



DFTB Manual

Amsterdam Modeling Suite 2023.1

www.scm.com

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1.1 Introduction

The DFTB engine implements density functional based tight-binding methods, which can be viewed as computationally very efficient approximations to density functional theory (DFT). As such it is a good engine for cheap 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 DFTB2023.1

- Improved SCC convergence with the *MultiStepper* (page 14).

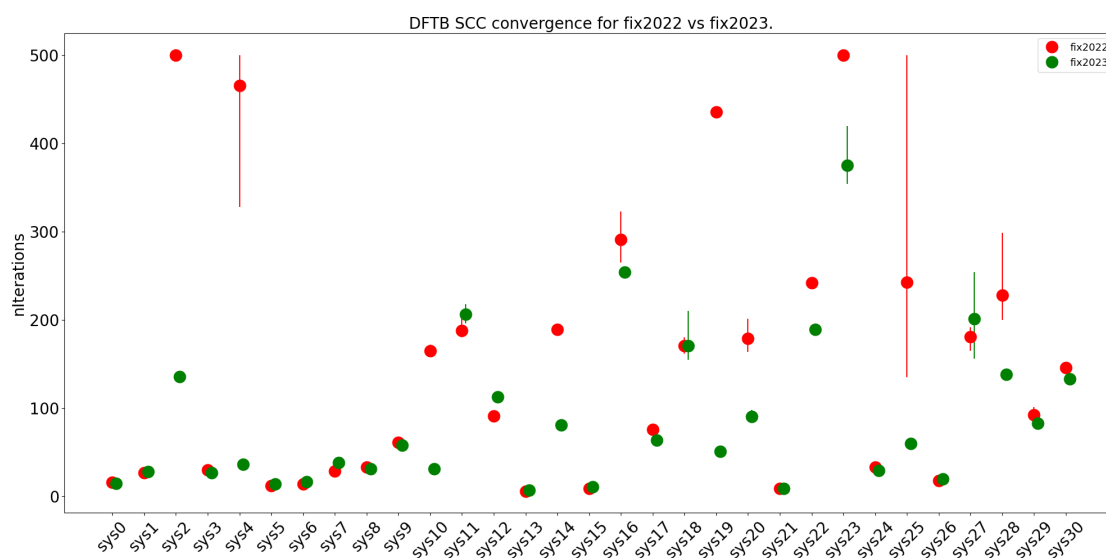


Fig. 1.1: Comparison of the number of SCC cycles needed. For easy systems there is not much difference, for more difficult systems, however, the fix2023 (green) is an improvement over the fix2022 (red). As there can be some randomness in the number of iterations the calculations are repeated five times (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.

1.2.2 New in DFTB2022.1

- Visualization of orbitals in AMSview now also works for calculations with (most) DFTB.org parameter sets.
- *Fragment orbital analysis* (page 37)
- *Charge transport (transfer integrals)* (page 47)

1.2.3 New in DFTB2021.1

- The D4 *dispersion correction* (page 8) has been added. It can be used with the Slater-Koster based model Hamiltonians and the DFTB.org parameter sets.

1.2.4 New in DFTB2020

- Calculations with the *GFN1-xTB model* (page 7) 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.

1.2.5 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 22) 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 22) are generally faster and scale much better on parallel machines.
 - The *GFN1-xTB model* (page 7) can now be used together with *k-space integration* (page 22).
 - *Unrestricted calculations* (page 10) can now also be performed in conjunction with *k-space integration* (page 22).
 - The orbital dependent (l-dependent) *SCC cycle* (page 10) is now compatible with *k-space integration* (page 22).
 - The *stress tensor* is now calculated analytically, making its calculation faster and the result more accurate.
- An *implicit solvation model* (page 9) (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.

1.2.6 New in DFTB2019.1

- Grimme's GFN1-xTB has been added as a new *model Hamiltonian* (page 7). 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 22).
- More robust SCC convergence:

- *Adaptive mixing* (page 10): 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.

1.2.7 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 to 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
```

(continues on next page)

(continued from previous page)

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
    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
```

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.

