721
H      0.36572698     16.33122360     10.98878373
H      3.28986843     10.73894681      6.74402515
H     -1.56541845      1.43349681     12.99246579
H      1.37493156      7.87195319      6.41363548
H      6.23021843     17.17740319      0.16519484
H      3.74550631     11.09356333      9.15380170
H     -2.02105634      1.78811333     10.58268924
H      0.91929367      7.51733667      4.00385893
H      6.68585632     16.82278667      2.57497138
H      4.35802904     12.59828784     11.01817560
```

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```
      H      -2.63357907       3.29283784       8.71831534
      H       0.30677094       6.01261216       2.13948502
      H       7.29837905      15.31806216       4.43934529
      H       5.18081420      16.17885133      10.49020037
      H      -3.45636423       6.87340133       9.24629056
      H      -0.51601422       2.43204867       2.66746025
      H       8.12116421      11.73749867       3.91137006
      H       9.42762559      15.63449202       1.17123747
      H      -1.82247560       6.32904202       5.40759284
      H      -4.76282560       2.97640798      11.98642316
      H       6.48727558      12.28185798       7.75006778
      H      -0.79240888      17.50142328       2.78677788
      H       8.39755887       8.19597328       3.79205244
      H       5.45720886       1.10947672      10.37088275
      H      -3.73275889      10.41492672       9.36560819
      H       1.04123418       0.53956949       2.40400293
      H       6.56391581       9.84501949       4.17482738
      H       3.62356581      18.07133051      10.75365769
      H      -1.89911583       8.76588051       8.98283325
      H       2.50141739       0.31172726       0.40272646
      H       5.10373261       9.61717726       6.17610385
      H       2.16338260      18.29917274      12.75493416
      H      -0.43893262       8.99372274       6.98155677
    End
    Lattice
       10.54550000       0.00000000       0.00000000
        0.00000000      18.61090000       0.00000000
       -5.88070002       0.00000000      13.15766063
    End
End

Engine DFTB
    Model DFTB3
    ResourcesDir DFTB.org/3ob-3-1
    DispersionCorrection D3-BJ
    KSpace Quality=GammaOnly
EndEngine

EOF
```

10.8.2 Example: Analytical stress tensor Urea

Download GO_Analytical_Ewald_Urea.run

```
#!/bin/sh
$AMSBIN/ams << eor

Task GeometryOptimization
System
    Atoms
          C      -0.353812500     2.476687500     1.569096000
          C       2.476687500    -0.353812500    -1.569096000
          O      -0.353812500     2.476687500    -1.899878400
          O       2.476687500    -0.353812500     1.899878400
          N       0.460805400    -2.369694600     0.863238400
```

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```
          N      -1.168430400     1.662069600     0.863238400
          N      -2.369694600    -1.168430400    -0.863238400
          N       1.662069600     0.460805400    -0.863238400
          H       1.073891700    -1.756608300     1.337736800
          H      -1.781516700     1.048983300     1.337736800
          H      -1.756608300    -1.781516700    -1.337736800
          H       1.048983300     1.073891700    -1.337736800
          H       0.418914000    -2.411586000    -0.130051200
          H      -1.126539000     1.703961000    -0.130051200
          H      -2.411586000    -1.126539000     0.130051200
          H       1.703961000     0.418914000     0.130051200
    End
    Lattice
          5.661000000     0.000000000     0.000000000
          0.000000000     5.661000000     0.000000000
          0.000000000     0.000000000     4.712000000
    End
End

NumericalDifferentiation
  StrainStepSize 0.00001
  Parallel nCoresPerGroup=1
End

GeometryOptimization
  OptimizeLattice yes
  Convergence Gradients=1e-3
  Method Fire
End


Engine DFTB
    Model DFTB3
    ResourcesDir DFTB.org/3ob-3-1
    DispersionCorrection D3-BJ
    Technical
      EwaldSummation Enabled=yes
      AnalyticalStressTensor yes
    End
    KSpace Quality=GammaOnly
EndEngine

eor
```

10.8.3 Example: Elastic tensor

Download ElasticTensor.run

```
#! /bin/sh


# === Diamond ===

AMS_JOBNAME=Diamond $AMSBIN/ams << EOF

```

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```
   Task GeometryOptimization

   Properties
       ElasticTensor Yes
   End

   System
      Atoms
         C  0.44625  0.44625  2.23125
         C  2.23125  2.23125  2.23125
         C -2.23125 -2.23125 -2.23125
         C -0.44625 -0.44625 -2.23125
         C -0.44625 -2.23125 -0.44625
         C  1.33875 -0.44625 -0.44625
         C -2.23125 -0.44625 -0.44625
         C -0.44625  1.33875 -0.44625
         C -0.44625 -0.44625  1.33875
         C  1.33875  1.33875  1.33875
         C -1.33875 -1.33875 -1.33875
         C  0.44625  0.44625 -1.33875
         C  0.44625 -1.33875  0.44625
         C  2.23125  0.44625  0.44625
         C -1.33875  0.44625  0.44625
         C  0.44625  2.23125  0.44625
      End
      Lattice
         0.0  3.57 3.57
         3.57 0.0  3.57
         3.57 3.57 0.0
      End
   End

   GeometryOptimization
       OptimizeLattice Yes
       Convergence Quality=Good
   End

   Symmetry Tolerance=1e-6

   Engine DFTB
       Model DFTB
       ResourcesDir DFTB.org/mio-1-1
       KSpace
           Type Symmetric
           Symmetric KInteg=3
       End
       Technical AnalyticalStressTensor=False # Not yet supported with symmetric k-
↪space grid.
   EndEngine

EOF


# === Boron-Nitride sheet ===

# 3x3 super-cell, default k-space sampling
```

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```
AMS_JOBNAME=BN_sheet $AMSBIN/ams << EOF

   Task GeometryOptimization

   Properties
       ElasticTensor Yes
   End

   System
      Atoms
         N  3.76095075   0.723795     0.0
         N  5.01460112   2.89518114   0.0
         B -3.76095112  -2.17138614   0.0
         B -2.50730075   0.0          0.0
         B -1.25365038   2.17138614   0.0
         B -1.25365037  -2.17138614   0.0
         B  0.0          0.0          0.0
         B  1.25365037   2.17138614   0.0
         B  1.25365038  -2.17138614   0.0
         B  2.50730075   0.0          0.0
         B  3.76095112   2.17138614   0.0
         N -2.50730112  -1.44759114   0.0
         N -1.25365075   0.723795     0.0
         N  -3.8e-07      2.89518114 0.0
         N  -3.7e-07     -1.44759114 0.0
         N  1.25365      0.723795     0.0
         N  2.50730037   2.89518114   0.0
         N  2.50730038  -1.44759114   0.0
      End
      Lattice
         7.52190225 0.0
         3.76095111 6.51415842
      End
   End

   GeometryOptimization
      OptimizeLattice Yes
      Convergence Quality=Good
   End

   Engine DFTB
      Model SCC-DFTB
      ResourcesDir DFTB.org/matsci-0-3
   EndEngine

EOF


# === Polyoxyethylene ===

# primitive cell with k-space sampling

AMS_JOBNAME=Polyoxyethylene $AMSBIN/ams << EOF

   Task GeometryOptimization

   Properties
```

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```
      ElasticTensor Yes
   End

   ElasticTensor
      StrainStepSize 0.002
   End

   System
      Atoms
         C   -0.279368361   -0.125344097   -0.026221791
         O    0.840592835   -0.919621431   -0.193214154
         H   -0.279527057    0.337014408    0.997733792
         H   -0.281697417    0.707951120   -0.778297849
      End
      Lattice
         2.240292981
      End
   End

   GeometryOptimization
      OptimizeLattice Yes
      Convergence Quality=Good
   End

   Engine DFTB
      Model SCC-DFTB
      ResourcesDir DFTB.org/3ob-3-1
      KSpace
          Type Symmetric
          Symmetric KInteg=5
      End
      Technical AnalyticalStressTensor=False # Not yet supported with symmetric k-
↪space grid.
   EndEngine

EOF


# Note: the elastic tensor is also printed to standard output.

echo ""
echo "Extract the elastic tensor of Diamond from the rkf file:"
$AMSBIN/amsreport Diamond.results/dftb.rkf -r "AMSResults%ElasticTensor#12.4f##6"

echo ""
echo "Extract the elastic tensor of Boron-Nitride from the rkf file:"
$AMSBIN/amsreport BN_sheet.results/dftb.rkf -r "AMSResults%ElasticTensor#12.4f##3"

echo ""
echo "Extract the elastic tensor of Polyoxyethylene from the rkf file:"
$AMSBIN/amsreport Polyoxyethylene.results/dftb.rkf -r "AMSResults%ElasticTensor#12.4f#
↪#1"
```

10.9 Molecular Dynamics

10.9.1 Example: Molecular dynamics

Download MD_aspirin.run

```
#!/bin/sh

$AMSBIN/ams << eor

Task MolecularDynamics

MolecularDynamics
    nSteps 3
    TimeStep 0.2
    InitialVelocities Type=zero
    Thermostat Type=berendsen BerendsenApply=local Tau=20 Temperature=1200
    Trajectory SamplingFreq=1
    Preserve CenterOfMass=true
    Print System=true
End

System
    Atoms [Bohr]
        C     1.05960877221036       -4.29661605444804      -0.634037783371545
        C     3.70944109230336       -4.29661605444804      -0.634037783371545
        C     5.01105409669631       -1.99043606903162      -0.634037783371545
        C     3.65522107511068       0.286575996219979      -0.625747555592921
        C    0.994311181450713       0.336536571102876      -0.603233360526924
        C   -0.284455036107599       -2.00337880211933      -0.623649959779319
        O   -0.281193369103746        2.57767407876400      -0.596339640231410
        C    -2.98801415491818       -2.09305007828785      -0.642322341972295
        O    -4.09533876437070      -0.211143806102700       -1.93967968350738
        C   -0.320197312880997        4.26468724370209        1.32592550924302
        C    0.933554602168619        3.32259649258268        3.72681289050655
        H    5.555390692156803E-002  -6.12434199368563      -0.648191830798464
        H     4.76167074144455       -6.09597720705304      -0.642072898145812
        H     7.09553143269668       -1.96900279721371      -0.645115356938515
        H     4.71261912474754        2.08377152287689      -0.639226970852763
        O    -4.22220929602639       -3.71173831148125       0.403176103305787
        H    -3.05020881565447        1.05602705297610       -2.76001350141399
        O    -1.32857587116215        6.31113951397156        1.15028115060619
        H    0.422139955826862        4.57364609951207        5.33966942939295
        H     3.02803425766575        3.36265301371865        3.55019154354933
        H    0.292508534546246        1.38261705197608        4.22808915708257
    End
End

Engine DFTB
   Model SCC-DFTB
   ResourcesDir Dresden
   SCC
       Iterations 200
       Converge charge=1e-7
   End
   Repulsion
       ForcePolynomial true
```

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```
   End
   DispersionCorrection Auto
EndEngine

eor
```

10.9.2 Example: MD ethylene graphene

Download MD_ethylene_graphene.run

```
#! /bin/sh

$AMSBIN/ams << eor

Task MolecularDynamics

MolecularDynamics
    nSteps 5
    Timestep 0.5
    InitialVelocities
        Type Input
        Values
            0.00386657     0.00248442    -0.00365340
           -0.00685900     0.00372959    -0.00251567
           -0.00337849     0.00427222    -0.00312621
           -0.00262074    -0.00701592     0.00113233
           -0.00235220     0.00716892    -0.00224433
            0.00709322    -0.00478422    -0.00385799
            0.00690609    -0.00701767    -0.00430586
           -0.00578471    -0.00685568     0.00719495
            0.00463927     0.00691165    -0.00160766
           -0.00711540     0.00707290    -0.00186106
           -0.00289722     0.00677257     0.00703130
           -0.00560551     0.00421418     0.00008108
            0.00702463     0.00110754    -0.00717058
            0.00314315    -0.00368145    -0.00711784
           -0.00210798     0.00468384     0.00543764
           -0.00720273    -0.00665179    -0.00407414
           -0.00396359     0.00614417     0.00608546
           -0.00297469     0.00647775    -0.00245696
           -0.00428470    -0.00120421    -0.00716899
           -0.00459898    -0.00721328    -0.00287459
           -0.05358934    -0.07103670    -0.05578240
            0.01565046    -0.06666639    -0.04444608
           -0.05206965    -0.08540528     0.03078936
            0.07612262     0.08571624    -0.05223484
        End
    End
    Trajectory SamplingFreq=1
    Preserve
       Momentum        false
       AngularMomentum false
    End
End
```

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```
System
    Atoms
        C 0.01890012557 0.006154556297 -0.463984544
        C 1.248840602 0.7162706363 -0.4639711139
        C 1.24893317 2.136550013 -0.4641652045
        C 2.478907661 2.846802734 -0.4641354681
        C -1.211067484 -2.124176808 -0.4643503578
        C 0.01889729551 -1.414034025 -0.4641656898
        C 2.478882829 0.006210752849 -0.4641273211
        C 3.708952915 0.7162947206 -0.4641642638
        C 3.708939806 2.13661872 -0.4640903058
        C 4.938979056 2.846735645 -0.4640971093
        C 1.248826397 -2.124236351 -0.4641422158
        C 2.478856391 -1.414110439 -0.4640214402
        C -2.441031711 0.006167945601 -0.4643418121
        C -1.211040211 0.7162194157 -0.4641998989
        C -1.211097135 2.136443052 -0.464194732
        C 0.01887926696 2.846648611 -0.4641145804
        C -3.671122781 -2.124300926 -0.46412142
        C -2.441117073 -1.414110304 -0.4642262685
        C -0.9347946789 -0.319377646 3.183251858
        C 0.2740530406 0.2112707751 3.083888257
        H 1.178725997 -0.4117555796 2.991115711
        H -1.839452684 0.3037579484 3.275246477
        H -1.095141972 -1.409988748 3.178469159
        H 0.4343907186 1.301893629 3.089576954
    End

    Lattice
        7.38 0.000000 0.0
        3.69 6.391267479 0.0
    End
End

Engine DFTB
   Model SCC-DFTB
   ResourcesDir Dresden
   Occupation Strategy=fermi Temperature=20
   KSpace
     Type Symmetric
     Symmetric KInteg=5
   End
EndEngine

eor
```

10.9.3 Example: MD hydrogen

Download MD_hydrogen.run

```
#!/bin/sh

$AMSBIN/ams << eor

Task MolecularDynamics

MolecularDynamics
    nSteps 3
    TimeStep 1
    InitialVelocities Type=Zero
    Thermostat Type=none
    Trajectory SamplingFreq=1
    Print System=true
    Preserve
       Momentum        false
       AngularMomentum false
    End
End

System
    Atoms [Bohr]
        H  -2.0  0.0  0.0
        H   2.0  0.0  0.0
    End
End

Engine DFTB
   Model SCC-DFTB
   ResourcesDir Dresden
   DispersionCorrection Auto
EndEngine

eor
```

10.9.4 Example: MD hydrogen long run

Download MD_hydrogen_longrun.run

```
#!/bin/sh

$AMSBIN/ams << eor

Task MolecularDynamics

MolecularDynamics
    nSteps 1000
    TimeStep 0.1
    InitialVelocities Type=zero
    Preserve Momentum=False AngularMomentum=False
    Thermostat Type=none
    Trajectory SamplingFreq=100
End
```

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```
System
    Atoms [Bohr]
        H  -2.0  0.0  0.0
        H   2.0  0.0  0.0
    End
End

Engine DFTB
   Model SCC-DFTB
   ResourcesDir Dresden
   Occupation Strategy=Fermi Temperature=5
   Repulsion
       forcePolynomial true
   End
   DispersionCorrection Auto
EndEngine

eor
```

10.9.5 Example: MD periodic

Download MD_periodic.run

```
#!/bin/sh

$AMSBIN/ams << eor

Task MolecularDynamics

MolecularDynamics
    nSteps 50
    TimeStep 0.5
    InitialVelocities Type=zero
    Thermostat Type=None
    Trajectory SamplingFreq=1
    Remap Range=AroundCenter
    Print System=true Velocities=true
    Preserve
       Momentum        false
       AngularMomentum false
    End
End

System
   Atoms
      H  0.0  0.0  0.0
      H  0.0  0.0  1.4
      H  2.0  0.0  0.0
      H  2.0  0.0  1.4
      H  4.0  0.0  0.0
      H  4.0  0.0  1.4
   End

   Lattice
```

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```
      0.0 5.0 5.0
      5.0 0.0 5.0
      5.0 5.0 0.0
   End
End

Engine DFTB
   ResourcesDir Dresden
   Model DFTB0
   KSpace Quality=GammaOnly
EndEngine

eor
```

10.10 Electronic transport, NEGF

10.10.1 Example: Electronic transport with NEGF

Download conductance.run

```
#!/bin/sh

# ==================================
# First test: Aluminum chain (DFTB0)
# ==================================

# Lead:
# =====

AMS_JOBNAME=Al_lead $AMSBIN/ams <<EOF
    Task SinglePoint
    System
        Atoms
            Al 0.0  0.0 0.0
            Al 2.83 0.0 0.0
            Al 5.66 0.0 0.0
            Al 8.49 0.0 0.0
        End

        Charge 0

        Lattice
            11.32 0.0 0.0
        End
    End

    Engine DFTB
       ResourcesDir QUASINANO2013.1
       StoreMatrices yes
       Model DFTB0
       Occupation Strategy=Fermi Temperature=5
       KSpace
         Type Symmetric
```

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```
         Symmetric KInteg=13
       End
    EndEngine
EOF

# Scattering region:
# ==================

AMS_JOBNAME=Al_scattering $AMSBIN/ams <<EOF
    Task SinglePoint
    System
        Atoms
            Al -14.15 0.0 0.0
            Al -11.32 0.0 0.0
            Al -8.49 0.0 0.0
            Al -5.66 0.0 0.0
            Al -2.83 0 0
            Al 0 0 0
            Al 2.83 0 0
            Al 5.66 0.0 0.0
            Al 8.49 0.0 0.0
            Al 11.32 0.0 0.0
            Al 14.15 0.0 0.0
        End

        Charge 0
    End

    Engine DFTB
       ResourcesDir QUASINANO2013.1
       StoreMatrices yes
       Model DFTB0
       Occupation Strategy=Fermi Temperature=5
    EndEngine
EOF

# Conductance:
# ============

$AMSBIN/conductance <<EOF
    EnergyGrid min=-5 max=5 num=500

    Files
       Leads      Al_lead.results/dftb.rkf
       Scattering Al_scattering.results/dftb.rkf
    End
EOF

mv ConductanceResults.kf Al_ConductanceResults.kf

echo "Extract DOS from the kf file Al_ConductanceResults.kf:"
$AMSBIN/amsreport Al_ConductanceResults.kf -r "results%dos#12.5f##1"

echo "Extract transmission from the kf file Al_ConductanceResults.kf:"
$AMSBIN/amsreport Al_ConductanceResults.kf -r "results%transmission#12.5f##1"
```

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```
# ==========================================
#   Second test: CO on gold chain (SCC-DFTB)
# ==========================================

# Lead:
# =====

AMS_JOBNAME=Au_lead $AMSBIN/ams <<EOF
    Task SinglePoint
    System
        Atoms
            Au 0.0 0.0 0.0
            Au 2.884996 0.0 0.0
            Au 5.769992 0.0 0.0
        End

        Charge 0

        Lattice
            8.654988 0.0 0.0
        End
    End
    Engine DFTB
       Model SCC-DFTB
       ResourcesDir QUASINANO2013.1
       Occupation Strategy=Fermi Temperature=5
       StoreMatrices yes
       KSpace
         Type Symmetric
         Symmetric KInteg=13
       End
    EndEngine
EOF

# Scattering region:
# ==================

AMS_JOBNAME=Au_scattering $AMSBIN/ams <<EOF
    Task SinglePoint
    System
        Atoms
            Au -20.194972   0.0 0.0
            Au -17.309976   0.0 0.0
            Au -14.42498    0.0 0.0
            Au -11.539984   0.0 0.0
            Au -8.654988    0.0 0.0
            Au -5.769992    0.0 0.0
            Au -2.884996    0.0 0.0
            Au 0.0          0.0 0.20
            Au 2.884996     0.0 0.0
            Au 5.769992     0.0 0.0
            Au 8.654988     0.0 0.0
            Au 11.539984    0.0 0.0
            O  0.0          0.0 3.12
            C  0.0          0.0 1.96
            Au 14.42498     0.0 0.0
            Au 17.309976    0.0 0.0
```

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```
            Au 20.194972    0.0 0.0
        End

        Charge 0

        Lattice
            43.27494 0.0 0.0
        End
    End

    Engine DFTB
       Model SCC-DFTB
       ResourcesDir QUASINANO2013.1
       Occupation Strategy=Fermi Temperature=5
       StoreMatrices yes
    EndEngine
EOF

# Conductance:
# ============

$AMSBIN/conductance <<EOF
    EnergyGrid min=-3.5 max=3 num=200

    Files
      Leads      Au_lead.results/dftb.rkf
      Scattering Au_scattering.results/dftb.rkf
    End
EOF

mv ConductanceResults.kf Au_ConductanceResults.kf

echo "Extract DOS from the kf file Au_ConductanceResults.kf:"
$AMSBIN/amsreport Au_ConductanceResults.kf -r "results%dos#12.5f##1"

echo "Extract transmission from the kf file Au_ConductanceResults.kf:"
$AMSBIN/amsreport Au_ConductanceResults.kf -r "results%transmission#12.5f##1"
```

10.10.2 Example: Charge transfer integrals Alq3 dimer

Download TransferIntegrals_dimer_Alq3.run

```
#! /bin/sh

# DFTB can calculate charge transfer integrals, that are needed in
# approximate methods that model charge transport properties. The molecular
# system typically should be build from 2 fragments. In this example charge
# transfer integrals are calculated between two Alq3 molecules. First these two
# molecules are calculated.
# Next the dimer is calculated and the charge transfer integrals between the
# two Alq3 molecules are calculated.

