Keywords of deMonNano

MOLECULES

Keyword to defines MOLECULES. After this line, their is one line per molecules with the unit numer and the molecule type like : 1 WAT except if MOLTYPE is used (see below). This keyword should appear in the input file at the very end. The running directory should contain a file named MOLECULES with for each molecule type a line like WAT NAT=3 (3 letters for the molecule name and the number of atoms). The NAT next lines are standard atom name plus xyz inputs (C 0.071715 0.071715 0.000000).

NMOL=

number of subsystems

MOLTYPE=

all units are of the same type of molecule defined after MOLTYPE=

PARAM

The path to the DFTB parameters folder will be written

PTYPE=

specifies the parameter : NSC for non SCC, MAT or BIO for SCC, OWN for personal file

CHARGE

This keyword specifies the charge of the system. for instance : CHARGE 3

GEOMETRY

This keyword It specifies the molecular geometry and should be placed at the end of the input file. It is followed by the molecular geometry

BOHR

Coordinates or bond distances are given in atomic units

ANGST

Coordinates or bond distances are given in Angstrom. (This is the default

CARTE

The molecular structure is given in Cartesian coordinates. This is the default.

MULTIPLICITY

This keyword specifies the multiplicity of the system, integer following MULTIPLICITY 3

OPTIMIZATION

This keyword controls the geometry optimization

MAX=

Maximum number of optimisation steps. The default is 100.

TOL=

Optimization convergence criterion for the energy. Default is 3E-4 Hartree.

GRADTOL=

Optimization convergence criterion for the gradients. Default is 4E-6 Hartree in general.

STEP=

Maximum step size in optimization (Bohr). Default is 0.3 Bohr.

CGRAD

Uses the conjugate gradient method. This is the default.

SDC=

Uses the steepest descent method for geometry optimisation with specified multipler of the gradient. The default is 0.1

SDC

Uses the steepest descent method for geometry optimisation

OUT=

Interval to output structure during optmimisation

MONTECARLO

Perform Monte Carlo simulation

MAX=

Indicates the number of steps after "="

SEED=

indicates value of the SEED if Monte Carlo simulation is intended

WALL=

Refuses any displacement leading to structure not entering in a sphere of radius specified after '=' in a0. If it is set to zero, there is no distance check. Defaults is 0.

MCTEMP

Additional information about for Monte Carlo simulation. Should appear after the MONTEC keyword.

TMC=

Temperature for MC simulation (no parallel tempering)

NTEMP=

Number of temperatures, defines a parallel tempering MONTE CARLO scheme

LIST

The set of temperatures is readen from a list. After the MCTEMP line are the NTEMP lines. Each line contain : the trajectory number, the temperature, the initial center of mass displacment step, the initial quaternion displacement step

GEOM

The set of temperatures follows a geometric pattern

LINEAR

The set of temperatures follows a linear pattern

TEMPMIN=

The smallest temperature

TEMPMAX=

The largest temperature

X=

inital displacement for smallest temperature

Q=

initial displacement for lowest temperature quaternion displacement

RESCALE=

Frequency to rescale displacement steps

SWAP=

Kind of swap, it can be NO (no exchange), SE(exchange only between successive temperatures, AE (all exchange-exchange MC, ie possible between all temperatures, this is all exchange)

SMOD=

number of steps without trying any swap

SPERCENT=

probability to try a swap each "SWAP" step

SDBG

print some information (mostly to debug)

OUT=

frequency for molden

SOUT=

frequency for output

PATHS

perform paths over the PES, only works with quaternion apporach. A deMon.pth.inp file contain the points defined with CHKPTS NAME=PT1 followed by a line per subsystem defined with quaternions (see quaternions keyword for this general input) like for instance :" 1 0.0 0.0 0.0 1.0 0.0 0.0 0.0"

NPTS=

number of points

NPTHS=

number of paths

FREQUENCY

This keyword activates frequency analysis.

VIB=

Scaling factor for the numerical step size

DIPOLE

This keyword activates the calculation of molecular electrostatic moments.

OUTFILE

writes the dipole in an output file

MDYNAMICS

This keyword activates the Born-Oppenheimer molecular dynamic (BOMD) simulation

ZERO

Start a trajectory with initial velocities of the nuclei set to zero. This is the default.

RANDOM=

Start a trajectory using random initial velocities, which have no net momentum or angular momentum and give the requested temperature specified after =.

RAN

Start a trajectory using random initial velocities, which have no net momentum or angular momentum and give the initial temperature of MDTEMP keyword.