In 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 systems' net charge, the lattice vector, 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)

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 precalculation 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 (recently also called DFTB2), which accounts for density fluctuations and improves results on polar bonds. Note that the self-consistent calculations is about an order of magnitude slower than calculations with the “plain” DFTB Hamiltonian.
- The third order extension known as DFTB3, which improve 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 as recently been 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 Schroedinger 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 280).

```
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 279).

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 corrections 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), thus the user may first want to evaluate if 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 the 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 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 upon 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 is the mix factor σ . The default method is the *MultiStepper* (page 14), which is explained separately. The older *DIIS* (page 20) method is more simple 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
  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 $2/\sqrt{n\text{Atoms}}$.

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.

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) Boltmann 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.

3.6.1 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

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

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 to loaded is controlled by the `SCF%MultiStepperPresetPath` key, and this may be an absolute path to your own preset.

The 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
    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=Trials. 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 SCFMultiStepper block is in the input, and Method=MultiStepper. If the path is not absolute, it is relative to \$AMSHOME/data/presets/multi_stepper'

3.6.2 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

```

(continues on next page)

(continued from previous page)

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.

3.7 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
  Quality [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).

Quality

Type Multiple Choice

Default value Normal

Options [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 'GammaOnly', only one point (the gamma point) will be used.

For the other options, the actual number of K points generated depends 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).

3.8 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.

3.9 Technical options

```

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

SPECTROSCOPY AND PROPERTIES

4.1 Electronic structure of periodic systems

```
Periodic
  EffectiveMass
    Enabled Yes/No
    KPointCoord float_list
    NumAbove integer
    NumBelow integer
    StepSize float
  End
  BandStructure
    Automatic Yes/No
    DeltaK float
    Enabled Yes/No
    FatBands Yes/No
    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

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.

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.**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 (<http://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 transitions: 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 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 30).

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 with

```
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 the exact 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. Weinholds Natural Bond Orbital (NBO) package, by E. Glendening et al. can be made, 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
```

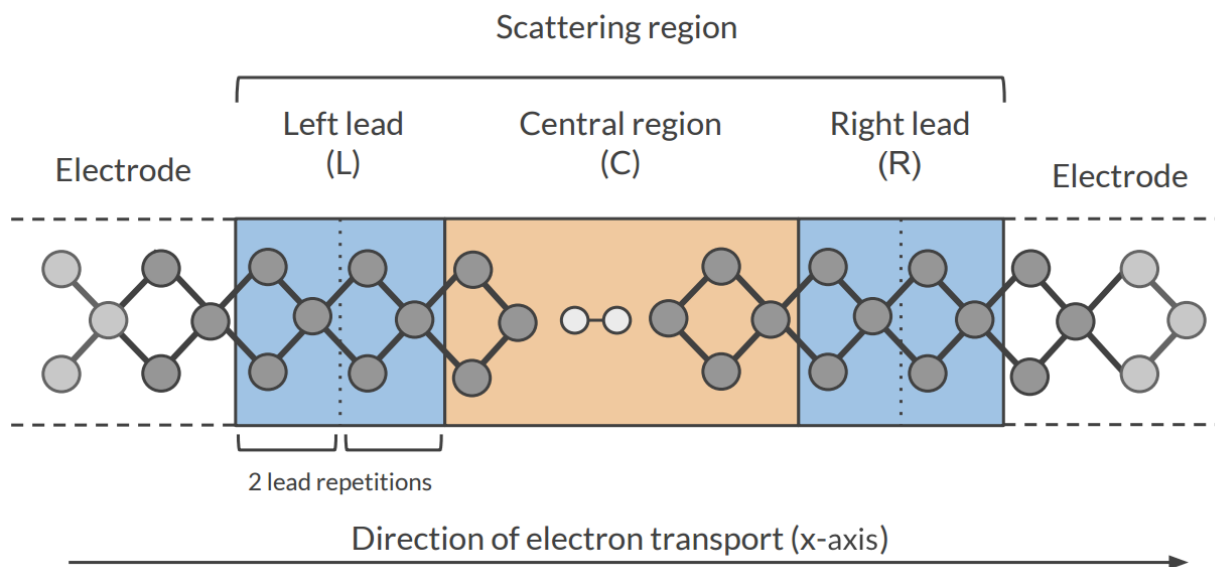

ELECTRONIC TRANSPORT (NEGF)

See also:

- DFTB-NEGF GUI tutorials
- *Example: Electronic transport with NEGF* (page 254)

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:

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

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:

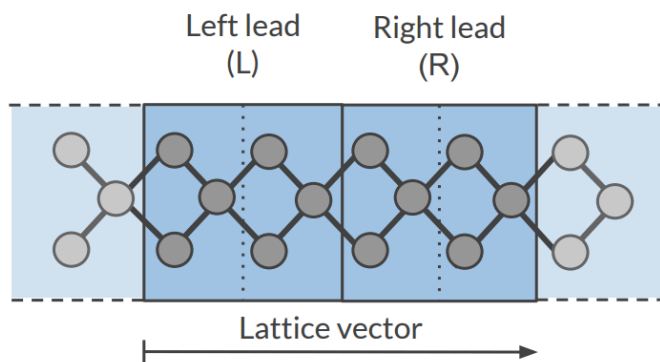
[PhD Thesis](https://opus.jacobs-university.de/frontdoor/index/index/docId/478) (https://opus.jacobs-university.de/frontdoor/index/index/docId/478) of Mahdi Ghorbani-Asl (DFTB-NEGF developer)