AMS_JOBNAME=Alq3_1 "$AMSBIN/ams" << eor
Task SinglePoint
System
```

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```
    Atoms
        C -1.2532452927 -4.2436531593 -5.6800115371
        C -1.6002356129 -3.628630899 -4.4625616847
        C -2.3166627009 -2.4309877283 -4.466594504
        C -2.6682692402 -1.8439166714 -5.756213841
        C -2.3561928593 -2.5170678195 -6.9843208241
        C -1.6512696758 -3.719830858 -6.9292054573
        C -2.6855114248 -1.7317753464 -3.3190778499
        C -3.3657320612 -0.5091752474 -3.4487721821
        C -3.6488978399 0.0190863447 -4.721744153
        C -6.9109250076 -0.5684531166 -11.3009872376
        C -5.5931161268 -0.1386952767 -11.1096306784
        C -5.0031197614 -0.304079768 -9.7837558297
        C -4.797153712 0.4447445829 -12.0961575197
        C -3.491952356 0.8534249078 -11.7692364116
        C -5.7470889275 -0.8818427552 -8.714163041500001
        C -1.521921939 1.464639922 -7.5667098728
        C -0.3075775491 2.1388971292 -7.6202165725
        C -0.2664221476 3.5171932557 -7.3450676891
        C -1.4267805963 4.251590413 -7.0047721214
        C -2.6719288124 3.6116632702 -6.9646019681
        C -2.7134395057 2.1895131201 -7.2740406478
        C -3.8852239978 4.2286266521 -6.6524870999
        C -5.0659713795 3.4588503508 -6.6506804594
        C -5.0388377042 2.0959764695 -6.9959791168
        C -2.9889404515 0.6766722553 -10.4634123477
        C -7.0510398913 -1.3002598893 -8.9510803531
        C -7.6304496018 -1.1364330624 -10.2294791139
        H -0.657764429 -5.1369220894 -5.6458579041
        H -1.2764482466 -4.0710495244 -3.5280887931
        H -1.3719846126 -4.2251249904 -7.8450077468
        H -2.4367067302 -2.1213847714 -2.3423018403
        H -3.6490248057 0.0467413072 -2.5658320516
        H -4.1461918087 0.9740729641 -4.7864213104
        H 0.597333457 1.6066837659 -7.8875907242
        H 0.679611233 4.0219553084 -7.444720368
        H -1.3549091409 5.3160323625 -6.8170100952
        H -3.919614268 5.2837735636 -6.4149944649
        H -6.0041856891 3.9054265542 -6.3685046202
        H -5.9539388661 1.5175984809 -6.9886625981
        H -7.598853678 -1.7608423553 -8.148837203799999
        H -8.6430324336 -1.4788592006 -10.4034071424
        H -7.376351861 -0.4808003889 -12.2746522104
        H -5.1822456956 0.5984619047 -13.0969032753
        H -2.8771937878 1.3227485141 -12.5240563582
        H -1.9932606643 1.025104893 -10.2292724091
        N -3.2837377695 -0.664491859 -5.8465663222
        N -3.8524864579 1.4991142677 -7.2859856873
        N -3.7633918961 0.0903193296 -9.5053497157
        O -2.7251315757 -1.9232489398 -8.1021556012
        O -5.1457683284 -0.9727214768 -7.5493429881
        O -1.6598493293 0.1830791333 -7.798390479
        Al -3.4400529704 -0.2815131096 -7.6838832318
    End
End

Engine DFTB
```

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```
   Model GFN1-xTB
EndEngine
eor

AMS_JOBNAME=Alq3_2 "$AMSBIN/ams" << eor
Task SinglePoint
System
    Atoms
        C 1.8794971861 -3.2423985149 -3.7055748349
        C 1.4011660396 -2.2204931545 -4.5483930567
        C 0.8274160672999999 -1.0717826595 -3.9973668319
        C 0.746983485 -0.9752989758 -2.5423512135
        C 1.2665725664 -2.0129450542 -1.7049850454
        C 1.8271673309 -3.1412429717 -2.2998034997
        C 0.2762842971 -0.0297851274 -4.7420249828
        C -0.3267411113 1.0480718286 -4.0713454755
        C -0.3857680483 1.0728768536 -2.6636208351
        C 2.7644548613 0.9617998245 4.0521806593
        C 1.7439042145 0.0941090718 3.642059507
        C 1.3996414133 0.0669834211 2.2243753192
        C 1.0246834424 -0.7518007473 4.4897696339
        C -0.0253912619 -1.5240836801 3.961651508
        C 2.1676852503 0.794508034 1.2632486424
        C -2.3492859035 -0.5066719029 0.0806199723
        C -3.6744350901 -0.9392987641 0.0975336336
        C -4.7079127213 -0.020618815 0.3771973267
        C -4.4394638678 1.3371214498 0.6598958034
        C -3.1321189427 1.8219755043 0.5974315921
        C -2.0642722189 0.8693320226 0.3369119755
        C -2.7721209304 3.1610944822 0.7475851159
        C -1.4144957483 3.5219566869 0.6650177522
        C -0.4278377382 2.5489518242 0.4378243493
        C -0.3586369631 -1.4383319818 2.594888547
        C 3.2148559649 1.5999922827 1.7099111367
        C 3.4831465281 1.7092530557 3.0921846639
        H 2.2914114296 -4.1270622441 -4.158196487
        H 1.4543744769 -2.3475597919 -5.6229273984
        H 2.1966824143 -3.9437878589 -1.6810430419
        H 0.2883188796 -0.0646089869 -5.8230215972
        H -0.771892801 1.8523200353 -4.6417846164
        H -0.8774279828 1.9026533162 -2.1773984742
        H -3.9039055772 -1.9755591047 -0.1103067723
        H -5.732849804 -0.3710752989 0.3801561174
        H -5.2465403092 2.0113655771 0.9117513642
        H -3.5314949482 3.913350028 0.8950780632000001
        H -1.1119084494 4.5521879649 0.766667497
        H 0.6089086397 2.8551248498 0.358222646
        H 3.7881190229 2.1752551515 0.9982104892
        H 4.2640858083 2.381823329 3.4210694665
        H 3.0118117692 1.0528196574 5.1034300383
        H 1.2574079525 -0.8033825665 5.5443969166
        H -0.5927560352 -2.1754873153 4.6136376386
        H -1.1882703275 -2.0188179907 2.2151671074
        N 0.1569126804 0.0531352413 -1.9348483597
        N -0.7873119119999999 1.2424726569 0.2843969979
        N 0.3730124556 -0.6434632843 1.7615285374
        O 1.1442860805 -1.8491466636 -0.405855127
```

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```
        O 1.7961887073 0.6871617202 0.0034904085
        O -1.3220788059 -1.2813762571 -0.1866654751
        Al 0.2305308242 -0.2883029309 -0.0814854552
    End
End

Engine DFTB
   Model GFN1-xTB
EndEngine
eor

AMS_JOBNAME=Alq3_dimer "$AMSBIN/ams" << eor
Task SinglePoint
System
    Atoms
        C -1.2532452927 -4.2436531593 -5.6800115371
        C -1.6002356129 -3.628630899 -4.4625616847
        C -2.3166627009 -2.4309877283 -4.466594504
        C -2.6682692402 -1.8439166714 -5.756213841
        C -2.3561928593 -2.5170678195 -6.9843208241
        C -1.6512696758 -3.719830858 -6.9292054573
        C -2.6855114248 -1.7317753464 -3.3190778499
        C -3.3657320612 -0.5091752474 -3.4487721821
        C -3.6488978399 0.0190863447 -4.721744153
        C -6.9109250076 -0.5684531166 -11.3009872376
        C -5.5931161268 -0.1386952767 -11.1096306784
        C -5.0031197614 -0.304079768 -9.7837558297
        C -4.797153712 0.4447445829 -12.0961575197
        C -3.491952356 0.8534249078 -11.7692364116
        C -5.7470889275 -0.8818427552 -8.714163041500001
        C -1.521921939 1.464639922 -7.5667098728
        C -0.3075775491 2.1388971292 -7.6202165725
        C -0.2664221476 3.5171932557 -7.3450676891
        C -1.4267805963 4.251590413 -7.0047721214
        C -2.6719288124 3.6116632702 -6.9646019681
        C -2.7134395057 2.1895131201 -7.2740406478
        C -3.8852239978 4.2286266521 -6.6524870999
        C -5.0659713795 3.4588503508 -6.6506804594
        C -5.0388377042 2.0959764695 -6.9959791168
        C -2.9889404515 0.6766722553 -10.4634123477
        C -7.0510398913 -1.3002598893 -8.9510803531
        C -7.6304496018 -1.1364330624 -10.2294791139
        H -0.657764429 -5.1369220894 -5.6458579041
        H -1.2764482466 -4.0710495244 -3.5280887931
        H -1.3719846126 -4.2251249904 -7.8450077468
        H -2.4367067302 -2.1213847714 -2.3423018403
        H -3.6490248057 0.0467413072 -2.5658320516
        H -4.1461918087 0.9740729641 -4.7864213104
        H 0.597333457 1.6066837659 -7.8875907242
        H 0.679611233 4.0219553084 -7.444720368
        H -1.3549091409 5.3160323625 -6.8170100952
        H -3.919614268 5.2837735636 -6.4149944649
        H -6.0041856891 3.9054265542 -6.3685046202
        H -5.9539388661 1.5175984809 -6.9886625981
        H -7.598853678 -1.7608423553 -8.148837203799999
        H -8.6430324336 -1.4788592006 -10.4034071424
        H -7.376351861 -0.4808003889 -12.2746522104
```

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```
    H -5.1822456956 0.5984619047 -13.0969032753
    H -2.8771937878 1.3227485141 -12.5240563582
    H -1.9932606643 1.025104893 -10.2292724091
    N -3.2837377695 -0.664491859 -5.8465663222
    N -3.8524864579 1.4991142677 -7.2859856873
    N -3.7633918961 0.0903193296 -9.5053497157
    O -2.7251315757 -1.9232489398 -8.1021556012
    O -5.1457683284 -0.9727214768 -7.5493429881
    O -1.6598493293 0.1830791333 -7.798390479
    Al -3.4400529704 -0.2815131096 -7.6838832318
    C 1.8794971861 -3.2423985149 -3.7055748349
    C 1.4011660396 -2.2204931545 -4.5483930567
    C 0.8274160672999999 -1.0717826595 -3.9973668319
    C 0.746983485 -0.9752989758 -2.5423512135
    C 1.2665725664 -2.0129450542 -1.7049850454
    C 1.8271673309 -3.1412429717 -2.2998034997
    C 0.2762842971 -0.0297851274 -4.7420249828
    C -0.3267411113 1.0480718286 -4.0713454755
    C -0.3857680483 1.0728768536 -2.6636208351
    C 2.7644548613 0.9617998245 4.0521806593
    C 1.7439042145 0.0941090718 3.642059507
    C 1.3996414133 0.0669834211 2.2243753192
    C 1.0246834424 -0.7518007473 4.4897696339
    C -0.0253912619 -1.5240836801 3.961651508
    C 2.1676852503 0.794508034 1.2632486424
    C -2.3492859035 -0.5066719029 0.0806199723
    C -3.6744350901 -0.9392987641 0.0975336336
    C -4.7079127213 -0.020618815 0.3771973267
    C -4.4394638678 1.3371214498 0.6598958034
    C -3.1321189427 1.8219755043 0.5974315921
    C -2.0642722189 0.8693320226 0.3369119755
    C -2.7721209304 3.1610944822 0.7475851159
    C -1.4144957483 3.5219566869 0.6650177522
    C -0.4278377382 2.5489518242 0.4378243493
    C -0.3586369631 -1.4383319818 2.594888547
    C 3.2148559649 1.5999922827 1.7099111367
    C 3.4831465281 1.7092530557 3.0921846639
    H 2.2914114296 -4.1270622441 -4.158196487
    H 1.4543744769 -2.3475597919 -5.6229273984
    H 2.1966824143 -3.9437878589 -1.6810430419
    H 0.2883188796 -0.0646089869 -5.8230215972
    H -0.771892801 1.8523200353 -4.6417846164
    H -0.8774279828 1.9026533162 -2.1773984742
    H -3.9039055772 -1.9755591047 -0.1103067723
    H -5.732849804 -0.3710752989 0.3801561174
    H -5.2465403092 2.0113655771 0.9117513642
    H -3.5314949482 3.913350028 0.8950780632000001
    H -1.1119084494 4.5521879649 0.766667497
    H 0.6089086397 2.8551248498 0.358222646
    H 3.7881190229 2.1752551515 0.9982104892
    H 4.2640858083 2.381823329 3.4210694665
    H 3.0118117692 1.0528196574 5.1034300383
    H 1.2574079525 -0.8033825665 5.5443969166
    H -0.5927560352 -2.1754873153 4.6136376386
    H -1.1882703275 -2.0188179907 2.2151671074
    N 0.1569126804 0.0531352413 -1.9348483597
    N -0.7873119119999999 1.2424726569 0.2843969979
```

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```
        N 0.3730124556 -0.6434632843 1.7615285374
        O 1.1442860805 -1.8491466636 -0.405855127
        O 1.7961887073 0.6871617202 0.0034904085
        O -1.3220788059 -1.2813762571 -0.1866654751
        Al 0.2305308242 -0.2883029309 -0.0814854552
    End
End

Engine DFTB
   Model GFN1-xTB
   Properties
      Fragments
         TransferIntegrals
         File Alq3_1.results/dftb.rkf
         File Alq3_2.results/dftb.rkf
      End
   End
EndEngine
eor
```

10.11 Analysis

10.11.1 Example: Bond orders

Download SP_bondorders.run

```
#!/bin/sh

AMS_JOBNAME=benzene $AMSBIN/ams << EOF

Task SinglePoint

System
    Atoms
         C      -1.398802120000       0.000000000000       0.000000000000
         C       1.398802120000       0.000000000000       0.000000000000
         C      -0.699401060000      -1.211398170000       0.000000000000
         C      -0.699401060000       1.211398170000       0.000000000000
         C       0.699401060000       1.211398170000       0.000000000000
         C       0.699401060000      -1.211398170000       0.000000000000
         H      -2.490090980000       0.000000000000       0.000000000000
         H      -1.245045490000       2.156482040000       0.000000000000
         H       1.245045490000       2.156482040000       0.000000000000
         H       2.490090980000       0.000000000000       0.000000000000
         H       1.245045490000      -2.156482040000       0.000000000000
         H      -1.245045490000      -2.156482040000       0.000000000000
    End
End

Properties
    BondOrders true
End
```

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```
Engine DFTB
   Model SCC-DFTB
   ResourcesDir DFTB.org/mio-1-1
EndEngine

EOF

AMS_JOBNAME=carotene $AMSBIN/ams << EOF

Task SinglePoint

System
    Atoms
      C      -1.67096000       1.41980000      -1.15887000
      C      -0.38686000       2.25210000      -1.41391000
      C      -1.74087000       0.49471000      -0.15347000
      C      -2.78739000       1.72912000      -2.05465000
      C       0.64868000       2.05301000      -0.28395000
      C       0.23104000       1.84552000      -2.77135000
      C      -0.70560000       3.76543000      -1.46182000
      C      -0.54745000       0.11313000       0.69574000
      C      -3.00351000      -0.21803000       0.26657000
      C      -3.76926000       0.89738000      -2.51350000
      C       0.78914000       0.59489000       0.13981000
      C      -4.86625000       1.29159000      -3.36539000
      C      -5.83916000       0.35729000      -3.66241000
      C      -4.93554000       2.71910000      -3.84917000
      C      -7.05227000       0.56749000      -4.37867000
      C      -8.05019000      -0.37384000      -4.49171000
      C      -9.34557000      -0.15733000      -5.06205000
      C     -10.30909000      -1.14399000      -4.91514000
      C      -9.64286000       1.17054000      -5.71730000
      C     -11.69180000      -1.05048000      -5.21459000
      C     -12.61955000      -2.01468000      -4.87148000
      C     -14.02165000      -1.83518000      -4.98190000
      C     -15.01934000      -2.67078000      -4.50243000
      C     -16.37196000      -2.20132000      -4.51598000
      C     -14.71829000      -4.01459000      -3.88235000
      C     -17.44392000      -2.81539000      -3.90884000
      C     -18.74098000      -2.23505000      -3.81068000
      C     -19.81891000      -2.70482000      -3.08600000
      C     -21.01079000      -1.89278000      -3.01886000
      C     -19.77834000      -4.00300000      -2.31809000
      C     -22.11699000      -2.17469000      -2.26831000
      C     -23.34229000      -1.38813000      -2.11260000
      C     -24.62364000      -2.22792000      -1.86832000
      C     -23.37421000      -0.02091000      -2.14864000
      C     -25.81771000      -1.33236000      -1.46707000
      C     -24.97031000      -3.02505000      -3.14664000
      C     -24.41619000      -3.23491000      -0.71197000
      C     -24.66206000       0.77221000      -2.09033000
      C     -22.15090000       0.86196000      -2.20093000
      C     -25.91751000      -0.06612000      -2.31089000
      H      -2.80910000       2.75370000      -2.43250000
      H       1.61418000       2.46808000      -0.61595000
      H       0.33480000       2.64516000       0.59383000
      H      -0.50118000       1.95999000      -3.58430000
```

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```
        H       1.10267000       2.47962000      -3.00160000
        H       0.55846000       0.79551000      -2.76878000
        H      -1.27083000       4.08204000      -0.57268000
        H       0.23706000       4.33391000      -1.48690000
        H      -1.27659000       4.05053000      -2.35573000
        H      -0.69913000       0.51646000       1.71643000
        H      -0.54631000      -0.98424000       0.82135000
        H      -3.05490000      -1.23815000      -0.15105000
        H      -3.01240000      -0.33500000       1.36235000
        H      -3.91214000       0.31400000      -0.03789000
        H      -3.75416000      -0.15646000      -2.22797000
        H       1.07957000      -0.02480000      -0.72369000
        H       1.58320000       0.48035000       0.89321000
        H      -5.69282000      -0.64720000      -3.25046000
        H      -4.00625000       2.99962000      -4.36844000
        H      -5.76674000       2.88684000      -4.54145000
        H      -5.05424000       3.41602000      -3.00441000
        H      -7.22923000       1.55534000      -4.80743000
        H      -7.87841000      -1.35648000      -4.03966000
        H      -9.98472000      -2.07170000      -4.43134000
        H      -8.86494000       1.42343000      -6.45273000
        H     -10.60514000       1.16993000      -6.23979000
        H      -9.66280000       1.98327000      -4.97344000
        H     -12.06891000      -0.12920000      -5.66646000
        H     -12.24343000      -2.93190000      -4.41065000
        H     -14.35090000      -0.88585000      -5.41809000
        H     -16.54169000      -1.22776000      -4.98799000
        H     -15.37918000      -4.79019000      -4.29660000
        H     -13.68496000      -4.33124000      -4.05827000
        H     -14.88466000      -3.99412000      -2.79324000
        H     -17.27327000      -3.77423000      -3.41639000
        H     -18.87740000      -1.27545000      -4.32124000
        H     -20.99304000      -0.98523000      -3.62576000
        H     -19.85755000      -3.82238000      -1.23433000
        H     -20.62535000      -4.64779000      -2.59868000
        H     -18.85754000      -4.56711000      -2.49752000
        H     -22.10976000      -3.13142000      -1.74142000
        H     -26.74148000      -1.93003000      -1.53138000
        H     -25.70276000      -1.04055000      -0.40816000
        H     -24.12173000      -3.65146000      -3.45913000
        H     -25.83556000      -3.68339000      -2.96560000
        H     -25.21348000      -2.35763000      -3.98638000
        H     -24.03490000      -2.73308000       0.18974000
        H     -25.38111000      -3.70177000      -0.46026000
        H     -23.72534000      -4.04703000      -0.97564000
        H     -24.71649000       1.28228000      -1.10831000
        H     -24.60164000       1.58888000      -2.83152000
        H     -21.95198000       1.22417000      -3.22414000
        H     -22.31941000       1.76042000      -1.58543000
        H     -21.24680000       0.35543000      -1.84399000
        H     -26.00957000      -0.32720000      -3.37736000
        H     -26.81690000       0.51083000      -2.04725000
    End
End

Properties
    BondOrders true
```

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```
End

Engine DFTB
   Model SCC-DFTB
   ResourcesDir DFTB.org/mio-1-1
EndEngine

EOF

for spin in no yes
do

AMS_JOBNAME=N2.spin=$spin $AMSBIN/ams << EOF
Task SinglePoint

System
   Atoms
      N 0.0 0.0 0.0
      N 0.0 0.0 1.098
   End
End

Properties
  BondOrders true
End

Engine DFTB
   Model SCC-DFTB
   ResourcesDir DFTB.org/mio-1-1
   SCC Unrestricted=$spin
EndEngine

EOF
done

AMS_JOBNAME=O2 $AMSBIN/ams << EOF
Task SinglePoint

System
   Atoms
      O 0.0 0.0 0.0
      O 0.0 0.0 1.208
   End
End

Properties
  BondOrders true
End

Engine DFTB
   Model SCC-DFTB
   ResourcesDir DFTB.org/mio-1-1
   SCC Unrestricted=yes
EndEngine

EOF
```

10.11.2 Example: Fragment Orbital analysis

Download Fragment_Orbitals.run

```
#!/bin/sh

# An illustration of the fragment orbital analysis with DFTB

# The molecular system GC is build from 2 fragment: Guanine and Cytosine.
# An atomic Mulliken population is calculated for these two molecules.
# For these molecules the fragment orbitals are atomic.
# Next the full GC system is calculated and the fragment orbital analysis is
# calculated based on Guanine and Cytosine orbitals.