READ

Start a new MD trajectory. Velocities of the nuclei are given in Cartesian form in the input file, immediately following the MDYNAMICS keyword.

RESET

This option resets all averages and the MD step of the trajectory. It only makes sense with the RESTART option, otherwise it has no effect.

WALL=

This option imposes a spherical potential around the system during an MD simulation. It only makes sense for a finite size system. The radius of the wall has to be provided in angstrom. The definition of the wall is ENER*(r-WALL)**EXP. WARNING: the wall is centered at the c.o.m. of the system which has to be in (0,0,0). The calculation will stop if not KEEPCOM=.true. or if OUT_PBC=.true.

ENER=

the ENER parameter in the definition of the wall. Value is in Hartree

EXP=

the EXP parameter in the definition of the wall.

QUATERNION

Keyword allowing input with quaternions. After this line, their is one line per molecule that should look like : 1 1.0 0.0 .0 1.0 0.0 0.0 0.0 (unit number, coordinates of center of mass, 4 quaternions numbers) This should be associated with the MOLECULE keyword.

BOHR

Coordinates or bond distances are given in atomic

ANGST

Coordinates or bond distances are given in Angstrom.

MDSTEPS

This keyword controls the steps of the molecular dynamic (MD) simulation

MAX=

Maximum number of MD steps. The default is 1.

OUT=

Step interval to update the deMon.mol file. The default is 10.

SOUT=

Step interval to update the deMon.out file. The default is 1.

TSIM=

Maximum MD run time in ps.

MDTEMP

Desired MD temperature in Kelvin. The default is 300.

TIMESTEP

This keyword specifies the time step of the molecular dynamic (MD) simulation in fs (also used in NEB)

MDBATH

This keyword specifies the temperature bath used in the molecular dynamic (MD) simulation.

SCAL

The velocities are scaled in order to control the temperature. This option is only meaningful for very large systems of for the first equilibration steps of a trajectory.

BERE

Berendsen thermostat is applied to the system as a whole.

NOSE

The Nose-Hoover chain thermostat is applied

LANGE

Local Langevin thermostat is applied individually to each atom.

STOCH_R

Stochastic Velocity-Rescaling thermostat is applied to the system as a whole.

ANDERSEN

The Andersen thermostat is applied

LOCA

Berendsen thermostat is applied individually to each atom

VAL=

> if (thermostat = SCALING) : number of steps between velocity resets / if (thermostat = BERENDSEN, LOCAL, LANGEVIN or STOCH_R) = Thermostat time constant in picoseconds[ps]. Default is = 0.5 ps.

NTHER=

Specifies the size of the chain used in the Nose-Hoover thermostat (i.e. the number of thermostats). The default value is NTHER = 4.

FREQTH=

Specifies the frequence of the Nose-Hoover thermostat. The defaut value is FREQTH = 100 cm-1.

NONE

No temperature bath. This is the default

CONSERVE

The keywords requests imposition of constraints on some or all mechanical constants of the overall motion of the system.

NONE

> Do not impose constraints. This is the default, except for MDYNAMICS RANDOM.

ALL

Equivalent to COM, ANG and MOM. This is the default for MDYNAMICS RANDOM

COM

Reset position of the centre of mass of the system to (0,0,0) on each MD step.

ANG

Reset overall angular momentum of the system to zero on each MD step. This constraint makes no sense, and is ignored, for periodic calculations

MOM

Reset overall momentum of motion of the system to zero on each MD step.

MDCONSTRAINTS

This keyword imposes atomic constraints during a molecular dynamics simulation (read pdf manual)

METADYNAMICS

Perform a metadynamics calculation in combination with molecular dynamics.

PLUMED1

Perform a metadynamics simulation using PLUMED 1.2. The input file for the MetaD papameters has to be plumed.dat. Please cite: M. Bonomi, D. Branduardi, G. Bussi, C. Camilloni, D. Provasi, P. Raiteri, D. Donadio, F. Marinelli, F. Pietrucci, R.A. Broglia and M. Parrinello, PLUMED: a portable plugin for free energy calculations with molecular dynamics, Comp. Phys. Comm. C180, 1961 (2009)'

PRNG

Defines the pseudo random number generator (PRNG) to use for stochastic thermostats

LSFR

Uses the Linear Feedback Shift Register (LFSR) generators of L'Ecuyer. Please cite: L'Ecuyer, P. (1999) Tables of maximally equidistributed combined LFSR (Linear Feedback Shift Register) generators', Math. of Comput., 68, 261-269. This is the default.