5.2 Simulations work flow

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

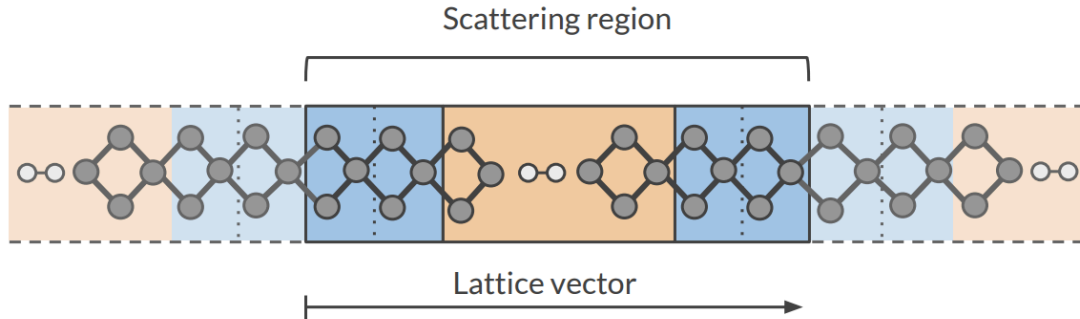
Tip: Use ADFInput (GUI) to set up your DFTB-NEGF calculation (see the [DFTB-NEGF GUI tutorials](#))

1): DFTB leads calculation A 1D-periodic DFTB calculation of the leads (*StoreMatrices* (page 26): yes, *KSpace* (page 22) 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 26): yes, gamma-only, *i.e.*, no *KSpace* (page 22) 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.

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, one 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 257)

In theoretical models of charge transport in organic materials, see Refs.¹²³, 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 the 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 LUMO's are considered. For hole mobility calculations the fragment HOMO's are considered.

To calculate the charge transfer integrals, spatial overlap integrals and site energies, the molecular system typically should be build from 2 fragments. See also the section on *Fragment orbital analysis* (page 37). 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. To calculate the matrix elements and overlap integrals based on all fragment orbitals one can use the key:

If 2 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 $V = (J - S(e_1 + e_2)/2)/(1 - S^2)$. Here e_1 , e_2 , are the site energies of fragment 1 and 2, respectively. J is the charge transfer integral, and S the overlap integral.

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

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 represent 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.

E_{Max}

Type Float

Default value 0.25

Unit Hartree

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

E_{min}

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.

EXAMPLES

The `$AMSHOME/examples/dftb` directory contains many different example files, covering various DFTB options.

7.1 Model Hamiltonians

7.1.1 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

```

7.1.2 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

```

7.1.3 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
```

7.1.4 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
```

7.1.5 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
```

7.1.6 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
```

7.1.7 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

```

7.1.8 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

7.1.9 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
```

7.1.10 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
```

7.1.11 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
```

7.1.12 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
```

7.1.13 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
```

7.1.14 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

```

7.1.15 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

```

7.1.16 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			

7.1.17 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
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H	13.51018455	-7.05296175	8.67255017
H	15.63980455	-8.28311175	8.67320017
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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
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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
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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
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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
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H	8.07537455	2.37845725	8.54192017
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H	12.39697355	4.83820925	8.54703017

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C	10.92390355	11.08010825	8.62322017
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C	8.84107455	9.87417825	8.62592017
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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
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B	-14.37469545	11.54140825	8.66010017
B	13.12031355	11.54945825	8.60922017
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H	-16.92696545	10.51931825	8.67320017
H	-14.76494545	14.26115825	8.67473017
H	-16.89478145	15.49164825	8.67190017
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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
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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
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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 23.25256355 -13.96422075 8.54703017
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C 20.38977455 -7.72440175 8.63670017
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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

```

7.1.18 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

```

7.1.19 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
```

7.1.20 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

```

7.1.21 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 QUASINANO20213.1
    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 QUASINANO20213.1
        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
```

7.1.22 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
```

7.1.23 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_ldesp.results/dftb.rkf

EOF

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

AMS_JOBNAME=gen_ldespq $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_ldespq $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
```

7.1.24 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

```

7.2 Geometry Optimization

7.2.1 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

```

7.2.2 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
```