AMS_JOBNAME=Guanine  $AMSBIN/ams<<eor
System
  Atoms
     N      -2.58004483      -0.57534828       0.00000000
     O       1.37445517       1.80325172       0.00000000
     N      -0.64954483       0.71205172       0.00000000
     C      -2.02304483       0.65505172       0.00000000
     N      -2.79744483       1.73455172       0.00000000
     C      -2.08284483       2.87605172       0.00000000
     C      -0.68984483       3.05555172       0.00000000
     C       0.12945517       1.88485172       0.00000000
     N      -2.59534483       4.15055172       0.00000000
     C      -1.51504483       5.02095172       0.00000000
     N      -0.36064483       4.40135172       0.00000000
     H      -2.02304483      -1.44274828       0.00000000
     H      -3.58904483      -0.61664828       0.00000000
     H      -0.11144483      -0.18554828       0.00000000
     H      -3.58074483       4.38415172       0.00000000
     H      -1.65544483       6.09615172       0.00000000
  End
end

Task SinglePoint

Engine DFTB
   Model SCC-DFTB
   ResourcesDir DFTB.org/mio-1-1
   Properties
      Fragments
      End
   End
EndEngine
eor

AMS_JOBNAME=Cytosine $AMSBIN/ams<<eor
System
  Atoms
     O      -1.04004483      -2.99644828       0.00000000
     N       2.81855517      -0.50844828       0.00000000
     N       0.88085517      -1.73164828       0.00000000
     C       3.00115517      -2.92044828       0.00000000
     C       0.19685517      -2.90274828       0.00000000
     N       0.95725517      -4.09354828       0.00000000
     C       2.31775517      -4.09434828       0.00000000
```

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```
      C       2.22455517      -1.70554828       0.00000000
      H       4.08765517      -2.90304828       0.00000000
      H       0.42435517      -4.95734827       0.00000000
      H       2.80565517      -5.06634827       0.00000000
      H       2.24745517       0.37825172       0.00000000
      H       3.82755517      -0.45254828       0.00000000
  End
end

Task SinglePoint

Engine DFTB
   Model SCC-DFTB
   ResourcesDir DFTB.org/mio-1-1
   Properties
      Fragments
      End
   End
EndEngine
eor

AMS_JOBNAME=GC $AMSBIN/ams<<eor
System
  Atoms
      N      -2.58004483      -0.57534828       0.00000000
      O       1.37445517       1.80325172       0.00000000
      N      -0.64954483       0.71205172       0.00000000
      C      -2.02304483       0.65505172       0.00000000
      N      -2.79744483       1.73455172       0.00000000
      C      -2.08284483       2.87605172       0.00000000
      C      -0.68984483       3.05555172       0.00000000
      C       0.12945517       1.88485172       0.00000000
      N      -2.59534483       4.15055172       0.00000000
      C      -1.51504483       5.02095172       0.00000000
      N      -0.36064483       4.40135172       0.00000000
      H      -2.02304483      -1.44274828       0.00000000
      H      -3.58904483      -0.61664828       0.00000000
      H      -0.11144483      -0.18554828       0.00000000
      H      -3.58074483       4.38415172       0.00000000
      H      -1.65544483       6.09615172       0.00000000
      O      -1.04004483      -2.99644828       0.00000000
      N       2.81855517      -0.50844828       0.00000000
      N       0.88085517      -1.73164828       0.00000000
      C       3.00115517      -2.92044828       0.00000000
      C       0.19685517      -2.90274828       0.00000000
      N       0.95725517      -4.09354828       0.00000000
      C       2.31775517      -4.09434828       0.00000000
      C       2.22455517      -1.70554828       0.00000000
      H       4.08765517      -2.90304828       0.00000000
      H       0.42435517      -4.95734827       0.00000000
      H       2.80565517      -5.06634827       0.00000000
      H       2.24745517       0.37825172       0.00000000
      H       3.82755517      -0.45254828       0.00000000
  End
end

Task SinglePoint
```

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```
Engine DFTB
   Model SCC-DFTB
   ResourcesDir DFTB.org/mio-1-1
   Properties
      Fragments
         File Guanine.results/dftb.rkf
         File Cytosine.results/dftb.rkf
      End
   End
EndEngine
eor
```

10.11.3 Example: 3D fields on a grid, QTAIM

Download DFTB_NAO.run

```
#! /bin/sh

# just to make sure that the properties are non zero at the first integration point
extend="-4.0"

export AMS_JOBNAME=Methane

$AMSBIN/ams << eor

Task SinglePoint

System
    Atoms
      C       0.000000000000       0.000000000000       0.000000000000
      H       0.863426938600       0.544775641100       0.352297349600
      H      -0.335313871500       0.422758012300      -0.935542767900
      H       0.264056533600      -1.036774276000      -0.147557605600
      H      -0.792169600700       0.069240623010       0.730803023900
    End
End

Engine DFTB
    ResourcesDir Demo
    Model DFTB0
EndEngine

eor

# cd Methane.results

$AMSBIN/nao << eor

Filename $AMS_JOBNAME.results/dftb.rkf

Grid
  Type Coarse
  ExtendX $extend
  ExtendY $extend
```

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```
  ExtendZ $extend
end

Fields
  rho
  rho(deformation)
  tau(valence)
  rho(deformation/fit)
  v(coulomb/atoms)
  v(coulomb/deformation)
  v(coulomb)
End

eor

echo ""
echo "Begin TOC of tape41 (Methane/props)"
$AMSBIN/pkf TAPE41
echo "End TOC of tape41 (Methane/props)"

rm TAPE41

# orbital plotting

$AMSBIN/nao << eor

Filename $AMS_JOBNAME.results/dftb.rkf

Grid
  Type Coarse
  ExtendX $extend
  ExtendY $extend
  ExtendZ $extend
end

Fields
  Orbitals 1
End

eor

echo ""
echo "Begin TOC of tape41 (Methane/orbitals)"
$AMSBIN/pkf TAPE41
echo "End TOC of tape41 (Methane/orbitals)"

rm TAPE41

# export to cube format

$AMSBIN/nao << eor

Filename $AMS_JOBNAME.results/dftb.rkf
ResultFilename CUBE

Grid
  Type Coarse
```

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```
  ExtendX $extend
  ExtendY $extend
  ExtendZ $extend
end

Fields
  rho
  rho(deformation)
  tau(valence)
  rho(deformation/fit)
  v(coulomb/atoms)
  v(coulomb/deformation)
  v(coulomb)
End

eor

echo ""
echo "Begin of cube file v(coulomb)"
head -n 12 v\(coulomb\).cube
echo "End of cube file v(coulomb)"

rm *.cube



# export single field on a .cube file

$AMSBIN/nao << eor

Filename $AMS_JOBNAME.results/dftb.rkf
ResultFilename CUBE

Grid
  Type Coarse
  ExtendX $extend
  ExtendY $extend
  ExtendZ $extend
end

Fields
  rho
End

eor

echo ""
echo "Begin of cube file"
head -n 12 rho.cube
echo "End of cube file"

rm rho.cube

# the order appears to be random
export NSCM=1

$AMSBIN/nao << eor
```

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```
Filename $AMS_JOBNAME.results/dftb.rkf

Grid
  Type Coarse
end

AIMCriticalPoints
  gridSpacing 0.2
End

eor

echo "kf file with QTAIM"

$AMSBIN/pkf $AMS_JOBNAME.results/dftb.rkf


# cd ..


echo "same test on periodic chain"

export AMS_JOBNAME=MethaneChain

$AMSBIN/ams << eor

Task SinglePoint

System
    Atoms [Angstrom]
        C 0.0 0.0 0.0
        H 1.079999998  0 0
        H -0.35604780   0                 1.019622459440336
        H -0.35604780   0.8830189521445  -0.50981122972017
        H -0.35604780  -0.8830189521445  -0.50981122972017
    End
    Lattice
        2.5 0.0 0.0
    End
End

Engine DFTB
   ResourcesDir Demo
   Model DFTB0
   UseSymmetry yes
   KSpace
     Type Symmetric
     Symmetric KInteg=3
   End
   Periodic
       BandStructure enabled=yes automatic=yes
   End
EndEngine

eor
```

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```
# cd MethaneChain.results

$AMSBIN/nao << eor

Filename $AMS_JOBNAME.results/dftb.rkf

Grid
  Type Coarse
  ExtendX $extend
  ExtendY $extend
  ExtendZ $extend
end

Fields
  rho
  rho(deformation)
  tau(valence)
  rho(deformation/fit)
  v(coulomb/atoms)
  v(coulomb/deformation)
  v(coulomb)
End

eor

echo "Begin TOC of tape41 (MethaneChain/props)"
$AMSBIN/pkf TAPE41
echo "End TOC of tape41 (MethaneChain/props)"

rm TAPE41

$AMSBIN/nao << eor

Filename $AMS_JOBNAME.results/dftb.rkf

Grid
  Type Coarse
  ExtendX $extend
  ExtendY $extend
  ExtendZ $extend
end

Fields
 Orbital band=1 kun=3
End

eor

echo "Begin TOC of tape41 (MethaneChain/orbitals)"
$AMSBIN/pkf TAPE41
echo "End TOC of tape41 (MethaneChain/orbitals)"

rm TAPE41

# the order appears to be random
export NSCM=1
```

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```
$AMSBIN/nao << eor

Filename $AMS_JOBNAME.results/dftb.rkf

Grid
  Type Coarse
end

AIMCriticalPoints
End

eor

echo "kf file with periodic QTAIM"
$AMSBIN/pkf $AMS_JOBNAME.results/dftb.rkf


cat << eor > coords.txt
1.0 0.0 0.0
0.2 0.4 0.0
eor

$AMSBIN/nao << eor

Filename $AMS_JOBNAME.results/dftb.rkf
ResultFilename result.txt

Grid
  Filename coords.txt
end

Fields
  v(coulomb)
End

eor

echo "Begin of result"
cat result.txt
echo "End of result"

echo "test on periodic chain with the gamma only method"

export AMS_JOBNAME=MethaneChainGamma

$AMSBIN/ams << eor

Task SinglePoint

System
    Atoms [Angstrom]
        C 0.0 0.0 0.0
        H 1.079999998  0 0
        H -0.35604780   0                 1.019622459440336
        H -0.35604780   0.8830189521445  -0.50981122972017
        H -0.35604780  -0.8830189521445  -0.50981122972017
    End
```

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```
    Lattice
        2.5 0.0 0.0
    End
End

Engine DFTB
   ResourcesDir Demo
   Model DFTB0
   KSpace Quality=GammaOnly
EndEngine

eor

# cd MethaneChainGamma.results

$AMSBIN/nao << eor

Filename $AMS_JOBNAME.results/dftb.rkf

Grid
  Type Coarse
  ExtendX $extend
  ExtendY $extend
  ExtendZ $extend
end

Fields
  rho
  rho(deformation)
  tau(valence)
  rho(deformation/fit)
  v(coulomb/atoms)
  v(coulomb/deformation)
  v(coulomb)
End

eor

echo ""
echo "Begin TOC of tape41 (MethaneChainGamma/props)"
$AMSBIN/pkf TAPE41
echo "End TOC of tape41 (MethaneChainGamma/props)"

rm TAPE41

# ------------- test with absolute path for AIM, which writes to the file ------------
↪------------

export AMS_JOBNAME=Methane.again

$AMSBIN/ams << eor

Task SinglePoint

System
    Atoms
```

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```
      C       0.000000000000       0.000000000000       0.000000000000
      H       0.863426938600       0.544775641100       0.352297349600
      H      -0.335313871500       0.422758012300      -0.935542767900
      H       0.264056533600      -1.036774276000      -0.147557605600
      H      -0.792169600700       0.069240623010       0.730803023900
    End
End

Engine DFTB
    ResourcesDir Demo
    Model DFTB0
EndEngine

eor

# the order appears to be random
export NSCM=1

base=$PWD
if test "$OS" = "Windows_NT"; then
 # ignore Windows line endings
 base=`pwd -W`
fi


$AMSBIN/nao << eor

Filename $base/$AMS_JOBNAME.results/dftb.rkf

Grid
  Type Coarse
end

AIMCriticalPoints
  gridSpacing 0.2
End

eor

echo "kf file with QTAIM"

$AMSBIN/pkf $AMS_JOBNAME.results/dftb.rkf
```

10.11.4 Example: Band structure with user-defined BZ path

Download Li_BZPlot.run

```
#! /bin/sh

# both the following runs follow the same path through the BZ

# first: automatic plot

AMS_JOBNAME=Li_auto $AMSBIN/ams << eor

```

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```
Task SinglePoint

System
    Atoms
        Li 0.0 0.0 0.0
    End
    Lattice
        -1.745 1.745 1.745
        1.745 -1.745 1.745
        1.745 1.745 -1.745
    End
End

Engine DFTB
   ResourcesDir Demo
   Model DFTB0
   KSpace
     Type Symmetric
     Symmetric KInteg=5
   End
   Periodic
       BandStructure enabled=yes automatic=yes fatbands=no
   End
EndEngine

eor

# second: user defined path

AMS_JOBNAME=Li_user $AMSBIN/ams << eor

Task SinglePoint

System
    Atoms
        Li 0.0 0.0 0.0
    End
    Lattice
        -1.745 1.745 1.745
        1.745 -1.745 1.745
        1.745 1.745 -1.745
    End
End

Engine DFTB
   ResourcesDir Demo
   Model DFTB0
   KSpace
     Type Symmetric
     Symmetric KInteg=5
   End
   Periodic
       BandStructure enabled=yes automatic=no fatbands=no
       BZPath
           Path
               0.0  0.0  0.0
               0.5 -0.5  0.5
```

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```
                0.0  0.0  0.5
                0.0  0.0  0.0
                0.25 0.25 0.25
                0.5 -0.5  0.5
            End
            Path
                0.25 0.25 0.25
                0.0  0.0  0.5
            End
        End
    End
EndEngine

eor

# The band structure is best visualized using the BandStructure GUI module.

echo 'Extract the band_curves section from the rkf files:'
$AMSBIN/dmpkf Li_auto.results/dftb.rkf 'band_curves'
$AMSBIN/dmpkf Li_user.results/dftb.rkf 'band_curves'
echo "Done"
```

10.11.5 Example: NBO analyse H2O

Download SP_DFTBNBO.run

```
#!/bin/sh

AMS_JOBNAME=water $AMSBIN/ams << EOF

Task SinglePoint

System
   Atoms [Bohr]
      O    0.0000000000    0.0000000000    0.0000000000
      H    1.7007535125    0.0000000000    0.0000000000
      H   -0.2953327481    1.6749152451    0.0000000000
   End
End

Properties
   BondOrders yes
End

Engine DFTB
   Model SCC-DFTB
   ResourcesDir DFTB.org/mio-1-1
   Properties
      NBOInput yes
   End
EndEngine

EOF

echo " "
```

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```
echo " "
echo "Contents of water.results/dftb-nboInput.FILE47 ="
echo " "
cat water.results/dftb-nboInput.FILE47