MRG32

Uses the Multiple Recursive Random Number Generators (MRG32) of L'Ecuyer. Please cite: L'Ecuyer, P. (1999) Good parameters and implementations for combined multiple recursive random number generators. Operations Research, 47(1), 159-164.

BOXMULLER

Uses the box-Muller transformation of a uniformally distributed variable to a random Gaussian distribution centered on 0 and of unitary variance.

ICDF

Uses the inverse cumulative distribution fonction method (ICDF) to transform a uniformally distributed variable to a random Gaussian distribution centered on 0 and of unitary variance.

PARATEMP

Perform a parallel-tempering molecular dynamics simulation. WARNING: to use this approach, the code has to be compiled using OpenMPI and the preprocessing option -DMPI. WARNING: in the actual implementation, one mpi process can handle only one replica.

TMINIMUM=

Miminum temperature of the MPDT algorithm

TMAXIMUM=

Maximum temperature of the MPDT algorithm

NUMREP=

Number of replicas in the MPDT algorithm

NBREQ=

Number of points to indicate as equilibration after an MDPT exchange in the deMon.out file. These points are indicated by a 1.0 in the last column of the file.

EXSTEP=

Numbef MD STEPS between MDPT exchanges

SHORT

If activited, this option avoids to write the average properties along the MDPT run in the deMon.out files

LINEAR

Linear distribution of temperatures between TMINIMUM and TMAXIMUM. The default is an exponential distribution.

DFTB

Perform a DFTB calculation

SCC

The self-consistent charge variant of DFTB. The default is non-SCC.

MEMOSCC

use previous atomic charges to restart the SCC process at a new geometry. This keyword automatically set SCC calculation (even without SCC keyword)

TOL=

The SCC convergence criterion in electron charges. The default is 1.0E-8.

MAX=

Maximum number of SCC cycles. The default is 100

MIX=

Mixing value for simple and Broyden mixing. The default is 0.2. This value is independent from the DFT mixing value

SIMPLE

Simple mixing instead of Broyden convergence acceleration is performed for SCC. This is per default switched off

L-DEP

> Angular momentum resolved SCC. Here, the self-consistent charge procedure is applied to Mulliken shell charges rather than to Mul- liken atomic charges.By default, this option is deactivated.

FERMI=

As FERMI, but with used-specified Fermi temperature (in K) following the keyword.

FERMI

The electron occupation follows a Fermi distribution

DISP=

London dispersion with a damping function. By default this option is switched off. DISP=1 Zhechkov et al., JCTC 2005 DISP=2 : Rapacioli et al., JCP, 2009

DISP

Equivalent to DISP=1. By default this option is switched off.

PRINT

This keyword controls optional printing.

MOE

Print molecular orbital energies and occupations

ASE

Print energies and forces for ASE

MOS=

Print molecular orbital energies, occupations and coefficients.

DE2

Print Hessian matrix.

MC

Print a lot of MC information. Type MC=X to print the energy informations every X steps.

DEBUG

Generate debug output

CARPAR

Activates a Car-Parrinello Molecular Dynamics simulation. This option is only available for DFTB. By default, this option is off.

FOM=

Ficticious orbital mass for Car-Parrinello DFTB (in atomic units).

LGTOL=

The requested tolerance to ensure orthonormality of the orbitals using a Lagrange multiplier. The default is 10*-10 in atomic units.

BO

The Car-Parrinello approach is used to reach the Born Oppenheimer surface at each point

DELMO=

Multiplier for MO energy gradient for the MO optimisation using the Car-Parrinello approach in conjunction with the steepest descent technique (requires CARPAR BO). The default is 0.1.

MOMD=

Same as the MOMD keyword, but specifying the friction parameter. The default is 10*10-2.

MOMD

Requests a molecular dynamics-like optimisation of the molecular orbitals: A Car-Parrinello MD is carried out. Whenever gradient and velocity of an orbital have opposite signs an additional friction term is added to the equations of motion.

MOLECULES

Keyword to defines MOLECULES. After this line, their is one line per molecules with the unit numer and the molecule type like : 1 WAT except if MOLTYPE is used (see below). This keyword should appear in the input file at the very end. The running directory should contain a file named MOLECULES with for each molecule type a line like WAT NAT=3 (3 letters for the molecule name and the number of atoms). The NAT next lines are standard atom name plus xyz inputs (C 0.071715 0.071715 0.000000).