7.2.3 Example: GO aspirin SCMGO

Download GO_SCMGO_aspirin_SCC.run

```
#!/bin/sh

$AMSBIN/ams << eor

task GeometryOptimization

Properties
  NormalModes True
End

GeometryOptimization
  method scmgo
  Convergence
    Gradients 1.0E-5
  end
End

System
```

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```

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

```

7.2.4 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
```

7.2.5 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

```

7.2.6 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
```


7.2.7 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"

```

7.2.8 Example: GO poly-ethylene

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

```

7.2.9 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
```

7.2.10 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=pbccatom "$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
    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
      C 1.303528070245188 -0.1416812092038768 0.7303699949711653
↪region=phenyl2

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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	┌
↔region=phenyl4				
H	2.017471491684088	3.023369029562452	3.242524256706377	┌
↔region=phenyl4				

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      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
  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
  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

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```
C 1.2274512359848 0.7092866246929653 -1.981478017299119
C 2.455989750017203 -0.000767672446473915 -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 -0.7103491590560944 -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 -3.547614761418386 -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
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
```

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```
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 2.127406352683383 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
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
```

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```
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
    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
```

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```
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
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
```

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```
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 -0.06737899999999999999 -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 -0.090550000000000001 3.867554
H 3.909847 0.420825 3.041412
H 2.839161 -0.79507399999999999999 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
H -0.857142 -3.347281 -2.055678
H 0.888225 -3.744967 -2.034598
H -0.156019 -4.368152 -3.348409
```

End

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```

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

```

7.2.11 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

Restrains
# 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
DifDist  2 3 1 4       0.2
Dihedral 4 1 2 3     180.0    0.1
End

```

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```
Engine DFTB
  Model GFN1-xTB
EndEngine
EOR
```

7.2.12 Example: GO BakerSet SCMGO

Download `SCMGO_BakerSet.run`

```
#!/bin/sh

for mol in $(find $AMSRESOURCES/Molecules/Misc/baker*.xyz)
do
  job=$(basename $mol)

  AMS_JOBNAME=$job $AMSBIN/ams << eor

  task GeometryOptimization

  GeometryOptimization
    Method SCMGO
    Convergence
      Gradients 1.0E-4
      Step 1.0e-3
    end
  end

  system
    GeometryFile $mol
  end

  engine dftb
    Model SCC-DFTB
    resourcesdir QUASINANO2015
  endengine
eor

echo 'Number of GO Steps '$mol' " " $(($AMSBIN/amsreport $job.results/ams.rkf -r
↪ "History%nEntries")
echo 'Final Energy '$mol' " " $(($AMSBIN/amsreport $job.results/dftb.rkf -r
↪ "AMSResults%Energy")
done
```

7.2.13 Example: GO polyethylene SCMGO plams

Download SCMGO_PE.run

```
$AMSBIN/plams $AMSHOME/examples/dftb/SCMGO_PE/SCMGO_PE.plms
```

Download SCMGO_PE.plms

```
import os
import random

# Set random seed to ensure reproducibility
random.seed(666)

def randomize_xyz(mol, random_size=0.01):
    mol_pert = mol.copy()
    for atom in mol_pert:
        transl = [random.uniform(-1,1)*random_size for i in range(3)]
        atom.translate(transl)
    return mol_pert

def run_optimization(molecule, settings, title):
    print("===== input for {} =====".format(title))
    job = AMSJob(molecule=molecule, settings=settings)
    print(job.get_input())
    job.run()
    energy = job.results.readrkf('AMSResults', 'Energy', file='dftb')
    nSteps = job.results.readrkf('History', 'nEntries', file='ams')
    return energy, nSteps

molecules_dir=os.path.join(os.environ['AMSHOME'],'atomicdata','Molecules','Misc')

molecules = []
for mol_name in sorted(os.listdir(molecules_dir)):
    if 'Polyethylene' in mol_name:
        molecules.append(Molecule(os.path.join(molecules_dir,mol_name)))

sett = Settings()
sett.input.ams.UseSymmetry = False
sett.input.ams.Task = 'GeometryOptimization'
sett.input.ams.GeometryOptimization.Method = 'SCMGO'
sett.input.ams.GeometryOptimization.Convergence.Gradients = 5.0E-5
sett.input.ams.GeometryOptimization.Convergence.Step = 4.0E-3

sett.input.dftb.model = 'DFTB0'
sett.input.dftb.resourcesdir = 'QUASINANO2015'

for mol in molecules:
    rand_small = randomize_xyz(mol,0.05)
    rand_large = randomize_xyz(mol,0.2)