$AMSBIN/gennbo6 water.results/dftb-nboInput.FILE47

echo " "
echo " "
echo "Contents of dftbnbo.37 = "
echo " "
cat dftbnbo.37

echo " "
echo " "
echo "Contents of dftbnbo.39 ="
echo " "
cat dftbnbo.39

echo " "
echo " "
echo "Contents of dftbnbo.49 ="
echo " "
cat dftbnbo.49
```

CHAPTER

ELEVEN

KEYWORDS

11.1 Links to manual entries

conductance:

dftb:

11.2 Summary of all keywords

11.2.1 Engine DFTB

`DispersionCorrection`

Type
Multiple Choice

Default value
None

Options
[None, Auto, UFF, ULG, D2, D3-BJ, D4]

GUI name
Dispersion

Description
This key is used to specify an empirical dispersion model. Please refer to the DFTB documentation for details on the different methods.

By default no dispersion correction will be applied. Setting this to auto applies the dispersion correction recommended in the DFTB parameter set's metainfo file. Note that the D3-BJ dispersion correction is enabled by default when using the GFN1-xTB model Hamiltonian, but can be disabled manually by setting this keyword to None.

KSpace

Type
Block

Description
Options for the k-space integration (i.e. the grid used to sample the Brillouin zone)

Analytical

Type
Bool

Default value
Yes

Description
For analytical integration the BZ is split into simplices, whereover the bands are interpolated, ater which the integrals can be performed analytically.

Alternatively, the set of eigenvalues in the discrete set of k-points are just handled as distinct molecular orbitals.

Using analytical=no can improve SCF convergence in combination with smearing/temperature.

Quality

Type
Multiple Choice

Default value
Auto

Options
[Auto, GammaOnly, Basic, Normal, Good, VeryGood, Excellent]

GUI name
K-space

Description
Select the quality of the K-space grid used to sample the Brillouin Zone. If ‘Auto’, the quality defined in the ‘NumericalQuality’ will be used. If ‘GammaOnly’, only one point (the gamma point) will be used.

The actual number of K points generated depends on this option and on the size of the unit cell. The larger the real space cell, the fewer K points will be generated.

The CPU-time and accuracy strongly depend on this option.

Regular

Type
Block

Description
Options for the regular k-space integration grid.

NumberOfPoints

Type
Integer List

Description
Use a regular grid with the specified number of k-points along each reciprocal lattice vector.

For 1D periodic systems you should specify only one number, for 2D systems two numbers, and for 3D systems three numbers.

`Symmetric`

Type
Block

Description
Options for the symmetric k-space integration grid.

`KInteg`

Type
Integer

GUI name
Accuracy

Description
Specify the accuracy for the Symmetric method.

1: absolutely minimal (only the G-point is used)

2: linear tetrahedron method, coarsest spacing

3: quadratic tetrahedron method, coarsest spacing

4,6,… (even): linear tetrahedron method

5,7…. (odd): quadratic method

The tetrahedron method is usually by far inferior.

`Type`

Type
Multiple Choice

Default value
Regular

Options
[Regular, Symmetric]

GUI name
K-space grid type

Description
The type of k-space integration grid used to sample the Brillouin zone (BZ) used.

'Regular': simple regular grid.

'Symmetric': symmetric grid for the irreducible wedge of the first BZ (useful when high-symmetry points in the BZ are needed to capture the correct physics of the system, graphene being a notable example).

`Model`

Type
Multiple Choice

Default value
GFN1-xTB

Options
[DFTB, SCC-DFTB, DFTB3, GFN1-xTB, NonSCC-GFN1-xTB]

Description
Selects the Hamiltonian used in the DFTB calculation:

- DFTB/DFTB0/DFTB1 for classic DFTB without a self-consistent charge cycle
- SCC-DFTB/DFTB2 with a self-consistency loop for the Mulliken charges
- DFTB3 for additional third-order contributions.
- GFN1-xTB for Grimme's extended tight-binding model in the GFN1 version.
- NonSCC-GFN1-xTB for a less accurate but faster version of GFN1-xTB without a self-consistency cycle

The choice has to be supported by the selected parameter set.

`Occupation`

Type
Block

Description
Configures the details of how the molecular orbitals are occupied with electrons.

`KT`

Type
Float

Unit
Hartree

Description
(KT) Boltzmann constant times temperature, used for electronic temperature with strategy is auto.

The default value is the default value for Temperature*3.166815423e-6.

This key and Temperature are mutually exclusive.

`NumBoltz`

Type
Integer

Default value
10

Description
The electronic temperature is done with a Riemann Stieltjes numerical integration, between zero and one occupation. This defines the number of points to be used.

`Strategy`

Type
Multiple Choice

Default value
Auto

Options
[Auto, Aufbau, Fermi]

GUI name
Occupation

Description
This optional key allows to specify the fill strategy to use for the molecular orbitals.

Can either be 'Aufbau' for simply filling the energetically lowest orbitals, or 'Fermi' for a smeared out Fermi-Dirac occupation. By default the occupation strategy is determined automatically, based on the other settings (such as the number of unpaired electrons).

`Temperature`

Type
Float

Default value
300.0

Unit
Kelvin

GUI name
Fermi temperature

Description
The Fermi temperature used for the Fermi-Dirac distribution. Ignored in case of aufbau occupations.

`Periodic`

Type
Block

Description
Block that sets various details of the calculation only relevant for periodic systems.

`BZPath`

Type
Block

Description
If [BandStructure%Automatic] is disabled, DFTB will compute the band structure for the user-defined path in the [BZPath] block. You should define the vertices of your path in fractional coordinates (with respect to the reciprocal lattice vectors) in the [Path] sub-block. If you want to make a jump in your path, you need to specify a new [Path] sub-block.

`Path`

Type
Non-standard block

Recurring
True

Description
A section of a k space path.

`BandStructure`

Type
Block

Description
Options for band structure plotting. This has no effect on the calculated energy. [Warning: The band structure is only computed in case of k-space sampling, i.e. it is not computed for Gamma-only calculations (see: Periodic%KSpace).]

`Automatic`

Type
Bool

Default value
Yes

GUI name
Automatic generate path

Description
Generate and use the standard path through the Brillouin zone.

If not, use the user defined path (set via Custom path in the GUI, or with the Periodic%BZPath keyword in the run script).

`DeltaK`

Type
Float

Default value
0.1

Unit
1/Bohr

GUI name
Interpolation delta-K

Description
Step size in reciprocal space for band structure interpolation. Using a smaller number will produce smoother band curves at an increased computational time.

`Enabled`

Type
Bool

Default value
Yes

GUI name
Calculate band structure

Description
Whether or not to calculate the band structure.

`FatBands`

Type
Bool

Default value
Yes

GUI name
Calculate fatbands

Description
Control the computation of the fat bands (only when the bandstructure is calculated).

The fat bands are the periodic equivalent of the Mulliken population analysis. The definition of the fat bands can be found in the Band Documentation.

KPathFinderConvention

Type
Multiple Choice

Default value
Setyawan-Curtarolo

Options
[Setyawan-Curtarolo, Hinuma]

Description
This option determines how the path through the Brillouin zone is generated when using the automatic k-point mode.

Available options:

- `Setyawan-Curtarolo` (default for 1D and 2D lattices): Uses our built-in KPath program to find a path through high-symmetry points based on the method by Setyawan and Curtarolo (https://doi.org/10.1016/j.commatsci.2010.05.010). For 2D lattices, the path is derived from the intersection of the 3D Brillouin zone with a plane. For 1D lattices, the path is simply Gamma-Z.
- `Hinuma`: Uses the external SeeKPath utility to generate the k-path (https://github.com/giovannipizzi/seekpath and https://doi.org/10.1016/j.commatsci.2016.10.015).

UseSymmetry

Type
Bool

Default value
Yes

Description
If set, only the irreducible wedge of the Wigner-Seitz cell is sampled. If not, the whole (inversion-unique) Wigner-Seitz cell is sampled. Only available for Setyawan and Curtarolo convention (see `KPathFinderConvention`).

DOS

Type
Block

Description
The subkeys of [DOS] allow to customize the calculation of the density of states.

EMax

Type
Float

Default value
0.75

Unit
Hartree

Description
Upper end of the energy interval in which the density of states is calculated.

`EMin`

Type
Float

Default value
-0.75

Unit
Hartree

Description
Lower end of the energy interval in which the density of states is calculated.

`Enabled`

Type
Bool

Default value
Yes

GUI name
Calculate DOS

Description
Whether or not to calculate the DOS. Note that the DOS will always be calculated when also the band structure is calculated.

`NSteps`

Type
Integer

Default value
300

Description
The number of energy intervals between [EMin] and [EMax] for which the density of states is calculated.

`EffectiveMass`

Type
Block

Description
In a semi-conductor, the mobility of electrons and holes is related to the curvature of the bands at the top of the valence band and the bottom of the conduction band.

With the effective mass option, this curvature is obtained by numerical differentiation.

The estimation is done with the specified step size, and twice the specified step size, and both results are printed to give a hint on the accuracy. By far the most convenient way to use this key is without specifying any options.

`Enabled`

Type
Bool

Default value
No

GUI name
Effective mass

Description
In a semi-conductor, the mobility of electrons and holes is related to the curvature of the bands at the top of the valence band and the bottom of the conduction band.

With the effective mass option, this curvature is obtained by numerical differentiation.

The estimation is done with the specified step size, and twice the specified step size, and both results are printed to give a hint on the accuracy. By far the most convenient way to use this key is without specifying any options.

`KPointCoord`

Type
Float List

Unit
1/Bohr

Recurring
True

GUI name
At K-point

Description
Coordinate of the k-points for which you would like to compute the effective mass.

`NumAbove`

Type
Integer

Default value
1

GUI name
Include N bands above

Description
Number of bands to take into account above the Fermi level.

`NumBelow`

Type
Integer

Default value
1

GUI name
Include N bands below

Description
Number of bands to take into account below the Fermi level.

`StepSize`

Type
Float

Default value
0.001

Description
Size of the step taken in reciprocal space to perform the numerical differentiation

`UseBandStructureInfoFromPath`

Type
Bool

Default value
Yes

Description
The (automatic) location of the HOMO and LUMO can be determined via band interpolation, or from the path as used by the BandStructure feature. The latter works better when they are located on the path. See also comments in the BandStructure block. To reproduce results from before ams2025 set to no.

`Properties`

Type
Block

Description
DFTB can calculate various properties of the simulated system. This block configures which properties will be calculated.

`Excitations`

Type
Block

Description
Contains all options related to the calculation of excited states, either as simple single orbitals transitions or from a TD-DFTB calculation.

`SingleOrbTrans`

Type
Block

Description
The simplest approximation to the true excitations are the single orbital transitions (sometimes called Kohn-Sham transitions), that is transitions where a single electron is excited from an occupied Kohn-Sham orbital into a virtual orbital. The calculation of these transitions is configured in this section. Note that the SingleOrbTrans section is optional even though the single orbital transitions are also needed for TD-DFTB calculations. If the section is not present all single orbital transitions will still be calculated and used in a subsequent TD-DFTB calculation, but no output will be produced.

`Enabled`

Type
Bool

Default value
No

GUI name
Single orbital transisitions: Calculate

Description
Calculate the single orbital transitions.

`Filter`

Type
Block

Description
This section allows to remove single orbital transitions based on certain criteria. All filters are disabled by default.

`OSMin`

Type
Float

GUI name
Minimum oscillator strength

Description
Removes single orbital transitions with an oscillator strength smaller than this threshold.

A typical value to start (if used at all) would be 1.0e-3.

`dEMax`

Type
Float

Unit
Hartree

Description
Removes single orbital transitions with an orbital energy difference larger than this threshold.

`dEMin`

Type
Float

Unit
Hartree

Description
Removes single orbital transitions with an orbital energy difference smaller than this threshold.

`PrintLowest`

Type
Integer

Default value
10

Description
The number of single orbital transitions that are printed to the screen and written to disk.

If not a TD-DFTB calculation, the default is to print the 10 lowest single orbital transitions.

In case of a TD-DFTB calculation it is assumed that the single orbital transitions are only used as an input for TD-DFTB and nothing will be printed unless PrintLowest is specified explicitly.

`TDDFTB`

Type
Block

Description
Calculations with time-dependent DFTB can be configured in the TDDFTB section and should in general give better results than the raw single orbital transitions. TD-DFTB calculates the excitations in the basis of the single orbital transitions, whose calculation is configured in the SingleOrbTrans section. Using a filter in SingleOrbTrans can therefore be used to reduce the size of the basis for TD-DFTB. One possible application of this is to accelerate the calculation of electronic absorption spectra by removing single orbital transitions with small oscillator strengths from the basis. Note that the entire TDDFTB section is optional. If no TDDFTB section is found, the behavior depends on the existence of the SingleOrbTrans section: If no SingleOrbTrans section is found (the Excitations section is completely empty then) a TD-DFTB calculation with default parameters will be performed. If only the SingleOrbTrans section is present no TD-DFTB calculation will be done.

`Calc`

Type
Multiple Choice

Default value
None

Options
[None, Singlet, Triplet]

GUI name
Type of excitations

Description
Specifies the multiplicity of the excitations to be calculated.

`DavidsonConfig`

Type
Block

Description
This section contains a number of keywords that can be used to override various internals of the Davidson eigensolver. The default values should generally be fine.

`ATCharges`

Type
Multiple Choice

Default value
Precalc

Options
[Precalc, OnTheFly]

GUI name
Transition charges

Description
Select whether the atomic transition charges are precalculated in advance or reevaluated during the iterations of the Davidson solver.

Precalculating the charges will improve the performance, but requires additional storage.

The default is to precalculate the atomic transition charges, but the precalculation may be disabled if not not enough memory is available.

`SafetyMargin`

Type
Integer

Default value
4

Description
The number of eigenvectors the Davidson method will calculate in addition to the ones requested by the user. With the Davidson eigensolver it is generally a good idea to calculate a few more eigenvectors than needed, as depending on the initial guess for the eigenvectors it can happen that the found ones are not exactly the lowest ones. This problem is especially prominent if one wants to calculate only a small number of excitations for a symmetric molecule, where the initial guesses for the eigenvectors might have the wrong symmetry. Note that the additionally calculated excitations will neither be written to the result file nor be visible in the output.

`Tolerance`

Type
Float

Default value
1e-09

Description
Convergence criterion for the norm of the residual.

`Diagonalization`

Type
Multiple Choice

Default value
Auto

Options
[Auto, Davidson, Exact]

GUI name
Method

Description
Select the method used to solve the TD-DFTB eigenvalue equation.

The most straightforward procedure is a direct diagonalization of the matrix from which the excitation energies and oscillator strengths are obtained. Since the matrix grows quickly with system size (number of used single orbital transitions squared), this option is possible only for small molecules.

The alternative is the iterative Davidson method, which finds a few of the lowest excitations within an error tolerance without ever storing the full matrix.

The default is to make this decision automatically based on the system size and the requested number of excitations.

`Lowest`

Type
Integer

Default value
10

GUI name
Number of excitations

Description
Specifies the number of excitations that are calculated.

Note that in case of the exact diagonalization all excitations are calculated, but only the lowest ones are printed to screen and written to the output file.

Also note that if limited both by number and by energy, (lowest and upto), DFTB will always use whatever results in the smaller number of calculated excitations.

`Print`

Type
String

Description
Specifies whether to print details on the contribution of the individual single orbital transitions to the calculated excitations.

`ScaleKernel`

Type
Float

Default value
1.0

Unit
None

Description
Set the scaling parameter of the response kernel.

A scaling approach can be used to identify plasmons in molecules. While single-particle excitations are only slightly affected by scaling of the response kernel, plasmonic excitations are sensitive to variations in the scaling parameter. Default no scaling is used (scaling parameter = 1.0)

`UpTo`

Type
Float

Unit
Hartree

GUI name
Excitations up to

Description
Set the maximum excitation energy.

Attempts to calculate all excitations up to a given energy by calculating a number of excitations equal to the number of single orbital transitions in this window. This is only approximately correct, so one should always add some safety margin.

Note that if limited both by number and by energy, (lowest and upto), DFTB will always use whatever results in the smaller number of calculated excitations.

TDDFTBGradients

Type
Block

Description
This block configures the calculation of analytical gradients for the TD-DFTB excitation energies, which allows the optimization of excited state geometries and the calculation of vibrational frequencies in excited states (see J. Comput. Chem., 28: 2589-2601). If the gradients are calculated, they will automatically be used for geometry optimizations or vibrational frequency calculations, if the corresponding Task is selected and only 1 excitation is selected. Vibrationally resolved UV/Vis spectroscopy (Franck-Condon Factors) can be calculated in combination with the FCF program or using the Vibrational Analysis Tools in AMS. See the ADF documentation on Vibrationally resolved electronic spectra or the AMS documentation for the Vibrational Analysis Tools.

Eigenfollow

Type
Bool

Default value
No

GUI name
Follow initial excitation

Description
If this option is set, DFTB uses the transition density in atomic orbital basis to follow the initially selected excited state during a geometry optimization. This is useful if excited state potential energy surfaces cross each other and you want to follow the surface you started on.

Excitation

Type
Integer List

GUI name
Excitation number

Description
Select which excited states to calculate the gradients for.

Gradients can only be calculated for an excited states that has been calculated using TD-DFTB. Make sure that enough excitations are calculated.

Fragments

Type
Block

Description
Fragment files

Analysis

Type
Bool

Default value
Yes

GUI name
Fragment analysis

Description
Mulliken population analysis in terms of fragment orbitals.

`EMax`

Type
Float

Default value
0.25

Unit
Hartree

Description
Upper end of the energy interval for which the orbitals are analyzed.

`Emin`

Type
Float

Default value
-0.75

Unit
Hartree

Description
Lower end of the energy interval for which the orbitals are analyzed.

`File`

Type
String

Recurring
True

Description
Path (either absolute or relative) of fragment file

`TIDegeneracyThreshold`

Type
Float

Default value
0.1

Unit
eV

Description
If the orbital energy of the fragment MO is within this threshold with fragment HOMO or

LUMO energy, then this fragment MO is included in the calculation of the transfer integrals. Relevant in case there is (near) degeneracy.

`TransferIntegrals`

Type
Bool

Default value
No

GUI name
Charge transfer integrals

Description
Calculate the charge transfer integrals, spatial overlap integrals and site energies.

Charge transfer integrals can be used in models that calculate transport properties.

`NBOInput`

Type
Bool

Default value
No

Description
Whether or not an input file for the NBO program is written to disk as nboInput.FILE47. The input file follows the FILE47 format as described in the NBO6 manual available on nbo6.chem.wisc.edu. By default, only the calculation of the natural bond orbitals and the natural localized molecular orbitals is enabled, but the nboInput.FILE47 file can be edited by hand to enable other analysis models. Please refer to the NBO6 manual for details.

`RESPONSE`

Type
Block

Description
Linear response module to compute electric (complex) polarizabilities

`Frequencies`

Type
Float List

Default value
[0.0]

Unit
eV

Description
List of frequencies of incident light

`LifeTime`

Type
Float

Unit
Hartree

Description
Phenomenological damping

`Solver`

Type
Block

Description
Solver details for CPKS

`Algorithm`

Type
Multiple Choice

Default value
EXACT

Options
[EXACT, ITER]

Description
Choice of solver for CPKS

`Debug`

Type
Bool

Default value
No

Description
Print technical information from solver

`NumIt`

Type
Integer

Default value
100

Description
Maximum number of iterations (ITER solver only)

`RMSE`

Type
Float

Default value
1e-06

Description
Threshold for convergence (ITER solver only)

`QMFQ`

Type
Block

Description
Block input key for QM/(w)FQ(FMu).