    e_unper, n_unper = run_optimization(molecule=mol, settings=sett, title=
↳ 'Unperturbed ({}>'.format(mol.properties.name))
```

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```

e_small, n_small = run_optimization(molecule=rand_small, settings=set, title=
↪'Small perturbation ({}).format(mol.properties.name))
e_large, n_large = run_optimization(molecule=rand_large, settings=set, title=
↪'Large perturbation ({}).format(mol.properties.name))

print("")
print("Summary for molecule {}".format(mol.properties.name))
print("Energy unperturbed: {}".format(e_unper))
print("Delta Energy medium perturbation : {}".format(abs(e_unper-e_small)))
print("Delta Energy large perturbation : {}".format(abs(e_unper-e_large)))
print("N steps small/medium/large perturbations: {} / {} / {}".format(n_unper,n_
↪small,n_large))
print("")

```

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

printf "\n\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

```

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```

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

rm -rf $AMS_JOBNAME.results

$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

```

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```

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)" >> $report
echo "">>$report

done
done

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

```

7.2.15 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

```

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```

    Excitations
      TDDFTB
        Calc singlet
        Lowest 1
        Diagonalization exact
      End
      TDDFTBGradients
        Excitation 1
      End
    End
  End
EndEngine
eor

```

7.2.16 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

```

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```
        End
      End
    End
  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
```


7.3 PESScan, Linear Transit, Transition State, NEB

7.3.1 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

```

7.3.2 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
```

7.3.3 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

```

7.3.4 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"

```

7.3.5 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

```

7.3.6 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"

```

7.3.7 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
```

7.4 Electronic structure of periodic systems

7.4.1 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

```

7.5 Excited States

7.5.1 Example: Fullerene excitations

Download SP_LR-TDDFTB_fullerene.run

```

#!/bin/sh

AMS_JOBNAME=SOOnly $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

```

7.5.2 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

```

7.5.3 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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```

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 evcontri
    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
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
EndEngine

eor

# =====
# Ketene
# =====

AMS_JOBNAME=ketene $AMSBIN/ams << eor

Task SinglePoint

```

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```
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

```

7.5.4 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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```

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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```

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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```

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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```

                ATCharges onTheFly
            End
        print evcontriBs
    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

```

7.5.5 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
  End

```

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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
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

```

7.5.6 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+'.npz'):
        print('Precalculated numerical gradient found -> reading from file')
        numgrad = np.load('./numgrad_precalc/'+teststr+'.npz')
    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)
        numgrad = Units.conversion_ratio('bohr', 'angstrom') * numgrad

```

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```

    # 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)

```

7.5.7 Example: Excitations SOT filter

Download SP_LR-TDDFTB_grimmefilter.run

```

#!/bin/sh

AMS_JOBNAME=noPertCorr $AMSBIN/ams << eor

Task SinglePoint

System
  Atoms
    Ir      0.04420    -0.00850    -0.05250
    N      -0.03840    -0.02260     2.09450

```

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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
C	-1.07890	-4.76580	-0.01610
H	-1.36750	-5.81370	-0.01700
C	-2.04030	-3.76920	-0.20280

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```

      H      -3.07920      -4.05800      -0.34770
      H       1.02320      -5.17010       0.31590
    End
  End
EndEngine

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
    H       3.90660      -0.04300       3.29620
    H       5.23270      -0.08580      -0.79660
    C       0.28050       0.12200      -2.02430

```

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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

End

TDDFTB

 Calc singlet

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(continued from previous page)

```

        Print evcontriBs
      End
    End
  End
EndEngine
eor

```

7.5.8 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
    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 false

End

Properties

Excitations

SingleOrbTrans

Filter

OSMin 0.0001

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        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
    C      5.02671217       1.78315021      -9.77819438
    C     -2.76322583      -0.21060941       0.58045389
    C      1.61310315       4.08163625      -4.15853296

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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
C	0.21729712	0.43018409	10.40014258

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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
C	-4.58861684	-0.45480589	7.38332328

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(continued from previous page)

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
End

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        printlowest 50
    End
    TDDFTB
        Calc singlet
        Lowest 20
        Print evcontriBs
    End
End
End
EndEngine

eor

echo 'SINGLET-TRIPLET (atomic) '

AMS_JOBNAME=ST_atomic $AMSBIN/ams << eor

Task SinglePoint

System
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    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
    C      1.61310315       4.08163625      -4.15853296
    H      1.65781749      -1.38443872     -10.88135435

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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
C	0.21729712	0.43018409	10.40014258
H	-3.02101125	-3.22412477	-1.01674298

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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
C	-4.58861684	-0.45480589	7.38332328
C	3.55447069	5.59373051	-4.79121698

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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
SingleOrbTrans
Filter
OSMin 0.0001
End
PrintLowest 50

(continues on next page)

(continued from previous page)

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        End
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        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
    C      1.61310315       4.08163625      -4.15853296
    H      1.65781749      -1.38443872     -10.88135435
    H      5.20362845       2.30053217     -10.72284683

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(continued from previous page)

N	0.98411405	-0.08507509	1.63291837
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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
C	0.21729712	0.43018409	10.40014258
H	-3.02101125	-3.22412477	-1.01674298
H	-1.33836424	0.41028647	-6.12174251

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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
C	-4.58861684	-0.45480589	7.38332328
C	3.55447069	5.59373051	-4.79121698
C	5.00971521	-1.65242908	-4.39564865

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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

End

PrintLowest 50

End

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```

        TDDFTB
            Calc triplet
            Lowest 20
            Print evcontriBs
        End
    End
End
EndEngine
eor

```

7.5.9 Example: Excitations benchmark

Download SP_LR-TDDFTB_tbe.run

```

#!/bin/sh

echo Singlet Excitations
for f in $(find $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>out
grep Excitation out
done
echo Ready

echo Triplet Excitations
for f in $(find $AMSHOME/examples/dftb/SP_LR-TDDFTB_tbe/molecules/*.xyz)
do
cat <<eor > in
System

```

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```

    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
End
EndEngine
eor
g=`basename $f .xyz`
echo $g
AMS_JOBNAME=${g}_ST $AMSBIN/ams <in>out
grep Excitation out
done
echo Ready

```

7.5.10 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
        C      -1.67096000      1.41980000      -1.15887000
        C      -0.38686000      2.25210000      -1.41391000
        C      -1.74087000      0.49471000      -0.15347000

```

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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	-0.711197000
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
H	-5.69282000	-0.64720000	-3.25046000
H	-4.00625000	2.99962000	-4.36844000
H	-5.76674000	2.88684000	-4.54145000

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```

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
    End
  End
End
End

```

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```
EndEngine
```

7.6 Vibrations, IR spectra, Normal Modes, VCD

7.6.1 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
  ResourcesDir Dresden
  DispersionCorrection Auto
EndEngine
```

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eor

7.6.2 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

eor
```

7.6.3 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
```

7.6.4 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
  End
  Charge -1
End

Engine DFTB
```

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```

Model SCC-DFTB
ResourcesDir Dresden
Repulsion
    forcePolynomial true
End
EndEngine
eor

```

7.6.5 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

AMS_JOBNAME=sym $AMSBIN/ams << eor

Task SinglePoint

```

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```

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

```

7.6.6 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
    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

```

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```

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

```

End

End

Engine DFTB

Model DFTB3

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```
ResourcesDir DFTB.org/3ob-3-1
DispersionCorrection D3-BJ
EndEngine
EOF
```

7.6.7 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
      End
    TDDFTBGradients
      Excitation 1
    End
  End
End
```

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```

End
EndEngine

eor

```

7.6.8 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')
    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()

```

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```

# ===== 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')))

# ===== 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'

```

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```

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')
    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]

```

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```

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)

```

7.6.9 Example: Vibrational circular dichroism

Download `FREQ_HNDT_VCD.run`

```

#!/bin/sh

$AMSBIN/ams << eor

Task SinglePoint

Properties
  VCD true
End

```

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```

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

```

7.7 Phonons

7.7.1 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
      0 2
    End
  End

  System
    Atoms
      C  0.000000000  -0.000000000  0.00000
      C  0.000000000  -1.420281662  0.00000
    End

    Lattice

```

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```

        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"

```

7.7.2 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

  NumericalPhonons
    StepSize 0.01
    SuperCell
      4
    End
  End

  System
    Atoms
      C  -2.42906152   -0.3445528299   -0.1353492062
      C  -1.146891508  -1.134644249    0.1353492061
    End
  End

```

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```

      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
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

```

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```

        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"

```

7.7.3 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
  End

  GeometryOptimization
    OptimizeLattice Yes
    Convergence Gradients=1e-5 StressEnergyPerAtom=1E-5
    Method Quasi-Newton
  End

  EngineAddons
    Pressure $P
  End

```

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```

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

```

7.8 Stress tensor, Elasticity

7.8.1 Example: Stress tensor

Download `SP_stresstensor.run`