AtomType

Type
Block

Recurring
True

Description
Definition of atomic types in MM environment

Alpha

Type
Float

Description
Polarizability of FQFMU atom

Area

Type
Float

Description
Effective charge-transfer area time between same-type wFQ atoms

Charge

Type
Float

Description
MM fixed charge (non-polarizable only)

Chi

Type
Float

Description
Electronegativity of FQ atom

Dfermi

Type
Float

Description
wFQ d parameter for Fermi damping

Efermi

Type
Float

Description
Fermi Energy of wFQ carbon-based structure

Eta

Type
Float

Description
Chemical Hardness of FQ atom

`R0`

Type
Float

Description
wFQ R0 parameter for Fermi damping

`Sfermi`

Type
Float

Description
wFQ s parameter for Fermi damping

`Sigma0`

Type
Float

Description
Static conductivity time of wFQ atom

`Symbol`

Type
String

Description
Symbol associated with atom type

`Tau`

Type
Float

Description
Scattering time of wFQ atom

`wFQFMuFile`

Type
String

Description
The absolute path to the wFQFMu interband polarizability file

`Coords`

Type
Non-standard block

Description
Coordinates and fragment information (FQ only)

`FDERESP`

Type
Bool

Default value
No

Description
In response calculations (TD), the polarization contribution of the FDE part is introduced at the FQ level [See F. Egidi et al. J. Chem. Phys. 2021, 154, 164107].

`Forcefield`

Type
Multiple Choice

Default value
FQ

Options
[FQ, FQFMU, wFQ, wFQ_RQ, wFQFmu, wFQFmu_RQRMU]

Description
Version of the FQ family of polarizable forcefields

`Frozen`

Type
Bool

Default value
No

Description
Expert option. Do not introduce polarization effect in response calculations.

`Kernel`

Type
Multiple Choice

Default value
OHNO

Options
[OHNO, COUL, GAUS]

Description
Expert option. KERNEL can be used to choose the functional form of the charge-charge interaction kernel between MM atoms. Recommended is to use the default OHNO. The COUL screening is the standard Coulomb interaction 1/r. The OHNO choice introduce the Ohno functional (see [K. Ohno, Theoret. Chim. Acta 2, 219 (1964)]), which depends on a parameter n that is set equal to 2. Finally, the GAUS screening models each FQ charge by means of a spherical Gaussian-type distribution, and the interaction kernel is obtained accordingly. For QM/FQFMU only GAUS SCREEN is implemented.

`LifeFrequency`

Type
Float

Default value
0.0

Description
Input frequency for calculating TDDFT/wFQ(Fmu) lifetimes

`LifeState`

Type
Integer

Default value
0

Description
Target excited state for state-specific TDDFT/wFQ(Fmu) lifetimes

`MolCharge`

Type
Float

Default value
0.0

Description
Total charge of each fragment (FQ only)

`NonEle`

Type
Multiple Choice

Default value
LJ

Options
[LJ, None]

Description
Whether to include non-electrostatic contributions to the energy. Default is the Lennard-Jones (LJ) model.

`QMSCREEN`

Type
Multiple Choice

Default value
GAUS

Options
[ERF, EXP, GAUS, NONE]

Description
Expert option. QMSCREEN can be used to choose the functional form of the charge-charge interaction kernel between MM atoms and the QM density. The screening types available are ERF (error function), EXP (exponential), GAUS (Gaussian), or NONE. The default is GAUS.

`QMSCREENFACTOR`

Type
Float

Default value
0.2

Description
Expert option. Sets the QM/MM interaction kernel screening length. Recommended is to use the default value 0.2 with the GAUS QM/MM screening function.

`ReadDynamicMatrix`

Type
String

Description
The absolute path to the decomposed wFQ(FMu) matrix file

`Repulsion`

Type
Block

Description
Configures various details of the repulsive potential.

`ResourcesDir`

Type
String

Description
The directory containing the parameter files. The path can be absolute or relative. Relative paths starting with ./ are considered relative to the directory in which the calculation is started, otherwise they are considered relative to $AMSRESOURCES/DFTB. This key is required for the Slater-Koster based DFTB models, but optional for xTB.

`SCC`

Type
Block

Description
This optional section configures various details of the self-consistent charge cycle. If the model Hamiltonian does not need a self-consistent solution (e.g. plain DFTB0), none of this information is used and the entire section will be ignored.

`AdaptiveMixing`

Type
Bool

Default value
Yes

Description
Change the mixing parameter based on the monitored energy. A significant increase of energy will strongly reduce the mixing. Then it will slowly grow back to the SCC%Mixing value.

`AlwaysClaimConvergence`

Type
Bool

Default value
No

Description
Even if the SCC does not converge, claim convergence.

`Converge`

Type
Block

Description
Controls the convergence criteria of the SCC cycle.

`Charge`

Type
Float

Default value
1e-08

GUI name
Charge convergence

Description
The maximum change in atomic charges between subsequent SCC iterations. If the charges change less, the SCC cycle is considered converged.

`Norm`

Type
Multiple Choice

Default value
L-Infinity

Options
[L2, L-Infinity]

Description
The LInfinity norm is the more stringent choice. The L2 norm is directly what is optimized by the DIIS procedure, it is scaled by the extra constant factor 2/sqrt(nAtoms).

`DIIS`

Type
Block

Description
Parameters influencing the DIIS self-consistency method

`Enabled`

Type
Bool

Default value
Yes

Description
If not enabled simple mixing without DIIS acceleration will be used.

`MaxSamples`

Type
Integer

Default value
20

Description
Specifies the maximum number of samples considered during the direct inversion of iteration of subspace (DIIS) extrapolation of the atomic charges during the SCC iterations. A smaller number of samples potentially leads to a more aggressive convergence acceleration, while a larger number often guarantees a more stable iteration. Due to often occurring linear dependencies within the set of sample vectors, the maximum number of samples is reached only in very rare cases.

`MaximumCoefficient`

Type
Float

Default value
10.0

Description
When the diis expansion coefficients exceed this threshold, the solution is rejected. The vector space is too crowded. The oldest vector is discarded, and the expansion is re-evaluated.

`MinSamples`

Type
Integer

Default value
-1

Description
When bigger than one, this affects the shrinking of the DIIS space on linear dependence. It will not reduce to a smaller space than MinSamples unless there is extreme dependency.

`MixingFactor`

Type
Float

Default value
0.15

Description
The parameter used to mix the DIIS linear combination of previously sampled atomic charge vectors with an analogous linear combination of charge vectors resulting from population analysis combination. It can assume real values between 0 and 1.

`HXDamping`

Type
Bool

Description
This option activates the DFTB3 style damping for H-X bonds. Note that this is always enabled if the DFTB%Model key is set to DFTB3. Not used with xTB.

`InheritMixFromPreviousResult`

Type
Bool

Default value
No

Description
For some run types, such as GeometryOptimization, a previous result is available. By using the charges from the previous geometry a better initial guess for the SCC procedure may be obtained.

Also the last mix factor from the previous result can be loaded, possibly speeding up the SCC.

`Iterations`

Type
Integer

Default value
500

Description
Allows to specify the maximum number of SCC iterations. The default should suffice for most standard calculations.

Convergence issues may arise due to the use of the Aufbau occupations for systems with small HOMO-LUMO gaps. In this case the use of a Fermi broadening strategy may improve convergence.

Choosing a smaller mixing parameter (see DFTB%SCC%Mixing) may also help with convergence issues: it often provides a more stable but slower way to converge the SCC cycle.

`Method`

Type
Multiple Choice

Default value
MultiStepper

Options
[DIIS, MultiStepper]

Description
The DIIS option is the old method. The MultiStepper is much more flexible and is controlled by the SCFMultiSolver block

`MinimumAdaptiveMixingFactor`

Type
Float

Default value
0.003

Description
In case of AdaptiveMixing the lower bound for the MixingFactor.

`MultiStepperPresetPath`

Type
String

Default value
DFTB/default2023.inc

Description
Name of file containing a SCFMultiStepper key block. This will be used if no Explicit SCF-MultiStepper block is in the input, and Method=MultiStepper.

If the path is not absolute, it is relative to $AMSHOME/data/presets/multi_stepper'

`OrbitalDependent`

Type
Bool

Description
Activates or disables orbital resolved calculations. If this key is absent the recommended settings from the parameter file's metainfo.

`SCFMultiStepper`

Type
Block

Description
To solve the self-consistent problem multiple steppers can be tried during stints using the ones that give the best progress.

`AlwaysChangeStepper`

Type
Bool

Default value
No

Description
When the progress is fine there is no reason to change the stepper. In practice this is always set to true, because also the Stepper%ExpectedSlope can be used to achieve similar behavior.

`ErrorGrowthAbortFactor`

Type
Float

Default value
1000.0

Description
Abort stint when the error grows too much, compared to the error at the start of the stint.

`FractionalStepFactor`

Type
Float

Default value
-1.0

Description
Multiply the step by this factor. If smaller than zero this is not used.

`MinStintCyclesForAbort`

Type
Integer

Default value
0

Description
Look at ErrorGrowthAbortFactor only when a number of steps has been completed since the start of the stint. A value of 0 means always.

`Stepper`

Type
Block

Recurring
True

Description
??

`AbortSlope`

Type
Float

Default value
100.0

Description
If the slope (at the end of a stint) is larger than this: abort the stepper

DIISStepper

Type
Block

Description
DIIS stepper

EDIISAlpha

Type
Float

Default value
0.01

Description
The extra energy vector is weighed by this factor. .

MaxCoefficient

Type
Float

Default value
20.0

Description
The largest allowed value of the expansion coefficients. If exceed the number of vectors is reduces until the criterion is met.

MaxVectors

Type
Integer

Default value
10

Description
Maximum number of previous densities to be used (size of the history).

MinVectors

Type
Integer

Default value
-1

Description
Try to prevent to make nVectors shrink below this value, by allowing for significantly larger coefficients.

Mix

Type
Float

Default value
0.2

Description
Also known as greed. It determines the amount of output density to be used. May be changed by the MixAdapter.

`ErrorGrowthAbortFactor`

Type
Float

Default value
-1.0

Description
Abort stint when the error grows too much, compared to the error at the start of the stint. Overrides global ErrorGrowthAbortFactor when set to a value > 0

`ExpectedSlope`

Type
Float

Default value
-100.0

Description
If the slope of the total SCF is better than this keep on going.

`FractionalStepFactor`

Type
Float

Default value
-1.0

Description
Multiply the step by this factor. If smaller than zero this is not used.

`MaxInitialError`

Type
Float

Description
Only use the stepper when error is smaller than this.

`MaxIterationNumber`

Type
Integer

Default value
-1

Description
Stepper will only be active for iterations smaller than this number. (Negative value means: Ignore this option)

`MaxStintNumber`

Type
Integer

Default value
-1

Description
Stepper will only be active for stints smaller than this number. (Negative value means: Ignore this option)

`MinInitialError`

Type
Float

Description
Only use the stepper when error is larger than this.

`MinIterationNumber`

Type
Integer

Default value
-1

Description
Stepper will only be active for iterations larger than this number.

`MinStintCyclesForAbort`

Type
Integer

Default value
0

Description
Look at ErrorGrowthAbortFactor only when a number of steps has been completed since the start of the stint. A value of 0 means always. Overrides global value.

`MinStintNumber`

Type
Integer

Default value
-1

Description
Stepper will only be active for stints larger than this number.

`MixAdapter`

Type
Block

Description
Generic mix adapter

`ErrorGrowthPanicFactor`

Type
Float

Default value
10.0

Description
When the error increases more than this factor, this mix is reduced a lot.

`GrowthFactor`

Type
Float

Default value
1.1

Description
When the mix is considered too low it is multiplied by this factor. Otherwise it is divided by it.

`MaxMix`

Type
Float

Default value
0.3

Description
Do not grow the mix above this value.

`MinMix`

Type
Float

Default value
0.1

Description
Do not shrink the mix below this value.

`NTrialMixFactors`

Type
Integer

Default value
3

Description
Only used with Type=Trial. Must be an odd number.

`TrialMode`

Type
Multiple Choice

Default value
CurrentMixCentered

Options
[CurrentMixCentered, FullRange]

Description
How are the NTrialMixFactors chosen?

`Type`

Type
Multiple Choice

Default value
Error

Options
[Error, Energy, UnpredictedStep, Trial]

Description
Adapt the mix factor based on the observed progress (slope).

`MixStepper`

Type
Block

Description
Simple mixing stepper, only using the previous (in/out) density.

`Mix`

Type
Float

Default value
0.1

Description
???.

`MultiSecantStepper`

Type
Block

Description
Multi secant stepper.

`MaxCoefficient`

Type
Float

Default value
20.0

Description
???.

`MaxVectors`

Type
Integer

Default value
10

Description
???.

`Mix`

Type
Float

Default value
0.2

Description
???.

`Variant`

Type
Multiple Choice

Default value
MSB2

Options
[MSB1, MSB2, MSR1, MSR1s]

Description
There are several version of the Multi secant method.

`StintLength`

Type
Integer

Description
Override global StintLength.

`StintLength`

Type
Integer

Default value
10

Description
A stepper is active during a number of SCF cycles, called a stint.

`UsePreviousStintForErrorGrowthAbort`

Type
Bool

Default value
No

Description
The error is normally checked against the first error of the stint. With this option that will be the one from the previous stint, if performed with the same stepper.

`SpinOrbit`

Type
Bool

Default value
No

Description
test

`Unrestricted`

Type
Bool

Default value
No

Description
Enables spin unrestricted calculations.

Only collinear spin polarization is supported, see Theor Chem Acc (2016) 135: 232, for details.

Must be supported by the chosen parameter set. Not yet compatible with DFTB3, k-space sampling periodic calculations or the xTB models.

`Solvation`

Type
Block

Description
Generalized Born solvation model with Solvent Accessible Surface Area (GBSA).

`GSolvState`

Type
Multiple Choice

Default value
Gas1MSolvent1M

Options
[Gas1BarSolvent, Gas1MSolvent1M, Gas1BarSolvent1M]

Description
Reference state for solvation free energy shift.

`Solvent`

Type
Multiple Choice

Default value
None

Options
[None, Acetone, Acetonitrile, CHCl3, CS2, DMSO, Ether, H2O, Methanol, THF, Toluene]

Description
Solvent used in the GBSA implicit solvation model.

`SurfaceGrid`

Type
Multiple Choice

Default value
230

Options
[230, 974, 2030, 5810]

Description
Number of angular grid points for the construction of the solvent accessible surface area. Usually the default number of grid point suffices, but in case of suspicious behaviors you can increase the number of points.

`Temperature`

Type
Float

Default value
298.15

Unit
Kelvin

Description
The temperature used when calculating the solvation free energy shift. Only used for 'Gas1BarSolvent' and 'Gas1BarSolvent1M' GSolvState options.

`UseGSASA`

Type
Bool

Default value
Yes

GUI name
Solvation Free Energy

Description
Include shift term and G(SASA) terms in the energy and gradient.

`StoreMatrices`

Type
Bool

Default value
No

Description
Determines whether the Hamiltonian and overlap matrices are stored in the binary result file.

`StoreOrbitals`

Type
Bool

Default value
Yes

Description
Determines whether the orbital coefficients are stored in the binary result file. They are needed for displaying orbitals and densities in amsview.

`Technical`

Type
Block

Description
This optional section is about technical aspects of the program that should not concern the normal user.

`AnalyticalStressTensor`

Type
Bool

Default value
Yes

Description
Whether to compute the stress tensor analytically. Note: This can only be used together with Ewald summation as it will give (slightly) wrong results with Madelung screening.

`EwaldSummation`

Type
Block

Description
Configures the details of the Ewald summation of the Coulomb interaction.

`CellRangeFactor`

Type
Float

Default value
2.0

Description
Smaller values will make the Ewald summation less accurate but faster.

`Enabled`

Type
Bool

Default value
Yes

Description
Whether to use Ewald summation for the long-range part of the Coulomb interaction. Otherwise screening is used.

`Tolerance`

Type
Float

Default value
1e-10

Description
Larger values will make the Ewald summation less accurate but faster.

`MatricesViaFullMaxSize`

Type
Integer

Default value
2047

Description
Matrices smaller than this size are constructed via a full matrix. This is faster, but uses more memory in the construction.

`Parallel`

Type
Block

Description
Calculation of the orbitals in several k-points is trivially parallel.

`nCoresPerGroup`

Type
Integer

Description
Number of cores in each working group.

`nGroups`

Type
Integer

Description
Total number of processor groups. This is the number of tasks that will be executed in parallel.

`nNodesPerGroup`

Type
Integer

GUI name
Cores per task

Description
Number of nodes in each group. This option should only be used on homogeneous compute clusters, where all used compute nodes have the same number of processor cores.

`ReuseKSpaceConfig`

Type
Bool

Default value
Yes

Description
Keep the number of k-points constant during a lattice optimization. Otherwise the PES might display jumps, because the number of points depends on the lattice vector sizes. If this option is on it will always use the number of k-points that was used from a previous result.

`Screening`

Type
Block

Description
For SCC-DFTB in periodic systems the Coulomb interaction can (instead of using Ewald summation) be screened with a Fermi-Dirac like function defined as S(r)=1/(exp((r-r_madel)/d_madel)+1). This section allows to change some details of the screening procedure. Note that Coulomb screening is only used if the Ewald summation is disabled.

`dMadel`

Type
Float

Unit
Bohr

Description
Sets the smoothness of the screening function. The default is 1/10 of [rMadel].

`rMadel`

Type
Float

Unit
Bohr

Description
Sets the range of the screening function. The default is 2x the norm of the longest lattice vector.

`UseGeneralizedDiagonalization`

Type
Bool

Default value
Yes

Description
Whether or not to use generalized diagonalization. Does not affect the results, but might be faster or slower.

`UnpairedElectrons`

Type
Integer

Default value
0

GUI name
Spin polarization

Description
This specifies the number of unpaired electrons (not the multiplicity!).

This number will then be used in the orbital-filling strategy. Has to be compatible with the total number of electrons, meaning it must be an even number if the total number of electrons is even and odd if the total number is odd. Must be an integer value.

Note that this does not activate spin polarization, it only affects the filling of the orbitals.

`XTBConfig`

Type
Block

Description
This block allows for minor tweaking.

`SlaterRadialThreshold`

Type
Float

Default value
1e-05

Description
Threshold determining the range of the basis functions. Using a larger threshold will speed up the calculation, but will also make the results less accurate.

`useXBTerm`

Type
Bool

Default value
No

Description
Whether to use the Halogen bonding (XB) term. This is not advised as it has a non-continuous PES.

11.2.2 conductance

`EnergyGrid`

Type
Block

Description
Energy grid for Transmission Function

`Max`

Type
Float

Default value
5.0

Unit
eV

Description
Max Energy (relative to Fermi energy)

`Min`

Type
Float

Default value
-5.0

Unit
eV

Description
Min energy (relative to Fermi energy)

`Num`

Type
Integer

Default value
200

Description
Number of energy values in which the interval Min-Max is subdivided

`Files`

Type
Block

Description
path of files

`HamiltonianElectrode`

Type
String

Default value
Description

`HamiltonianMolecule`

Type
String

Default value
Description

`Leads`

Type
String

Default value
Description
Path (either absolute or relative) of the lead results file

`OverlapElectrode`

Type
String

Default value
Description

`OverlapMolecule`

Type
String

Default value
Description

`Scattering`

Type
String

Default value

Description
Path (either absolute or relative) of the scattering region results

`Output`

Type
Block

Description
options describing what should be printed

`OldOutput`

Type
Bool

Default value
No

Description

`Physics`

Type
Block

Description
Block describing the physics of the system

`FermiEnergy`

Type
Block

Description
Block describing the physics of the system

`Electrode`

Type
Float

Default value
0.0

Description
Fermi energy of the electrode

`Technical`

Type
Block

Description
options describing technical parts of the calculation

`Eta`

Type
Float

Default value
1e-05

Description
To avoid poles of the Green's function, a small imaginary number is added to the energy

`overwriteLeads`

Type
Bool

Default value
Yes

Description
If true, Hamiltonians H_L and H_R are taken from the DFTB-leads calculation. If False, they are taken from the DFTB scattering-region calculation

`setOffDiagonalToZero`

Type
Bool

Default value
Yes

Description
If true, H_LR and S_LR are explicitly set to zero. If False, they are taken from the DFTB scattering-region calculation.

CHAPTER

TWELVE

KF OUTPUT FILES

12.1 Accessing KF files

KF files are Direct Access binary files. KF stands for Keyed File: KF files are keyword oriented, which makes them easy to process by simple procedures. Internally all the data on KF files is organized into sections containing variables, so each datum on the file can be identified by the combination of section and variable.

All KF files can be opened using the KFbrowser GUI program:

```
$AMSBIN/kfbrowser path/to/ams.rkf
```

By default KFbrowser shows a just a curated summary of the results on the file, but you can make it show the raw section and variable structure by switching it to expert mode. To do this, click on **File → Expert Mode** or press **ctrl/cmd + e**.

KF files can be opened and read with Command line tools.

For working with the data from KF files, it is often useful to be able to read them from Python. Using the AMS Python Stack, this can easily be done with the AKFReader class:

```
>>> from scm.akfreader import AKFReader
>>> kf = AKFReader("path/to/ams.rkf")
>>> "Molecule%Coords" in kf
True
>>> kf.description("Molecule%Coords")
{
    '_type': 'float_array',
    '_shape': [3, 'nAtoms'],
    '_comment': 'Coordinates of the nuclei (x,y,z)',
    '_unit': 'Bohr'
}
>>> kf.read("Molecule%Coords")
array([[-11.7770694 ,  -4.19739597,   0.04934546],
       [ -9.37471321,  -2.63234227,  -0.13448698],
        ...
       [ 10.09508738,  -1.06191208,   1.45286913],
       [ 10.11689333,  -1.5080196 ,  -1.87916127]])
```

Tip: For a full overview of the available methods in AKFReader, see the AKFReader API documentation.

12.2 Sections and variables on dftb.rkf

12.2.1 AMSResults

KF Section: AMSResults

Content: Generic results of the DFTB evaluation.

AMSResults%AAT_Transpose

Type
float_array

Description
VCD atomic axial tensors (AATs).

Shape
[3, 3, Molecule%nAtoms]

AMSResults%Bonds

Type
subsection

Description
Bond info

AMSResults%Bonds.Atoms

Type
archived_int_array

Description
?

AMSResults%Bonds.CellShifts

Type
archived_int_array

Description
?

AMSResults%Bonds.description

Type
string

Description
A string containing a description of how the bond orders were calculated / where they come from

AMSResults%Bonds.hasCellShifts

Type
bool

Description
Whether there are cell shifts (relevant only in case of periodic boundary conditions)

AMSResults%Bonds.Index

Type
archived_int_array

Description
index(i) points to the first element of Atoms, Orders, and CellShifts belonging to bonds from atom 'i'. Index(1) is always 1, Index(nAtoms+1) is always nBonds + 1

AMSResults%Bonds.nLattVec

Type
int

Description
Number of lattice vectors (0:molecule, 1:chain, 2:slab, 3:bulk). This determines how the lattice displacements for bonds are interpreted.

AMSResults%Bonds.Orders

Type
archived_float_array

Description
The bond orders.

AMSResults%BulkModulus

Type
float

Description
The Bulk modulus (conversion factor from hartree/bohr^3 to GPa: 29421.026)

Unit
hartree/bohr^3

AMSResults%Charges

Type
float_array

Description
Net atomic charges as computed by the engine (for example, the Charges for a water molecule might be [-0.6, 0.3, 0.3]). The method used to compute these atomic charges depends on the engine.

Unit
e

Shape
[Molecule%nAtoms]

AMSResults%DipoleGradients

Type
float_array

Description
Derivative of the dipole moment with respect to nuclear displacements.

Shape
[3, 3, Molecule%nAtoms]

AMSResults%DipoleMoment

Type
float_array

Description
Dipole moment vector (x,y,z)

Unit
e*bohr

Shape
[3]

`AMSResults%ElasticTensor`

Type
float_array

Description
The elastic tensor in Voigt notation (6x6 matrix for 3D periodic systems, 3x3 matrix for 2D periodic systems, 1x1 matrix for 1D periodic systems).

Unit
hartree/bohr^nLatticeVectors

Shape
[:, :]

`AMSResults%Energy`

Type
float

Description
The energy computed by the engine.

Unit
hartree

`AMSResults%fractionalOccupation`

Type
bool

Description
Whether of not we have fractionally occupied orbitals (i.e. not all occupations are integer numbers).

`AMSResults%Gradients`

Type
float_array

Description
The nuclear gradients.

Unit
hartree/bohr

Shape
[3, Molecule%nAtoms]

`AMSResults%Hessian`

Type
float_array

Description
The Hessian matrix

Unit
hartree/bohr^2

Shape
[3*Molecule%nAtoms, 3*Molecule%nAtoms]

`AMSResults%HOMOEnergy`

Type
float_array

Description
Molecular Orbital Info: energy of the HOMO.

Unit
hartree

Shape
[nSpin]

`AMSResults%HOMOIndex`

Type
int_array

Description
Molecular Orbital Info: index in the arrays orbitalEnergies and orbitalOccupations corresponding to the HOMO.

Shape
[nSpin]

`AMSResults%HOMOLUMOGap`

Type
float_array

Description
Molecular Orbital Info: HOMO-LUMO gap per spin.

Unit
hartree

Shape
[nSpin]

`AMSResults%LUMOEnergy`

Type
float_array

Description
Molecular Orbital Info: energy of the LUMO.

Unit
hartree

Shape
[nSpin]

`AMSResults%LUMOIndex`

Type
int_array

Description
Molecular Orbital Info: index in the arrays orbitalEnergies and orbitalOccupations corresponding to the LUMO.

Shape
[nSpin]

AMSResults%Molecules

Type
subsection

Description
Molecules

AMSResults%Molecules.AtCount

Type
archived_int_array

Description
shape=(nMolType), Summary: number of atoms per formula.

AMSResults%Molecules.Atoms

Type
archived_int_array

Description
shape=(nAtoms), atoms(index(i):index(i+1)-1) = atom indices of molecule i

AMSResults%Molecules.Count

Type
archived_int_array

Description
Mol count per formula.

AMSResults%Molecules.Formulas

Type
string

Description
Summary: unique molecule formulas

AMSResults%Molecules.Index

Type
archived_int_array

Description
shape=(nMol+1), index(i) = index of the first atom of molecule i in array atoms(:)

AMSResults%Molecules.Type

Type
archived_int_array

Description
shape=(nMol), type of the molecule, reference to the summary arrays below

AMSResults%nOrbitals

Type
int

Description
Molecular Orbital Info: number of orbitals.

AMSResults%nSpin

Type
int

Description
Molecular Orbital Info: number spins (1: spin-restricted or spin-orbit coupling, 2: spin unrestricted).

AMSResults%orbitalEnergies

Type
float_array

Description
Molecular Orbital Info: the orbital energies.

Unit
hartree

Shape
[nOrbitals, nSpin]

AMSResults%orbitalOccupations

Type
float_array

Description
Molecular Orbital Info: the orbital occupation numbers. For spin restricted calculations, the value will be between 0 and 2. For spin unrestricted or spin-orbit coupling the values will be between 0 and 1.

Shape
[nOrbitals, nSpin]

AMSResults%PESPointCharacter

Type
string

Description
The character of a PES point.

Possible values
['local minimum', 'transition state', 'stationary point with >1 negative frequencies', 'non-stationary point']

AMSResults%PoissonRatio

Type
float

Description
The Poisson ratio

AMSResults%ShearModulus

Type
float

Description
The Shear modulus (conversion factor from hartree/bohr^3 to GPa: 29421.026)

Unit
hartree/bohr^3

AMSResults%SmallestHOMOLUMOGap

Type
float

Description
Molecular Orbital Info: the smallest HOMO-LUMO gap irrespective of spin (i.e. min(LUMO) - max(HOMO)).

Unit
hartree

AMSResults%StressTensor

Type
float_array

Description
The clamped-ion stress tensor in Cartesian notation.

Unit
hartree/bohr^nLatticeVectors

Shape
[:, :]

AMSResults%YoungModulus

Type
float

Description
The Young modulus (conversion factor from hartree/bohr^3 to GPa: 29421.026)

Unit
hartree/bohr^3

12.2.2 band_curves

KF Section: band_curves
Content: Band dispersion curves.

band_curves%brav_type

Type
string

Description
Type of the lattice.

band_curves%Edge_#_bands

Type
float_array

Description
The band energies

Shape
[nBands, nSpin, :]

band_curves%Edge_#_direction

Type
float_array

Description
Direction vector.

Shape
[nDimK]

band_curves%Edge_#_fatBands

Type
float_array

Description
Fat band split up of the bands

Shape
[nBas, nBands, nSpin, :]

band_curves%Edge_#_kPoints

Type
float_array

Description
Coordinates for points along the edge.

Shape
[nDimK, :]

band_curves%Edge_#_labels

Type
lchar_string_array

Description
Labels for begin and end point of the edge.

Shape
[2]

band_curves%Edge_#_lGamma

Type
bool

Description
Is gamma point?

band_curves%Edge_#_nKPoints

Type
int

Description
The nr. of k points along the edge.

band_curves%Edge_#_vertices

Type
float_array

Description
Begin and end point of the edge.

Shape
[nDimK, 2]

band_curves%Edge_#_xFor1DPlotting

Type
float_array

Description
x Coordinate for points along the edge.

Shape
[:]

band_curves%indexLowestBand

Type
int

Description
?

band_curves%nBands

Type
int

Description
Number of bands.

band_curves%nBas

Type
int

Description
Number of basis functions.

band_curves%nDimK

Type
int

Description
Dimension of the reciprocal space.

band_curves%nEdges

Type
int

Description
The number of edges. An edge is a line-segment through k-space. It has a begin and end point and possibly points in between.

band_curves%nEdgesInPath

Type
int

Description
A path is built up from a number of edges.

band_curves%nSpin

Type
int

Description
Number of spin components.

Possible values
[1, 2]

band_curves%path

Type
int_array

Description
If the (edge) index is negative it means that the vertices of the edge abs(index) are swapped e.g. path = (1,2,3,0,-3,-2,-1) goes though edges 1,2,3, then there's a jump, and then it goes back.

Shape
[nEdgesInPath]

band_curves%path_source

Type
string

Description
Source or program used to generate the path.

Possible values
['input', 'kpath', 'seekpath']

band_curves%path_type

Type
string

Description
?

12.2.3 BandStructure

KF Section: BandStructure
Content: Info regarding the band structure.

BandStructure%BandGap

Type
float

Description
The band gap. For molecules this is the HOMO-LUMO gap.

Unit
hartree

BandStructure%bandsEnergyRange

Type
float_array

Description
The energy ranges (min/max) of the bands

Unit
hartree

Shape
[2, nBand, nSpin]

BandStructure%BottomConductionBand

Type
float

Description
The bottom of the conduction band

Unit
hartree

BandStructure%CoordsBottomConductionBand

Type
float_array

Description
The coordinates in k-space of the bottom of the conduction band

Unit
1/bohr

Shape
[nDimK]

BandStructure%CoordsTopValenceBand

Type
float_array

Description
The coordinates in k-space of the top of the valence band

Unit
1/bohr

Shape
[nDimK]

BandStructure%DerivativeDiscontinuity

Type
float

Description
Correction to be added to the band gap to get the fundamental gap. (band only)

Unit
hartree

BandStructure%FermiEnergy

Type
float

Description
Fermi level

Unit
hartree

BandStructure%HasGap

Type
bool

Description
Whether the system has a gap.

BandStructure%HomoBandIndex

Type
int

Description
The index of the highest occupied band

BandStructure%HomoDegeneracy

Type
int

Description
How many states are exactly at the HOMO level

BandStructure%HomoSpinIndex

Type
int

Description
In case of an unrestricted calculation: which of the two spins has the HOMO?

BandStructure%LumoBandIndex

Type
int

Description
The index of the lowest unoccupied band

BandStructure%LumoDegeneracy

Type
int

Description
How many states are exactly at the LUMO level

BandStructure%LumoSpinIndex

Type
int

Description
In case of an unrestricted calculation: which of the two spins has the LUMO?

BandStructure%nBand

Type
int

Description
The number of bands for which the band ranges are stored.

BandStructure%nDimK

Type
int

Description
The number of dimensions for the k-coordinates for CoordsTopValenceBand and CoordsBottomConductionBand.

BandStructure%nSpin

Type
int

Description
If 1: spin restricted calculation. For unrestricted results it has the value of 2.

Possible values
[1, 2]

BandStructure%TopValenceBand

Type
float

Description
The top of the valence band

Unit
hartree

12.2.4 BandStructure(FromPath)

KF Section: BandStructure(FromPath)
Content: Info regarding the band structure.

BandStructure(FromPath)%BandGap

Type
float

Description
The band gap. For molecules this is the HOMO-LUMO gap.

Unit
hartree

BandStructure(FromPath)%bandsEnergyRange

Type
float_array

Description
The energy ranges (min/max) of the bands

Unit
hartree

Shape
[2, nBand, nSpin]

BandStructure(FromPath)%BottomConductionBand

Type
float

Description
The bottom of the conduction band

Unit
hartree

BandStructure(FromPath)%CoordsBottomConductionBand

Type
float_array

Description
The coordinates in k-space of the bottom of the conduction band

Unit
1/bohr

Shape
[nDimK]

BandStructure(FromPath)%CoordsTopValenceBand

Type
float_array

Description
The coordinates in k-space of the top of the valence band

Unit
1/bohr

Shape
[nDimK]

BandStructure(FromPath)%DerivativeDiscontinuity

Type
float

Description
Correction to be added to the band gap to get the fundamental gap. (band only)

Unit
hartree

BandStructure(FromPath)%FermiEnergy

Type
float

Description
Fermi level

Unit
hartree

BandStructure(FromPath)%HasGap

Type
bool

Description
Whether the system has a gap.

`BandStructure(FromPath)%HomoBandIndex`

Type
int

Description
The index of the highest occupied band

`BandStructure(FromPath)%HomoDegeneracy`

Type
int

Description
How many states are exactly at the HOMO level

`BandStructure(FromPath)%HomoSpinIndex`

Type
int

Description
In case of an unrestricted calculation: which of the two spins has the HOMO?

`BandStructure(FromPath)%LumoBandIndex`

Type
int

Description
The index of the lowest unoccupied band

`BandStructure(FromPath)%LumoDegeneracy`

Type
int

Description
How many states are exactly at the LUMO level

`BandStructure(FromPath)%LumoSpinIndex`

Type
int

Description
In case of an unrestricted calculation: which of the two spins has the LUMO?

`BandStructure(FromPath)%nBand`

Type
int

Description
The number of bands for which the band ranges are stored.

`BandStructure(FromPath)%nDimK`

Type
int

Description
The number of dimensions for the k-coordinates for CoordsTopValenceBand and CoordsBottomConductionBand.

BandStructure(FromPath)%nSpin

Type
int

Description
If 1: spin restricted calculation. For unrestricted results it has the value of 2.

Possible values
[1, 2]

BandStructure(FromPath)%TopValenceBand

Type
float

Description
The top of the valence band

Unit
hartree

12.2.5 BZcell(primitive cell)

KF Section: BZcell(primitive cell)
Content: The Brillouin zone of the primitive cell.

BZcell(primitive cell)%boundaries

Type
float_array

Description
Normal vectors for the boundaries.

Shape
[ndim, nboundaries]

BZcell(primitive cell)%distances

Type
float_array

Description
Distance to the boundaries.

Shape
[nboundaries]

BZcell(primitive cell)%idVerticesPerBound

Type
int_array

Description
The indices of the vertices per bound.

Shape
[nvertices, nboundaries]

BZcell(primitive cell)%latticeVectors

Type
float_array

Description
The lattice vectors.

Shape
[3, :]

BZcell(primitive cell)%nboundaries

Type
int

Description
The nr. of boundaries for the cell.

BZcell(primitive cell)%ndim

Type
int

Description
The nr. of lattice vectors spanning the Wigner-Seitz cell.

BZcell(primitive cell)%numVerticesPerBound

Type
int_array

Description
The nr. of vertices per bound.

Shape
[nboundaries]

BZcell(primitive cell)%nvertices

Type
int

Description
The nr. of vertices of the cell.

BZcell(primitive cell)%vertices

Type
float_array

Description
The vertices of the bounds.

Unit
a.u.

Shape
[ndim, nvertices]

12.2.6 DFTBEngineRestart

KF Section: DFTBEngineRestart

Content: Stuff needed for restarting the DFTB engine

12.2.7 DOS

KF Section: DOS

Content: Info regarding the DOS

`DOS%Atom per basis function`

Type
int_array

Description
Atom index per basis function.

`DOS%COOP per basis pair`

Type
float_array

Description
COOP per basis pair.

Shape
[nEnergies, nSpin, :, :]

`DOS%DeltaE`

Type
float

Description
The energy difference between sampled DOS energies. When there is no DOS at all a certain energy range can be skipped.

Unit
hartree

`DOS%DOS per basis function`

Type
float_array

Description
DOS contributions per basis function, based on Mulliken analysis.

Shape
[nEnergies, nSpin, :]

`DOS%Energies`

Type
float_array

Description
The energies at which the DOS is sampled.

Unit
hartree

Shape
[nEnergies]

DOS%Fermi Energy

Type
float

Description
The fermi energy.

Unit
hartree

DOS%IntegrateDeltaE

Type
bool

Description
If enabled it means that the DOS is integrated over intervals of DeltaE. Sharp delta function like peaks cannot be missed this way.

DOS%L-value per basis function

Type
int_array

Description
quantum number l for all basis functions.

DOS%M-value per basis function

Type
int_array

Description
quantum number m for all basis functions.

DOS%nEnergies

Type
int

Description
The nr. of energies to use to sample the DOS.

DOS%nSpin

Type
int

Description
The number of spin components for the DOS.

Possible values
[1, 2]

DOS%Overlap population per basis pai

Type
float_array

Description
? note that the word 'pair' is cut of due to the finite length of the kf variables name…

DOS%Population per basis function

Type
float_array

Description
?

DOS%Symmetry per basis function

Type
int_array

Description
?

DOS%Total DOS

Type
float_array

Description
The total DOS.

Shape
[nEnergies, nSpin]

12.2.8 DOS_Phonons

KF Section: DOS_Phonons
Content: Phonon Density of States

DOS_Phonons%DeltaE

Type
float

Description
The energy difference between sampled DOS energies. When there is no DOS at all a certain energy range can be skipped.

Unit
hartree

DOS_Phonons%Energies

Type
float_array

Description
The energies at which the DOS is sampled.

Unit
hartree

Shape
[nEnergies]

DOS_Phonons%Fermi Energy

Type
float

Description
The fermi energy.

Unit
hartree

DOS_Phonons%IntegrateDeltaE

Type
bool

Description
If enabled it means that the DOS is integrated over intervals of DeltaE. Sharp delta function like peaks cannot be missed this way.

DOS_Phonons%nEnergies

Type
int

Description
The nr. of energies to use to sample the DOS.

DOS_Phonons%nSpin

Type
int

Description
The number of spin components for the DOS.

Possible values
[1, 2]

DOS_Phonons%Total DOS

Type
float_array

Description
The total DOS.

Shape
[nEnergies, nSpin]

12.2.9 Dynamical Polarizability

KF Section: Dynamical Polarizability
Content: ?

Dynamical Polarizability%frequency #

Type
float

Description
?

Dynamical Polarizability%imagPolar #

Type
float_array

Description
?

Dynamical Polarizability%nr of frequencies

Type
int

Description
?

Dynamical Polarizability%realPolar #

Type
float_array

Description
?

12.2.10 EffectiveMass

KF Section: EffectiveMass

Content: In the effective mass approximation the curvature of the bands is a measure of the charge mobility. The curvature is obtained by numerical differentiation. The mass is the inverse of the curvature.

EffectiveMass%EffectiveMasses

Type
float_array

Description
Inverse curvatures at the extrema. Several bands may be sampled at once.

Unit
a.u.

Shape
[Molecule%nLatticeVectors, MaxNBands, nKPoints, nSpin]

EffectiveMass%ErrorEffectiveMasses

Type
float_array

Description
Estimated errors from using two different step sizes for finite difference calculations.

Unit
a.u.

Shape
[Molecule%nLatticeVectors, MaxNBands, nKPoints, nSpin]

EffectiveMass%iBandHigh

Type
int_array

Description
See comment for iBandLow.

Shape
[nKPoints]

EffectiveMass%iBandLow

Type
int_array

Description
For point k bands iBandLo(k) to iBandHi(k) are considered

Shape
[nKPoints]

EffectiveMass%kCoordinates

Type
float_array

Description
The coordinates in k-space of the top of the valence band(s) or bottom of conduction band(s).

Unit
1/bohr

Shape
[Molecule%nLatticeVectors, nKPoints]

EffectiveMass%MaxNBands

Type
int

Description
Maximum number of curvatures calculated for all k points.

EffectiveMass%nKPoints

Type
int

Description
The number of k points for which the effective mass is calculated. These should always be extrema (minimum or maximum) of the bands.

EffectiveMass%nSpin

Type
int

Description
If 1: spin restricted calculation. For unrestricted results it has the value of 2.

Possible values
[1, 2]

12.2.11 Excitations SOT A

KF Section: Excitations SOT A

Content: Single oribtal transitions. Ask Robert about this.

`Excitations SOT A%contr #`

Type
float_array

Description
Contributions to excitation #.

Shape
[:]

`Excitations SOT A%contr index #`

Type
int_array

Description
Indices (org/new) for contributions to excitation #.

Shape
[:, 2]

`Excitations SOT A%contr irep index #`

Type
int_array

Description
Irrep indices (org/new) for contributions to excitation #.

Shape
[:, 2]

`Excitations SOT A%contr transdip #`

Type
float_array

Description
Contributions to transition dipole #.

Shape
[3, :]

`Excitations SOT A%eigenvec #`

Type
float_array

Description
Eigenvectors for excitation #.

Shape
[:]

`Excitations SOT A%excenergies`

Type
float_array

Description
Excitation energies.

Shape
[:]

`Excitations SOT A%gradient #`

Type
float_array

Description
Gradient for excitation #.

Shape
[3, Molecule%nAtoms]

`Excitations SOT A%nr of contributions #`

Type
int

Description
Number of contributions for excitation #.

`Excitations SOT A%nr of excenergies`

Type
int

Description
Number of excitation energies.

`Excitations SOT A%oscillator strengths`

Type
float_array

Description
Oscillator strengths.

Shape
[nr of excenergies]

`Excitations SOT A%transition dipole moments`

Type
float_array

Description
Transition dipole moments.

Shape
[3, nr of excenergies]

12.2.12 Excitations SS A

KF Section: Excitations SS A

Content: Singlet-singlet.

Excitations SS A%contr #

Type
float_array

Description
Contributions to excitation #.

Shape
[:]

Excitations SS A%contr index #

Type
int_array

Description
Indices (org/new) for contributions to excitation #.

Shape
[:, 2]

Excitations SS A%contr irep index #

Type
int_array

Description
Irrep indices (org/new) for contributions to excitation #.

Shape
[:, 2]

Excitations SS A%contr transdip #

Type
float_array

Description
Contributions to transition dipole #.

Shape
[3, :]

Excitations SS A%eigenvec #

Type
float_array

Description
Eigenvectors for excitation #.

Shape
[nTransUse]

Excitations SS A%excenergies

Type
float_array

Description
Excitation energies.

Shape
[nr of excenergies]

`Excitations SS A%gradient #`

Type
float_array

Description
Gradient for excitation #.

Shape
[3, Molecule%nAtoms]

`Excitations SS A%nr of contributions #`

Type
int

Description
Number of contributions for excitation #.

`Excitations SS A%nr of excenergies`

Type
int

Description
Number of excitation energies.

`Excitations SS A%nTransUse`

Type
int

Description
Number of single orbital transitions.

`Excitations SS A%oscillator strengths`

Type
float_array

Description
Oscillator strengths.

Shape
[nr of excenergies]

`Excitations SS A%transition dipole moments`

Type
float_array

Description
Transition dipole moments.

Shape
[3, nr of excenergies]

12.2.13 Excitations ST A

KF Section: Excitations ST A

Content: Singlet-triplet.

Excitations ST A%contr #

Type
float_array

Description
Contributions to excitation #.

Shape
[:]

Excitations ST A%contr index #

Type
int_array

Description
Indices (org/new) for contributions to excitation #.

Shape
[:, 2]

Excitations ST A%contr irep index #

Type
int_array

Description
Irrep indices (org/new) for contributions to excitation #.

Shape
[:, 2]

Excitations ST A%contr transdip #

Type
float_array

Description
Contributions to transition dipole #.

Shape
[3, :]

Excitations ST A%eigenvec #

Type
float_array

Description
Eigenvectors for excitation #.

Shape
[nTransUse]

Excitations ST A%excenergies

Type