```

#!/bin/sh
$AMSBIN/ams << EOF

Task SinglePoint

Properties
  StressTensor True
End

System
  Atoms
    C1      -3.27413732      17.07951309      11.46590854
    C1       4.99858729       7.77406309       8.27058240
    C1       7.93893730       1.53138691       1.69175208
    C1      -0.33378731      10.83683691       4.88707823
    C1      -2.62283362      13.61069415      10.36587591
    C1       4.34728360       4.30524415       9.37061503
    C1       7.28763360       5.00020585       2.79178471
    C1       0.31751639      14.30565585       3.78704560

```

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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
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

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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
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

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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
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

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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
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

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```

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

```

7.8.2 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
    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

```

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```

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

```

7.8.3 Example: Elastic tensor

Download ElasticTensor.run

```

#!/bin/sh

# === Diamond ===
AMS_JOBNAME=Diamond $AMSBIN/ams << EOF

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

```

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```

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

AMS_JOBNAME=BN_sheet $AMSBIN/ams << EOF

Task GeometryOptimization

Properties
  ElasticTensor Yes
End

System
  Atoms
    N 3.76095075 0.723795 0.0

```

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```

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
ElasticTensor Yes
End

ElasticTensor
StrainStepSize 0.002
End

System
Atoms
C -0.279368361 -0.125344097 -0.026221791
O 0.840592835 -0.919621431 -0.193214154

```

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```

      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"

```

7.9 Molecular Dynamics

7.9.1 Example: Molecular dynamics

Download MD_aspirin.run

```

#!/bin/sh

$AMSBIN/ams << eor

Task MolecularDynamics

```

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```

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
  End
  DispersionCorrection Auto
EndEngine

eor

```

7.9.2 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

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
  
```

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```

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

```

7.9.3 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

```

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```
        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
```

7.9.4 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

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
```

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```
eor
```

7.9.5 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
  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
    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
```

7.10 Electronic transport, NEGF

7.10.1 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
      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
```

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```

        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"

# =====
#   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

```

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```
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
    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
```

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```

# 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"

```

7.10.2 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
  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

```

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```
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 -1.27644482466 -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
  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
```

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```

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
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 "$SAMSBIN/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

```

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```
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
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
```

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```
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
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
```

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```
eor
```

7.11 Analysis

7.11.1 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

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
```

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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
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

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```
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
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
```

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```

    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

```

7.11.2 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

```

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```
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
    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
```

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```

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

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

```

7.11.3 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
  ExtendZ $extend
end

Fields
  rho
  rho(deformation)
  tau(valence)
  rho(deformation/fit)
  v(coulomb/atoms)
  v(coulomb/deformation)
  v(coulomb)
End

eor

echo ""

```

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```
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
  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
```

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```
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

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
```

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```

# 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

# 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)

```

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```
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

$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
```

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```
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

  Lattice
    2.5 0.0 0.0
  End
End

Engine DFTB
  ResourcesDir Demo
  Model DFTB0
  KSpace Quality=GammaOnly
EndEngine

eor

# cd MethaneChainGamma.results
```

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```

$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
    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

```

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```

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

```

7.11.4 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

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

```

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```
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
        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.
```

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```

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"

```

7.11.5 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 " "
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 ="

```

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```
echo " "  
cat dftbnbo.39  
  
echo " "  
echo " "  
echo "Contents of dftbnbo.49 ="  
echo " "  
cat dftbnbo.49
```

PARAMETERIZATIONS

8.1 Parameter meta-info

There is a file named `metainfo.yaml` in each resources directory (see *ResourcesDir* (page 8)), for example `DFTB.org/Bob-3-1/metainfo.yaml`, which contains information about the capabilities of a parameter set. The file is in accordance with the **YAML** (<http://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 `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) can not 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: http://www.scm.com

reference: |
  M. Wahiduzzaman, A. F. Oliveira, P. Philippsen, 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.

8.2 Slater-Koster based DFTB

The most popular parameter sets for Slater-Koster based DFTB are *distributed with the AMS package* (page 280). Other parameter sets can easily be *added* (page 281).

Often parameter files are designed for a specific purpose, which may be different from your application, and therefore may give not 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.

8.2.1 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 fo 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 to visit the [DFTB.org](http://www.dftb.org) (<http://www.dftb.org>) web site 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 288) set of DFTB parameter files available in the AMS package is designed by Mohammad Wahiduzzaman et al. 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 288) 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 288). These parameter files are kept in the directory \$AMSHOME/atomicdata/DFTB/Dresden.

8.2.2 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 280) 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 282), the *metainfo.yaml file* (page 279) and the optionally some *additional .yaml files* (page 282) as well as *binary .rkf files containing the basis functions* (page 283).