float_array

Description
Excitation energies.

Shape
[nr of excenergies]

`Excitations ST A%gradient #`

Type
float_array

Description
Gradient for excitation #.

Shape
[3, Molecule%nAtoms]

`Excitations ST A%nr of contributions #`

Type
int

Description
Number of contributions for excitation #.

`Excitations ST A%nr of excenergies`

Type
int

Description
Number of excitation energies.

`Excitations ST A%nTransUse`

Type
int

Description
Number of single orbital transitions.

`Excitations ST A%oscillator strengths`

Type
float_array

Description
Oscillator strengths.

Shape
[nr of excenergies]

`Excitations ST A%transition dipole moments`

Type
float_array

Description
Transition dipole moments.

Shape
[3, nr of excenergies]

12.2.14 FOPopulations

KF Section: FOPopulations

Content: ?

FOPopulations%fo_grosspop(#)

Type
float_array

Description
Gross population of fragment orbitals in full system.

Shape
[FragmentOrbitals%nOrbitals]

FOPopulations%fo_index(#)

Type
int_array

Description
Fragment orbital number for each stored fragment orbital contribution per molecular orbital.

FOPopulations%fo_pop(#)

Type
float_array

Description
Stored fragment orbital contribution per molecular orbital.

FOPopulations%nEntries

Type
int

Description
The number of sets. At the moment it should be 1, only nSpin=1 and nKpoints=1 supported.

FOPopulations%number of contributions(#)

Type
int_array

Description
Number of stored fragment orbital contributions per molecular orbital

Shape
[FragmentOrbitals%nOrbitals]

12.2.15 FragmentOrbitals

KF Section: FragmentOrbitals

Content: ?

FragmentOrbitals%AtomicFragmentOrbitals

Type
bool

Description
Whether atomic fragment orbitals are used.

FragmentOrbitals%BaseNameFragFile

Type
lchar_string_array

Description
Not used if AtomicFragmentOrbitals is true. Guess for reasonable fragment names in case of the AMS-GUI.

Shape
[nFragments]

FragmentOrbitals%Coefficients(#)

Type
float_array

Description
Fragment orbital coefficients in the basis of all fragment basis functions.

Shape
[nBasisFunctions, nOrbitals]

FragmentOrbitals%Energies(#)

Type
float_array

Description
Fragment orbital energies.

Shape
[nOrbitals]

FragmentOrbitals%Fragment

Type
int_array

Description
On which fragment is a fragment orbital.

Shape
[nOrbitals]

FragmentOrbitals%FragmentSymbols

Type
lchar_string_array

Description
Unique name of the fragments, typically name includes the chemical formula and a number.

Shape
[nFragments]

FragmentOrbitals%iFO

Type
int_array

Description
Orbital number of the fragment orbital in the fragment on which the fragment orbital is located.

Shape
[nOrbitals]

FragmentOrbitals%MOinFO(#)

Type
float_array

Description
Molecular orbital (MO) coefficients in the basis of fragment orbitals (FO).

Shape
[nOrbitals, nOrbitals]

FragmentOrbitals%nBasisFunctions

Type
int

Description
Total number of basis functions (summed over fragments). At the moment nBasisFunctions equals nOrbitals.

FragmentOrbitals%nEntries

Type
int

Description
The number of sets. At the moment it should be 1, only nSpin=1 and nKpoints=1 supported.

FragmentOrbitals%nFragments

Type
int

Description
Number of fragments

FragmentOrbitals%nOrbitals

Type
int

Description
Total number of orbitals (summed over fragments).

FragmentOrbitals%Occupations(#)

Type
float_array

Description
Fragment orbital occupation numbers.

Shape
[nOrbitals]

FragmentOrbitals%Overlaps(#)

Type
float_array

Description
Overlap fragment orbitals

Shape
[nOrbitals, nOrbitals]

FragmentOrbitals%SiteEnergies(#)

Type
float_array

Description
The Site energy of a fragment orbital (FO) is defined as the diagonal Fock matrix element of the Fock matrix of the full system in FO representation.

Shape
[nOrbitals]

FragmentOrbitals%SubSpecies

Type
lchar_string_array

Description
Symmetry labels of fragment orbitals. In case of AtomicFragmentOrbitals the subspecies are atomic like S, P:x, etcetera. Otherwise symmetry NOSYM is used and the subspecies are all A.

Shape
[nOrbitals]

12.2.16 General

KF Section: General
Content: General information about the DFTB calculation.

General%account

Type
string

Description
Name of the account from the license

General%engine input

Type
string

Description
The text input of the engine.

General%engine messages

Type
string

Description
Message from the engine. In case the engine fails to solves, this may contains extra information on why.

General%file-ident

Type
string

Description
The file type identifier, e.g. RKF, RUNKF, TAPE21…

General%jobid

Type
int

Description
Unique identifier for the job.

General%program

Type
string

Description
The name of the program/engine that generated this kf file.

General%release

Type
string

Description
The version of the program that generated this kf file (including svn revision number and date).

General%termination status

Type
string

Description
The termination status. Possible values: 'NORMAL TERMINATION', 'NORMAL TERMINATION with warnings', 'NORMAL TERMINATION with errors', 'ERROR', 'IN PROGRESS'.

General%title

Type
string

Description
Title of the calculation.

General%uid

Type
string

Description
SCM User ID

General%version

Type
int

Description
Version number?

12.2.17 KFDefinitions

KF Section: KFDefinitions

Content: The definitions of the data on this file

`KFDefinitions%json`

Type
string

Description
The definitions of the data on this file in json.

12.2.18 kspace

KF Section: kspace

Content: Info regarding the k-space integration…

`kspace%avec`

Type
float_array

Description
The lattice stored as a 3xnLatticeVectors matrix. Only the ndimk,ndimk part has meaning.

Unit
bohr

Shape
[3, :]

`kspace%bvec`

Type
float_array

Description
The inverse lattice stored as a 3x3 matrix. Only the ndimk,ndimk part has meaning.

Unit
1/bohr

Shape
[ndim, ndim]

`kspace%bzvol`

Type
float

Description
The volume of the BZ zone. In 2D it is the surface and in 1D it is the length. The unit is bohr raised to the power ndim.

`kspace%iDimkEffective`

Type
int_array

Description
Which latttice vectors are really used for the k-space integration.

Shape
[nDimkEffective]

kspace%isKunComplex

Type
bool_array

Description
Whether or not the Hamiltonian matrix is complex for a unique k-point.

Shape
[kuniqu]

kspace%kequiv

Type
int_array

Description
When kequiv(i)=i the k-point is unique.

Shape
[kt]

kspace%kequn

Type
int_array

Description
When looping over all k-points, the unique index is kun=kequn(k).

Shape
[kt]

kspace%kinteg

Type
int

Description
In case a symmetric grid is used this is the parameter used to create it.

kspace%klbl

Type
lchar_string_array

Description
labels describing the k-points

Shape
[kt]

kspace%klblun

Type
lchar_string_array

Description
labels describing the unique k-points

Shape
[kuniqu]

kspace%klnear

Type
bool

Description
Whether or not linear k-space integration is used (symmetric method with even kinteg).

kspace%ksimpl

Type
int_array

Description
Index array defining the simplices, referring to the xyzpt array.

Shape
[nvertk, nsimpl]

kspace%kt

Type
int

Description
The total number of k-points used by the k-space to sample the unique wedge of the Brillouin zone.

kspace%ktBoltz

Type
float

Description
band only?.

kspace%kuniqu

Type
int

Description
The number of symmetry unique k-points where an explicit diagonalization is needed. Smaller or equal to kt.

kspace%ndim

Type
int

Description
The nr. of lattice vectors.

kspace%ndimk

Type
int

Description
The nr. of dimensions used in the k-space integration.

kspace%nDimkEffective

Type
int

Description
Normally ndimk is equal to the number of lattice vectors. For very large lattice vectors the k-space dispersion is ignored, leading to a lower dimensional band structure.

kspace%noperk

Type
int

Description
The nr. of operators in k-space. band only?

kspace%nsimpl

Type
int

Description
The number of simplices constructed from the k-points to span the IBZ.

kspace%numBoltz

Type
int

Description
Number of energies to sample around the fermi energy. band only?

kspace%numEquivSimplices

Type
int_array

Description
Simplices may be equivalent due to symmetry operations..

Shape
[nsimpl]

kspace%nvertk

Type
int

Description
The number of vertices that each simplex has.

kspace%operk

Type
float_array

Description
Symmetry operators in k-space. band only?

Unit
bohr

Shape
[ndim, ndim, noperk]

kspace%xyzpt

Type
float_array

Description
The coordinates of the k-points.

Unit
1/bohr

Shape
[ndimk, kt]

12.2.19 kspace(primitive cell)

KF Section: kspace(primitive cell)
Content: should not be here!!!

`kspace(primitive cell)%avec`

Type
float_array

Description
The lattice stored as a 3xnLatticeVectors matrix. Only the ndimk,ndimk part has meaning.

Unit
bohr

Shape
[3, :]

`kspace(primitive cell)%bvec`

Type
float_array

Description
The inverse lattice stored as a 3x3 matrix. Only the ndimk,ndimk part has meaning.

Unit
1/bohr

Shape
[ndim, ndim]

`kspace(primitive cell)%kt`

Type
int

Description
The total number of k-points used by the k-space to sample the unique wedge of the Brillouin zone.

`kspace(primitive cell)%kuniqu`

Type
int

Description
The number of symmetry unique k-points where an explicit diagonalization is needed. Smaller or equal to kt.

`kspace(primitive cell)%ndim`

Type
int

Description
The nr. of lattice vectors.

`kspace(primitive cell)%ndimk`

Type
int

Description
The nr. of dimensions used in the k-space integration.

`kspace(primitive cell)%xyzpt`

Type
float_array

Description
The coordinates of the k-points.

Unit
1/bohr

Shape
[ndimk, kt]

12.2.20 Low Frequency Correction

KF Section: Low Frequency Correction
Content: Configuration for the Head-Gordon Dampener-powered Free Rotor Interpolation.

`Low Frequency Correction%Alpha`

Type
float

Description
Exponent term for the Head-Gordon dampener.

`Low Frequency Correction%Frequency`

Type
float

Description
Frequency around which interpolation happens, in 1/cm.

`Low Frequency Correction%Moment of Inertia`

Type
float

Description
Used to make sure frequencies of less than ca. 1 1/cm don't overestimate entropy, in kg m^2.

12.2.21 Matrices

KF Section: Matrices

Content: Section that can contain any number of real matrices

Matrices%Data(#)

Type
float_array

Description
The array, rank and dimensions as specified by Dimensions.

Matrices%Dimensions(#)

Type
int_array

Description
The dimensions of the array

Matrices%Name(#)

Type
string

Description
The name of the matrix.

Matrices%nEntries

Type
int

Description
The number of matrices

Matrices%Type(#)

Type
string

Description
The type such as Real, and perhaps Complex?

12.2.22 Mobile Block Hessian

KF Section: Mobile Block Hessian

Content: Mobile Block Hessian.

Mobile Block Hessian%Coordinates Internal

Type
float_array

Description
?

Mobile Block Hessian%Free Atom Indexes Input

Type
int_array

Description
?

Mobile Block Hessian%Frequencies in atomic units

Type
float_array

Description
?

Mobile Block Hessian%Frequencies in wavenumbers

Type
float_array

Description
?

Mobile Block Hessian%Input Cartesian Normal Modes

Type
float_array

Description
?

Mobile Block Hessian%Input Indexes of Block #

Type
int_array

Description
?

Mobile Block Hessian%Intensities in km/mol

Type
float_array

Description
?

Mobile Block Hessian%MBH Curvatures

Type
float_array

Description
?

Mobile Block Hessian%Number of Blocks

Type
int

Description
Number of blocks.

Mobile Block Hessian%Sizes of Blocks

Type
int_array

Description
Sizes of the blocks.

Shape
[Number of Blocks]

12.2.23 Molecule

KF Section: Molecule
Content: The input molecule of the calculation.

`Molecule%AtomicNumbers`

Type
int_array

Description
Atomic number 'Z' of the atoms in the system

Shape
[nAtoms]

`Molecule%AtomMasses`

Type
float_array

Description
Masses of the atoms

Unit
a.u.

Values range
[0, '\infinity']

Shape
[nAtoms]

`Molecule%AtomSymbols`

Type
string

Description
The atom's symbols (e.g. 'C' for carbon)

Shape
[nAtoms]

`Molecule%bondOrders`

Type
float_array

Description
The bond orders for the bonds in the system. The indices of the two atoms participating in the bond are defined in the arrays 'fromAtoms' and 'toAtoms'. e.g. bondOrders[1]=2, fromAtoms[1]=4 and toAtoms[1]=7 means that there is a double bond between atom number 4 and atom number 7

`Molecule%Charge`

Type
float

Description
Net charge of the system

Unit
e

Molecule%Coords

Type
float_array

Description
Coordinates of the nuclei (x,y,z)

Unit
bohr

Shape
[3, nAtoms]

Molecule%eeAttachTo

Type
int_array

Description
UNUSED IN AMS>=2026. A multipole may be attached to an atom. This influences the energy gradient.

Molecule%eeChargeWidth

Type
float

Description
If charge broadening was used for external charges, this represents the width of the charge distribution.

Molecule%eeEField

Type
float_array

Description
The external homogeneous electric field.

Unit
hartree/(e*bohr)

Shape
[3]

Molecule%eeLatticeVectors

Type
float_array

Description
UNUSED IN AMS>=2026. The lattice vectors used for the external point- or multipole-charges.

Unit
bohr

Shape
[3, eeNLatticeVectors]

`Molecule%eeMulti`

Type
float_array

Description
The values of the external point- or multipole- charges.

Unit
a.u.

Shape
[eeNZlm, eeNMulti]

`Molecule%eeNLatticeVectors`

Type
int

Description
UNUSED IN AMS>=2026. The number of lattice vectors for the external point- or multipole- charges.

`Molecule%eeNMulti`

Type
int

Description
The number of external point- or multipole- charges.

`Molecule%eeNZlm`

Type
int

Description
When external point- or multipole- charges are used, this represents the number of spherical harmonic components. E.g. if only point charges were used, eeNZlm=1 (s-component only). If point charges and dipole moments were used, eeNZlm=4 (s, px, py and pz).

`Molecule%eeUseChargeBroadening`

Type
bool

Description
Whether or not the external charges are point-like or broadened.

`Molecule%eeXYZ`

Type
float_array

Description
The position of the external point- or multipole- charges.

Unit
bohr

Shape
[3, eeNMulti]

Molecule%EngineAtomicInfo

Type
string_fixed_length

Description
Atom-wise info possibly used by the engine.

Molecule%fromAtoms

Type
int_array

Description
Index of the first atom in a bond. See the bondOrders array

Molecule%latticeDisplacements

Type
int_array

Description
The integer lattice translations for the bonds defined in the variables bondOrders, fromAtoms and toAtoms.

Molecule%LatticeVectors

Type
float_array

Description
Lattice vectors

Unit
bohr

Shape
[3, nLatticeVectors]

Molecule%nAtoms

Type
int

Description
The number of atoms in the system

Molecule%nAtomsTypes

Type
int

Description
The number different of atoms types

Molecule%nLatticeVectors

Type
int

Description
Number of lattice vectors (i.e. number of periodic boundary conditions)

Possible values
[0, 1, 2, 3]

Molecule%toAtoms

Type
int_array

Description
Index of the second atom in a bond. See the bondOrders array

12.2.24 MoleculeSuperCell

KF Section: MoleculeSuperCell

Content: The system used for the numerical phonon super cell calculation.

MoleculeSuperCell%AtomicNumbers

Type
int_array

Description
Atomic number 'Z' of the atoms in the system

Shape
[nAtoms]

MoleculeSuperCell%AtomMasses

Type
float_array

Description
Masses of the atoms

Unit
a.u.

Values range
[0, '\infinity']

Shape
[nAtoms]

MoleculeSuperCell%AtomSymbols

Type
string

Description
The atom's symbols (e.g. 'C' for carbon)

Shape
[nAtoms]

MoleculeSuperCell%bondOrders

Type
float_array

Description
The bond orders for the bonds in the system. The indices of the two atoms participating in the bond are defined in the arrays 'fromAtoms' and 'toAtoms'. e.g. bondOrders[1]=2, fromAtoms[1]=4 and toAtoms[1]=7 means that there is a double bond between atom number 4 and atom number 7

MoleculeSuperCell%Charge

Type
float

Description
Net charge of the system

Unit
e

MoleculeSuperCell%Coords

Type
float_array

Description
Coordinates of the nuclei (x,y,z)

Unit
bohr

Shape
[3, nAtoms]

MoleculeSuperCell%eeAttachTo

Type
int_array

Description
UNUSED IN AMS>=2026. A multipole may be attached to an atom. This influences the energy gradient.

MoleculeSuperCell%eeChargeWidth

Type
float

Description
If charge broadening was used for external charges, this represents the width of the charge distribution.

MoleculeSuperCell%eeEField

Type
float_array

Description
The external homogeneous electric field.

Unit
hartree/(e*bohr)

Shape
[3]

MoleculeSuperCell%eeLatticeVectors

Type
float_array

Description
UNUSED IN AMS>=2026. The lattice vectors used for the external point- or multipole-charges.

Unit
bohr

Shape
[3, eeNLatticeVectors]

`MoleculeSuperCell%eeMulti`

Type
float_array

Description
The values of the external point- or multipole- charges.

Unit
a.u.

Shape
[eeNZlm, eeNMulti]

`MoleculeSuperCell%eeNLatticeVectors`

Type
int

Description
UNUSED IN AMS>=2026. The number of lattice vectors for the external point- or multipole- charges.

`MoleculeSuperCell%eeNMulti`

Type
int

Description
The number of external point- or multipole- charges.

`MoleculeSuperCell%eeNZlm`

Type
int

Description
When external point- or multipole- charges are used, this represents the number of spherical harmonic components. E.g. if only point charges were used, eeNZlm=1 (s-component only). If point charges and dipole moments were used, eeNZlm=4 (s, px, py and pz).

`MoleculeSuperCell%eeUseChargeBroadening`

Type
bool

Description
Whether or not the external charges are point-like or broadened.

`MoleculeSuperCell%eeXYZ`

Type
float_array

Description
The position of the external point- or multipole- charges.

Unit
bohr

Shape
[3, eeNMulti]

MoleculeSuperCell%EngineAtomicInfo

Type
string_fixed_length

Description
Atom-wise info possibly used by the engine.

MoleculeSuperCell%fromAtoms

Type
int_array

Description
Index of the first atom in a bond. See the bondOrders array

MoleculeSuperCell%latticeDisplacements

Type
int_array

Description
The integer lattice translations for the bonds defined in the variables bondOrders, fromAtoms and toAtoms.

MoleculeSuperCell%LatticeVectors

Type
float_array

Description
Lattice vectors

Unit
bohr

Shape
[3, nLatticeVectors]

MoleculeSuperCell%nAtoms

Type
int

Description
The number of atoms in the system

MoleculeSuperCell%nAtomsTypes

Type
int

Description
The number different of atoms types

MoleculeSuperCell%nLatticeVectors

Type
int

Description
Number of lattice vectors (i.e. number of periodic boundary conditions)

Possible values
[0, 1, 2, 3]

MoleculeSuperCell%toAtoms

Type
int_array

Description
Index of the second atom in a bond. See the bondOrders array

12.2.25 NAOSetCells

KF Section: NAOSetCells

Content: For periodic systems neighboring cells need to be considered. More cells are needed for more diffuse basis sets.

NAOSetCells%Coords(#{entry})

Type
float_array

Description
Cell coordinates for a basis set.

Shape
[3, nCells(#{entry})]

NAOSetCells%Name(#{entry})

Type
string

Description
The name of the basis set.

NAOSetCells%nAtoms(#{entry})

Type
int

Description
Number of atoms for a basis set.

NAOSetCells%nCells(#{entry})

Type
int

Description
Number of cells needed for a basis set.

NAOSetCells%nEntries

Type
int

Description
The number of entries (basis sets), for basis sets like valence and core, fit, etc..

NAOSetCells%SkipAtom(#{entry})

Type
bool_array

Description
Sometimes the functions of an atom do not require a cell at all.

Shape
[nAtoms(#{entry}), nCells(#{entry})]

12.2.26 NumericalBasisSets

KF Section: NumericalBasisSets

Content: Specification of numerical atomic basis sets, consisting of a numerical radial table and a spherical harmonic: R_{nl} Y_{lm}.

`NumericalBasisSets%BasisType(#{set},#{type})`

Type
string

Description
Something like valence or core for (type,set). Will not depend on type.

`NumericalBasisSets%bField for GIAO(#{set},#{type})`

Type
float_array

Description
Band only. Finite magnetic field strength for GIAOs.

Shape
[3]

`NumericalBasisSets%d2RadialFuncs(#{set},#{type})`

Type
float_array

Description
The second derivative of the radial functions (for a type,set).

Shape
[NumRad(#{type}), nRadialFuncs(#{set},#{type})]

`NumericalBasisSets%dRadialFuncs(#{set},#{type})`

Type
float_array

Description
The derivative of the radial functions (for a type,set).

Shape
[NumRad(#{type}), nRadialFuncs(#{set},#{type})]

`NumericalBasisSets%Element(#{type})`

Type
string

Description
The chemical element (H,He,Li) for a type.

NumericalBasisSets%GridType(#{type})

Type
string

Description
What kind of radial grid is used. Currently this is always logarithmic.

NumericalBasisSets%ljValues(#{set},#{type})

Type
int_array

Description
Normally for each radial function the l value. In case of spin-orbit there is also a j value (for a type,set).

Shape
[2, nRadialFuncs(#{set},#{type})]

NumericalBasisSets%MaxRad(#{type})

Type
float

Description
Maximum value of the radial grid (for a type).

NumericalBasisSets%MinRad(#{type})

Type
float

Description
Minimum value of the radial grid (for a type).

NumericalBasisSets%nRadialFuncs(#{set},#{type})

Type
int

Description
The number of radial functions (for a type,set).

NumericalBasisSets%nSets

Type
int

Description
The number of basis sets stored for each type. For instance if you store core and the valence basis sets it is two.

NumericalBasisSets%nTypes

Type
int

Description
The number of types: elements with a different basis set. Normally this is just the number of distinct elements in the system.

NumericalBasisSets%NumRad(#{type})

Type
int

Description
The number of radial points (for a type).

`NumericalBasisSets%RadialFuncs(#{set},#{type})`

Type
float_array

Description
The radial functions (for a type,set).

Shape
[NumRad(#{type}), nRadialFuncs(#{set},#{type})]

`NumericalBasisSets%RadialMetaInfo(#{set},#{type})`

Type
float_array

Description
Info about the radial functions. Whether it is a NAO or STO. For instance for an STO the alpha value. All encoded in a real array of fixed size.

Shape
[:, nRadialFuncs(#{set},#{type})]

`NumericalBasisSets%SpherHarmonicType(#{set},#{type})`

Type
string

Description
Either zlm or spinor (type,set). Will not depend on type.

12.2.27 Orbitals

KF Section: Orbitals
Content: Info regarding the orbitals…

`Orbitals%Coefficients(#)`

Type
float_array

Description
for each entry the orbital expansion coefficients.

Shape
[nBasisFunctions, nOrbitals]

`Orbitals%CoefficientsImag(#)`

Type
float_array

Description
for each entry the imaginary part of the orbital expansion coefficients.

Shape
[nBasisFunctions, nOrbitals]

Orbitals%CoefficientsReal(#)

Type
float_array

Description
for each entry the real part of the orbital expansion coefficients.

Shape
[nBasisFunctions, nOrbitals]

Orbitals%Energies(#)

Type
float_array

Description
for each entry the eigen values.

Shape
[nOrbitals]

Orbitals%nBasisFunctions

Type
int

Description
Total number of basis functions.

Orbitals%nEntries

Type
int

Description
The number of sets. For a molecule this is nSpin, for a solid it is nKpoints*nSpin.

Orbitals%nOrbitals

Type
int

Description
The number of orbitals stored for an entry. This can be equal or less than nBasisFunctions

Orbitals%Occupations(#)

Type
float_array

Description
for each entry the Occupations.

Shape
[nOrbitals]

12.2.28 phonon_curves

KF Section: phonon_curves
Content: Phonon dispersion curves.

phonon_curves%brav_type

Type
string

Description
Type of the lattice.

phonon_curves%Edge_#_bands

Type
float_array

Description
The band energies

Shape
[nBands, nSpin, :]

phonon_curves%Edge_#_direction

Type
float_array

Description
Direction vector.

Shape
[nDimK]

phonon_curves%Edge_#_kPoints

Type
float_array

Description
Coordinates for points along the edge.

Shape
[nDimK, :]

phonon_curves%Edge_#_labels

Type
lchar_string_array

Description
Labels for begin and end point of the edge.

Shape
[2]

phonon_curves%Edge_#_lGamma

Type
bool

Description
Is gamma point?

phonon_curves%Edge_#_nKPoints

Type
int

Description
The nr. of k points along the edge.

phonon_curves%Edge_#_vertices

Type
float_array

Description
Begin and end point of the edge.

Shape
[nDimK, 2]

phonon_curves%Edge_#_xFor1DPlotting

Type
float_array

Description
x Coordinate for points along the edge.

Shape
[:]

phonon_curves%indexLowestBand

Type
int

Description
?

phonon_curves%nBands

Type
int

Description
Number of bands.

phonon_curves%nBas

Type
int

Description
Number of basis functions.

phonon_curves%nDimK

Type
int

Description
Dimension of the reciprocal space.

phonon_curves%nEdges

Type
int

Description
The number of edges. An edge is a line-segment through k-space. It has a begin and end point and possibly points in between.

phonon_curves%nEdgesInPath

Type
int

Description
A path is built up from a number of edges.

phonon_curves%nSpin

Type
int

Description
Number of spin components.

Possible values
[1, 2]

phonon_curves%path

Type
int_array

Description
If the (edge) index is negative it means that the vertices of the edge abs(index) are swapped e.g. path = (1,2,3,0,-3,-2,-1) goes though edges 1,2,3, then there's a jump, and then it goes back.

Shape
[nEdgesInPath]

phonon_curves%path_source

Type
string

Description
Source or program used to generate the path.

Possible values
['input', 'kpath', 'seekpath']

phonon_curves%path_type

Type
string

Description
?

12.2.29 Phonons

KF Section: Phonons

Content: Information on the numerical phonons (super cell) setup. NB: the reciprocal cell of the super cell is smaller than the reciprocal primitive cell.

`Phonons%Modes`

Type
float_array

Description
The normal modes with the translational symmetry of the super cell.

Shape
[3, nAtoms, 3, NumAtomsPrim, nK]

`Phonons%nAtoms`

Type
int

Description
Number of atoms in the super cell.

`Phonons%nK`

Type
int

Description
Number of gamma-points (of the super cell) that fit into the primitive reciprocal cell.

`Phonons%NumAtomsPrim`

Type
int

Description
Number of atoms in the primitive cell.

`Phonons%xyzKSuper`

Type
float_array

Description
The coordinates of the gamma points that fit into the primitive reciprocal cell.

Shape
[3, nK]

12.2.30 Plot

KF Section: Plot

Content: Generic section to store x-y plots.

`Plot%numPlots`

Type
int

Description
Number of plots.

`Plot%NumPoints(#)`

Type
int

Description
Number of x points for plot #.

`Plot%NumYSeries(#)`

Type
int

Description
Number of y series for plot #.

`Plot%Title(#)`

Type
string

Description
Title of plot #

`Plot%XLabel(#)`

Type
string

Description
X label for plot #.

`Plot%XUnit(#)`

Type
string

Description
X unit for plot #.

`Plot%XValues(#)`

Type
float_array

Description
X values for plot #.

Shape
[:]

`Plot%YLabel(#)`

Type
string

Description
Y label for plot #.

`Plot%YUnit(#)`

Type
string

Description
Y unit for plot #.

`Plot%YValues(#)`

Type
float_array

Description
Y values for plot #. Array has extra column NumYSeries.

12.2.31 Properties

KF Section: Properties
Content: Generic container for properties.

12.2.32 QMFQ

KF Section: QMFQ
Content: Why is this in the ams.rkf file and not in the adf.rkf file?

`QMFQ%atoms to index`

Type
int_array

Description
?

`QMFQ%atoms to mol label`

Type
int_array

Description
?

`QMFQ%charge constraints`

Type
float_array

Description
?

`QMFQ%external xyz`

Type
float_array

Description
?

QMFQ%fde atoms to index

Type
int_array

Description
?

QMFQ%fde atoms to mol label

Type
int_array

Description
?

QMFQ%fde charge constraints

Type
float_array

Description
?

QMFQ%fde external xyz

Type
float_array

Description
?

QMFQ%fde index to mol label

Type
int_array

Description
?

QMFQ%fde type index

Type
int_array

Description
?

QMFQ%index to mol label

Type
int_array

Description
?

QMFQ%type alpha

Type
float_array

Description
?

QMFQ%type chi

Type
float_array

Description
?

QMFQ%type eta

Type
float_array

Description
?

QMFQ%type index

Type
int_array

Description
?

QMFQ%type name

Type
string

Description
?

QMFQ%type rmu

Type
float_array

Description
?

QMFQ%type rq

Type
float_array

Description
?

12.2.33 QTAIM

KF Section: QTAIM
Content: Bader analysis (Atoms In Molecule): critical points and bond paths.

QTAIM%CoordinatesAlongBPs

Type
float_array

Description
The position of each step point. (bond path index, step index, 3)

Unit
bohr

Shape
[nBondPaths, :, 3]

`QTAIM%CoordinatesCPs`

Type
float_array

Description
Coordinates of the critical points.

Unit
bohr

Shape
[nCriticalPoints, 3]

`QTAIM%DensityAlongBPs`

Type
float_array

Description
The density at that point along the bond path. (bond path index, step index)

Shape
[nBondPaths, :]

`QTAIM%DensityAtCPs`

Type
float_array

Description
Density at the critical points.

Shape
[nCriticalPoints]

`QTAIM%GradientAlongBPs`

Type
float_array

Description
The gradient at that point along the bond path. (bond path index, step index, 3)

Shape
[nBondPaths, :, 3]

`QTAIM%GradientAtCPs`

Type
float_array

Description
Density gradients at the critical points.

Shape
[nCriticalPoints, 3]

`QTAIM%HessianAlongBPs`

Type
float_array

Description
The gradient at that point along the bond path. (bond path index, step index, 6)

Shape
[nBondPaths, :, 6]

`QTAIM%HessianAtCPs`

Type
float_array

Description
Density Hessian at the critical points (6 values, being the upper triangle of the Hessian).

Shape
[nCriticalPoints, 6]

`QTAIM%nBondPaths`

Type
int

Description
Number of bond paths.

`QTAIM%nCriticalPoints`

Type
int

Description
Number of critical points.

`QTAIM%nStepsBondPaths`

Type
int_array

Description
The number of steps each bond path is made of.

Shape
[nBondPaths]

`QTAIM%RankSignatureCPs`

Type
lchar_string_array

Description
Type of critical points. Possible values are: Atom, Cage, Bond, Ring.

Shape
[nCriticalPoints]

12.2.34 RadialAtomicFunctions

KF Section: RadialAtomicFunctions

Content: Info regarding spherical atom centered functions.

RadialAtomicFunctions%d2RadialFunc(#{func},#{type})

Type
float_array

Description
Second derivative of the radial function.

Shape
[NumericalBasisSets%NumRad(#{type})]

RadialAtomicFunctions%dRadialFunc(#{func},#{type})

Type
float_array

Description
Derivative of the radial function.

Shape
[NumericalBasisSets%NumRad(#{type})]

RadialAtomicFunctions%FunctionType(#{func},#{type})

Type
string

Description
FunctionType(a,b) gives the name of function a for type b. It could have a value like core density.

RadialAtomicFunctions%nFunctions

Type
int

Description
The number of radial functions stored for each type. For instance if you store the core and the valence density it is two.

RadialAtomicFunctions%nTypes

Type
int

Description
The number of types: elements with a different basis set. Normally this is just the number of distinct elements in the system.

RadialAtomicFunctions%RadialFunc(#{func},#{type})

Type
float_array

Description
RadialFunc(a,b) gives the radial table for function a for type b

Shape
[NumericalBasisSets%NumRad(#{type})]

12.2.35 SCCLogger

KF Section: SCCLogger

Content: Details on the SCC logger.

12.2.36 Symmetry

KF Section: Symmetry

Content: Info regarding the symmetry of the system.

`Symmetry%nOperators`

Type
int

Description
The number of symmetry operations.

`Symmetry%nsym excitations`

Type
int

Description
The number of symmetries for excitations..

`Symmetry%PointGroupOperators`

Type
float_array

Description
The Point group part of the operators.

Shape
[3, 3, nOperators]

`Symmetry%symlab excitations`

Type
lchar_string_array

Description
labels.

Shape
[nsym excitations]

`Symmetry%Translations`

Type
float_array

Description
The (fractional lattice) translations part of the operators.

Shape
[3, nOperators]

12.2.37 Thermodynamics

KF Section: Thermodynamics

Content: Thermodynamic properties computed from normal modes.

Thermodynamics%Enthalpy

Type
float_array

Description
Enthalpy.

Unit
a.u.

Shape
[nTemperatures]

Thermodynamics%Entropy rotational

Type
float_array

Description
Rotational contribution to the entropy.

Unit
a.u.

Shape
[nTemperatures]

Thermodynamics%Entropy total

Type
float_array

Description
Total entropy.

Unit
a.u.

Shape
[nTemperatures]

Thermodynamics%Entropy translational

Type
float_array

Description
Translational contribution to the entropy.

Unit
a.u.

Shape
[nTemperatures]

Thermodynamics%Entropy vibrational

Type
float_array

Description
Vibrational contribution to the entropy.

Unit
a.u.

Shape
[nTemperatures]

`Thermodynamics%Gibbs free Energy`

Type
float_array

Description
Gibbs free energy.

Unit
a.u.

Shape
[nTemperatures]

`Thermodynamics%Heat Capacity rotational`

Type
float_array

Description
Rotational contribution to the heat capacity.

Unit
a.u.

Shape
[nTemperatures]

`Thermodynamics%Heat Capacity total`

Type
float_array

Description
Total heat capacity.

Unit
a.u.

Shape
[nTemperatures]

`Thermodynamics%Heat Capacity translational`

Type
float_array

Description
Translational contribution to the heat capacity.

Unit
a.u.

Shape
[nTemperatures]

Thermodynamics%Heat Capacity vibrational

Type
float_array

Description
Vibrational contribution to the heat capacity.

Unit
a.u.

Shape
[nTemperatures]

Thermodynamics%Inertia direction vectors

Type
float_array

Description
Inertia direction vectors.

Shape
[3, 3]

Thermodynamics%Internal Energy rotational

Type
float_array

Description
Rotational contribution to the internal energy.

Unit
a.u.

Shape
[nTemperatures]

Thermodynamics%Internal Energy total

Type
float_array

Description
Total internal energy.

Unit
a.u.

Thermodynamics%Internal Energy translational

Type
float_array

Description
Translational contribution to the internal energy.

Unit
a.u.

Shape
[nTemperatures]

Thermodynamics%Internal Energy vibrational

Type
float_array

Description
Vibrational contribution to the internal energy.

Unit
a.u.

Shape
[nTemperatures]

Thermodynamics%lowFreqEntropy

Type
float_array

Description
Entropy contributions from low frequencies (see 'lowFrequencies').

Unit
a.u.

Shape
[nLowFrequencies]

Thermodynamics%lowFreqHeatCapacity

Type
float_array

Description
Heat capacity contributions from low frequencies (see 'lowFrequencies').

Unit
a.u.

Shape
[nLowFrequencies]

Thermodynamics%lowFreqInternalEnergy

Type
float_array

Description
Internal energy contributions from low frequencies (see 'lowFrequencies').

Unit
a.u.

Shape
[nLowFrequencies]

Thermodynamics%lowFrequencies

Type
float_array

Description
Frequencies below 20 cm^-1 (contributions from frequencies below 20 cm^-1 are not included in vibrational sums, and are saved separately to 'lowFreqEntropy', 'lowFreqInternalEnergy' and 'lowFreqInternalEnergy'). Note: this does not apply to RRHO-corrected quantities.

Unit
cm^-1

Shape
[nLowFrequencies]

`Thermodynamics%Moments of inertia`

Type
float_array

Description
Moments of inertia.

Unit
a.u.

Shape
[3]

`Thermodynamics%nLowFrequencies`

Type
int

Description
Number of elements in the array lowFrequencies.

`Thermodynamics%nTemperatures`

Type
int

Description
Number of temperatures.

`Thermodynamics%Pressure`

Type
float

Description
Pressure used.

Unit
atm

`Thermodynamics%RRHOCorrectedHeatCapacity`

Type
float_array

Description
Heat capacity T*S corrected using the 'low vibrational frequency free rotor interpolation corrections'.

Unit
a.u.

Shape
[nTemperatures]

`Thermodynamics%RRHOCorrectedInternalEnergy`

Type
float_array

Description
Internal energy T*S corrected using the 'low vibrational frequency free rotor interpolation corrections'.

Unit
a.u.

Shape
[nTemperatures]

Thermodynamics%RRHOCorrectedTS

Type
float_array

Description
T*S corrected using the 'low vibrational frequency free rotor interpolation corrections'.

Unit
a.u.

Shape
[nTemperatures]

Thermodynamics%Temperature

Type
float_array

Description
List of temperatures at which properties are calculated.

Unit
a.u.

Shape
[nTemperatures]

Thermodynamics%TS

Type
float_array

Description
T*S, i.e. temperature times entropy.

Unit
a.u.

Shape
[nTemperatures]

12.2.38 TransferIntegrals

KF Section: TransferIntegrals

Content: Charge transfer integrals relevant for hole or electron mobility calculations. Electronic coupling V (also known as effective (generalized) transfer integrals J_eff) V = (J-S(e1+e2)/2)/(1-S^2). For electron mobility calculations the fragment LUMOs are considered. For hole mobility calculations the fragment HOMOs are considered.

`TransferIntegrals%Determinant`

Type
float

Description
Determinant related to overlap integrals used in ADF FOCDFT%electrontransfer.

`TransferIntegrals%e1(electron)`

Type
float

Description
Site energy LUMO fragment 1.

Unit
hartree

`TransferIntegrals%e1(hole)`

Type
float

Description
Site energy HOMO fragment 1.

Unit
hartree

`TransferIntegrals%e2(electron)`

Type
float

Description
Site energy LUMO fragment 2.

Unit
hartree

`TransferIntegrals%e2(hole)`

Type
float

Description
Site energy HOMO fragment 2.

Unit
hartree

`TransferIntegrals%Electronic coupling`

Type
float

Description
Electronic coupling calculated by ADF FOCDFT%electrontransfer.

`TransferIntegrals%J(charge recombination 12)`

Type
float

Description
Charge transfer integral HOMO fragment 1 - LUMO fragment 2 for charge recombination 1-2.

Unit
hartree

`TransferIntegrals%J(charge recombination 21)`

Type
float

Description
Charge transfer integral LUMO fragment 1 - HOMO fragment 2 for charge recombination 2-1.

Unit
hartree

`TransferIntegrals%J(electron)`

Type
float

Description
Charge transfer integral LUMO fragment 1 - LUMO fragment 2 for electron transfer.

Unit
hartree

`TransferIntegrals%J(hole)`

Type
float

Description
Charge transfer integral HOMO fragment 1 - HOMO fragment 2 for hole transfer.

Unit
hartree

`TransferIntegrals%S(charge recombination 12)`

Type
float

Description
Overlap integral HOMO fragment 1 - LUMO fragment 2 for charge recombination 1-2.

`TransferIntegrals%S(charge recombination 21)`

Type
float

Description
Overlap integral LUMO fragment 1 - HOMO fragment 2 for charge recombination 2-1.

`TransferIntegrals%S(electron)`

Type
float

Description
Overlap integral LUMO fragment 1 - LUMO fragment 2.

`TransferIntegrals%S(hole)`

Type
float

Description
Overlap integral HOMO fragment 1 - HOMO fragment 2.

`TransferIntegrals%V(charge recombination 12)`

Type
float

Description
Effective charge transfer integral HOMO fragment 1 - LUMO fragment 2 for charge recombination 1-2.

Unit
hartree

`TransferIntegrals%V(charge recombination 21)`

Type
float

Description
Effective charge transfer integral LUMO fragment 1 - HOMO fragment 2 for charge recombination 2-1.

Unit
hartree

`TransferIntegrals%V(electron)`

Type
float

Description
Effective transfer integral LUMO fragment 1 - LUMO fragment 2 for electron transfer.

Unit
hartree

`TransferIntegrals%V(hole)`

Type
float

Description
Effective transfer integral HOMO fragment 1 - HOMO fragment 2 for hole transfer.

Unit
hartree

`TransferIntegrals%Vtot(charge recombination 12)`

Type
float

Description
Total electronic coupling for charge recombination 1-2.

Unit
hartree

TransferIntegrals%Vtot(charge recombination 21)

Type
float

Description
Total electronic coupling for charge recombination 2-1.

Unit
hartree

TransferIntegrals%Vtot(electron)

Type
float

Description
Total electronic coupling for electron transfer.

Unit
hartree

TransferIntegrals%Vtot(hole)

Type
float

Description
Total electronic coupling for hole transfer.

Unit
hartree

12.2.39 Vibrations

KF Section: Vibrations
Content: Information related to molecular vibrations.

Vibrations%ExcitedStateLifetime

Type
float

Description
Raman excited state lifetime.

Unit
hartree

Vibrations%ForceConstants

Type
float_array

Description
The force constants of the vibrations.

Unit
hartree/bohr^2

Shape
[nNormalModes]

`Vibrations%Frequencies[cm-1]`

Type
float_array

Description
The vibrational frequencies of the normal modes.

Unit
cm^-1

Shape
[nNormalModes]

`Vibrations%Intensities[km/mol]`

Type
float_array

Description
The intensity of the normal modes.

Unit
km/mol

Shape
[nNormalModes]

`Vibrations%IrReps`

Type
lchar_string_array

Description
Symmetry symbol of the normal mode.

Shape
[nNormalModes]

`Vibrations%ModesNorm2`

Type
float_array

Description
Norms of the rigid motions.

Shape
[nNormalModes+nRigidModes]

`Vibrations%ModesNorm2*`

Type
float_array

Description
Norms of the rigid motions (for a given irrep…?).

Shape
[nNormalModes+nRigidModes]

Vibrations%nNormalModes

Type
int

Description
Number of normal modes.

Vibrations%NoWeightNormalMode(#)

Type
float_array

Description
?.

Shape
[3, Molecule%nAtoms]

Vibrations%NoWeightRigidMode(#)

Type
float_array

Description
?

Shape
[3, Molecule%nAtoms]

Vibrations%nRigidModes

Type
int

Description
Number of rigid modes.

Vibrations%nSemiRigidModes

Type
int

Description
Number of semi-rigid modes.

Vibrations%PVDOS

Type
float_array

Description
Partial vibrational density of states.

Values range
[0.0, 1.0]

Shape
[nNormalModes, Molecule%nAtoms]

Vibrations%RamanDepolRatioLin

Type
float_array

Description
Raman depol ratio (lin).

Shape
[nNormalModes]

Vibrations%RamanDepolRatioNat

Type
float_array

Description
Raman depol ratio (nat).

Shape
[nNormalModes]

Vibrations%RamanIncidentFreq

Type
float

Description
Raman incident light frequency.

Unit
hartree

Vibrations%RamanIntens[A^4/amu]

Type
float_array

Description
Raman intensities

Unit
A^4/amu

Shape
[nNormalModes]

Vibrations%ReducedMasses

Type
float_array

Description
The reduced masses of the normal modes.

Unit
a.u.

Values range
[0, '\infinity']

Shape
[nNormalModes]

Vibrations%RotationalStrength

Type
float_array

Description
The rotational strength of the normal modes.

Shape
[nNormalModes]

`Vibrations%TransformationMatrix`

Type
float_array

Description
?

Shape
[3, Molecule%nAtoms, nNormalModes]

`Vibrations%VROACIDBackward`

Type
float_array

Description
VROA Circular Intensity Differential: Backward scattering.

Unit
10ˉ3

Shape
[nNormalModes]

`Vibrations%VROACIDDePolarized`

Type
float_array

Description
VROA Circular Intensity Differential: Depolarized scattering.

Unit
10ˉ3

Shape
[nNormalModes]

`Vibrations%VROACIDForward`

Type
float_array

Description
VROA Circular Intensity Differential: Forward scattering.

Unit
10ˉ3

Shape
[nNormalModes]

`Vibrations%VROACIDPolarized`

Type
float_array

Description
VROA Circular Intensity Differential: Polarized scattering.

Unit
10¯3

Shape
[nNormalModes]

Vibrations%VROADeltaBackward

Type
float_array

Description
VROA Intensity: Backward scattering.

Unit
10¯3 A^4/amu

Shape
[nNormalModes]

Vibrations%VROADeltaDePolarized

Type
float_array

Description
VROA Intensity: Depolarized scattering.

Unit
10¯3 A^4/amu

Shape
[nNormalModes]

Vibrations%VROADeltaForward

Type
float_array

Description
VROA Intensity: Forward scattering.

Unit
10¯3 A^4/amu

Shape
[nNormalModes]

Vibrations%VROADeltaPolarized

Type
float_array

Description
VROA Intensity: Polarized scattering.

Unit
10¯3 A^4/amu

Shape
[nNormalModes]

`Vibrations%ZeroPointEnergy`

Type
float

Description
Vibrational zero-point energy.

Unit
hartree

12.2.40 WScell(reciprocal_space)

KF Section: WScell(reciprocal_space)
Content: The Wigner Seitz cell of reciprocal space, i.e. the Brillouin zone.

`WScell(reciprocal_space)%boundaries`

Type
float_array

Description
Normal vectors for the boundaries.

Shape
[ndim, nboundaries]

`WScell(reciprocal_space)%distances`

Type
float_array

Description
Distance to the boundaries.

Shape
[nboundaries]

`WScell(reciprocal_space)%idVerticesPerBound`

Type
int_array

Description
The indices of the vertices per bound.

Shape
[nvertices, nboundaries]

`WScell(reciprocal_space)%latticeVectors`

Type
float_array

Description
The lattice vectors.

Shape
[3, :]

`WScell(reciprocal_space)%nboundaries`

Type
int

Description
The nr. of boundaries for the cell.

`WScell(reciprocal_space)%ndim`

Type
int

Description
The nr. of lattice vectors spanning the Wigner-Seitz cell.

`WScell(reciprocal_space)%numVerticesPerBound`

Type
int_array

Description
The nr. of vertices per bound.

Shape
[nboundaries]

`WScell(reciprocal_space)%nvertices`

Type
int

Description
The nr. of vertices of the cell.

`WScell(reciprocal_space)%vertices`

Type
float_array

Description
The vertices of the bounds.

Unit
a.u.

Shape
[ndim, nvertices]

CHAPTER

THIRTEEN

FAQ

13.1 Which DFTB parameters are available?

The DFTB module in the Amsterdam Modeling Suite ships with the following parameter sets:

- GFN1-xTB (https://doi.org/10.1021/acs.jctc.7b00118): extended tight-binding parameters for elements H-Rn (all spd elements). Can be used for all properties.
- Quasinano 2013 (https://dx.doi.org/10.1021/ct4004959): electronic parameters for H-Po, La, Th, enabling electronic properties like band structures, DOS, UV/VIS, NEGF.
- Quasinano 2015 (https://dx.doi.org/10.1021/acs.jctc.5b00702): + repulsive parameters for H-Ca, Br, enabling geometry optimization, IR spectra, MD.
- Dresden parameters: C, H, O, N, P, S, Al, Si, Ti, Cu, Na, see **$ADFHOME/atomicdata/DFTB/Dresden/README**
- DFTB.org (https://www.dftb.org/) parameters (see README or the DFTB.org website for latest info). Encrypted parameters may also be evaluated during a trial.
- Dispersion corrections available (Grimme's D2 & D3(BJ), London, UFF).

See the *documentation on the available DFTB parameter sets* (page 68).

13.2 Can I use Grimme's D3(BJ) dispersion corrections?

Yes, with DFTB3 and either the Quasinano or the DFTB.org 3ob parameter sets. With other DFTB methods and parameter sets you can use D2, London (ULG), or UFF dispersion.

13.3 Do you have the extended Tight-Binding (xTB) parameters?

We have implemented Grimme's first GFN-xTB method (GFN1-xTB). The second set (GFN2-xTB) usually does not improve accuracy much and has not yet been implemented.

13.4 Can I include electric fields?

Yes.

13.5 Can I study 1D periodic systems like carbon nanotubes?

Yes, DFTB can be applied to 0D systems (molecules), 1D systems (polymers, nanotubes), 2D systems (surfaces), and 3D systems (bulk).

For 1D and 2D systems, we have proper periodic boundary conditions. So you do not need to work with large unit cells and slab-gap approximations.

All DFTB parameters can be used for any periodicity.

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