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 the Slater-Koster files are encrypted though, 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](http://www.dftb.org/fileadmin/DFTB/public/misc/slakoformat.pdf) (<http://www.dftb.org/fileadmin/DFTB/public/misc/slakoformat.pdf>) of the Slater-Koster file format can be found at [DFTB.org](http://www.dftb.org) (<http://www.dftb.org>).

Additional .yaml files

The Slater-Koster file format (<http://www.dftb.org/fileadmin/DFTB/public/misc/slakoformat.pdf>) 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 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.

8.3 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 8) 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.)

REQUIRED CITATIONS

When you publish results in the scientific literature that were obtained with programs of 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, in case you have used them.

9.1 General references

For calculations with the Density Functional Tight Binding (DFTB) engine: AMS DFTB 2023.1, SCM, Theoretical Chemistry, Vrije Universiteit, Amsterdam, The Netherlands, <http://www.scm.com>. Optionally, you may add the following list of authors and contributors: R. Rüger, A. Yakovlev, P. Philippsen, 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>)

9.2 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. Philippsen, 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. Philippsen, 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/nm700184k>)

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](http://www.dftb.org) (<http://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>)

REFERENCES

10.1 Slater-Koster based DFTB

10.1.1 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](https://doi.org/10.1002/(SICI)1097-461X(1996)58:2%3C185::AID-QUA7%3E3.0.CO;2-U))

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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) ([http://onlinelibrary.wiley.com/doi/10.1002/\(SICI\)1521-3951\(200001\)217:1%3C41::AID-PSSB41%3E3.0.CO;2-V/abstract](http://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) ([http://onlinelibrary.wiley.com/doi/10.1002/\(SICI\)1521-3951\(200001\)217:1%3C357::AID-PSSB357%3E3.0.CO;2-J/abstract](http://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) (<http://www.rsc.org/publishing/journals/CP/article.asp?doi=b105782k>)

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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) (<http://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>)

10.1.2 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 TDDFTB 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>)

10.1.3 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>)

10.1.4 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 für 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>)

10.1.5 DFTB.org

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

10.2 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>)

10.3 External programs and Libraries

[Click here](#) for the list of programs and/or libraries used in the AMS package. On some platforms optimized libraries have been used and/or vendor specific MPI implementations.

KEYWORDS

11.1 Links to manual entries

conductance:

- *EnergyGrid* (page 43)
- *Files* (page 44)
- *Technical* (page 44)

dftb:

- *DispersionCorrection* (page 8)
- *KSpace* (page 22)
- *Model* (page 8)
- *Occupation* (page 13)
- *Periodic* (page 27)
- *Properties* (page 31)
- *ResourcesDir* (page 8)
- *SCC* (page 10)
- *Solvation* (page 9)
- *StoreMatrices* (page 26)
- *Technical* (page 24)
- *UnpairedElectrons* (page 13)
- *XTBConfig* (page 23)

11.2 Summary of all keywords

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).

Quality**Type** Multiple Choice**Default value** Normal**Options** [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 'GammaOnly', only one point (the gamma point) will be used.

For the other options, the actual number of K points generated depends 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) Boltmann 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.

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.

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

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 transissions: 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 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/FQ(FMu).

AtomType

Type Block

Recurring True

Description Definition of atomic types in MM environment

Alpha

Type Float

Description Polarizability of FQFMU atom

Charge

Type Float

Description MM fixed charge (non-polarizable only)

Chi

Type Float

Description Electronegativity of FQ atom

Eta

Type Float

Description Chemical Hardness of FQ atom

Symbol

Type String

Description Symbol associated with atom type

Coords

Type Non-standard block

Description Coordinates and fragment information (FQ only)

Forcefield

Type Multiple Choice

Default value FQ

Options [FQ, FQFMU, NOPOL]

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.

MolCharge

Type Float

Default value 0.0

Description Total charge of each fragment (FQ only)

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 SCFMultiStepper 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=Trials. 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.

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.

12.1 Which DFTB parameters are available?

The DFTB module in the Amsterdam Modeling Suite ships with the following parameters:

- **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** (<http://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** (<http://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** (<http://www.dftb.org/>) parameters (see Readme or dftb.org website for latest info). Encrypted parameters may also be evaluated during trial
- Dispersion corrections available (Grimme's D2 & D3(BJ), London, UFF)

See the *documentation on the available DFTB parameter sets* (page 280).

12.2 Can I use Grimme's D3(BJ) dispersion corrections?

Yes, with DFTB3 and either the Quasinano or the DFTB.org 3ob parameters sets. With other DFTB methods and parameter sets you can use D2, London (ULG) or UFF dispersion.

12.3 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.

12.4 Can I include electric fields?

Yes.

12.5 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 all periodicity.

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