NMOL=

number of subsystems

RIGID

In the case of Monte Carlo exploration, these subsystems

ALLATOMS

The subsystems will never be treated as rigid

MOLTYPE=

all units are of the same type of molecule defined after MOLTYPE=

CUTSYS

Separate the system in subsystems (not necessary if MOLECULES keyword is used)

NMOL=

number of subsystems

RIGID

In the case of Monte Carlo exploration, these subsystems will be treated as rigid

ALLATOMS

The subsystems will never be treated as rigid

NATMOL=

number of atoms per subsystem (all molecules have the

PARAM

The path to the DFTB parameters folder will be written

PTYPE=

specifies the parameter : NSC for non SCC, MAT or BIO for SCC, OWN for personal file

CHARGE

This keyword specifies the charge of the system. for instance : CHARGE 3

GEOMETRY

This keyword It specifies the molecular geometry and should be placed at the end of the input file. It is followed by the molecular geometry

BOHR

Coordinates or bond distances are given in atomic units

ANGST

Coordinates or bond distances are given in Angstrom. (This is the default

CARTE

The molecular structure is given in Cartesian coordinates. This is the default.

MIXED

The first atoms of the molecular structure are defined by Cartesian coordinates and the following ones are defined by a Z-Matrix.

ZMATR

The molecular structure is defined by a Z-Matrix

MULTIPLICITY

This keyword specifies the multiplicity of the system, integer following MULTIPLICITY 3

OPTIMIZATION

This keyword controls the geometry optimization

MAX=

Maximum number of optimisation steps. The default is 100.

TOL=

Optimization convergence criterion for the energy. Default is 3E-4 Hartree.

GRADTOL=

Optimization convergence criterion for the gradients. Default is 4E-6 Hartree in general.

STEP=

Maximum step size in optimization (Bohr). Default is 0.3 Bohr.

CGRAD

Uses the conjugate gradient method. This is the default.

NUCFRIC=

Perform optimisation via MD with additional friction term with a user-defined mulitplier to the dissipative term.

NUCFRIC

Perform geometry optimisation via MD with additional friction term for degrees of freedom where velocity and gradient have opposite sign. The multiplier of the dissipative term is by default 0.6

SDC=

Uses the steepest descent method for geometry optimisation with specified multipler of the gradient. The default is 0.1

SDC

Uses the steepest descent method for geometry optimisation

NUCFRIC=

Perform optimisation via MD with additional friction term with a user-defined mulitplier to the dissipative term.

NUCFRIC

Perform geometry optimisation via MD with additional friction term for degrees of freedom where velocity and gradient have opposite sign. The multiplier of the dissipative term is by default 0.6

OUT=

Interval to output structure during optmimisation

NEB

This keyword controls the NEB search of transition states. If no option, a default calculation was made (NEB PTITR=13 OPT=COMB TYPROT=SVD NODEBUG).

PTITR=

Number of intermediate image in NEB strings between initial points

PTMAX=

Maximum number of image for NEB, at the end of FIRE OPTIMIZATION if this number is not reach, add two new images around each maximum and make a new OPTIMIZATION.

TYPROT=

Specify the type of rotation (SVD only at the moment)

TYPROT

Perform rotation of images to match with each others at each step of NEB. It takes default rotation to position the 3 first atoms allways in the same plan.

KNEB=

Set de spring constant. Default is 0.0972 Hartree/Bohr

NDEBUG=

For NEB. Write information in debug files and set interval.

NODEBUG

For NEB. No information file.

OPT=

Select one of the 3 types of NEB OPTIMIZATION of standard NEB (OPT=GRAD, FIRE, COMB(FIRE+GRAD)). OPT=DELR skip standard NEB, in TSNEB= (mandatory in this case) create a new rope with TS fixed point

FTOL=

Optimization energetic convergence criterion for the OPT FIRE. Default is 5.10E-3 Hartree.

MAX=

It corresponds to maximum displacement for FIRE search (default is 0.188 Bohr)

GRADTOL=

It corresponds to the gradient convergency criterion (default = 1e-3 Hartree).

TOLITER=

Set convergence threshold for OPT Gradient (default is 1E-6)

STEP=

> The default is 100. Number of maximal steps for gradient convergency below threshold

TSOPT=

Same as TSOPT followed with a NEB optimization select one of the 3 types of NEB OPTIMIZATION implemented (TSOPT=GRAD, FIRE, COMB(FIRE+GRAD)

TSOPT

Optimize the different transistion states using frequency analysis (following one negative frequency)

TSTOL=

In the case of TSOPT it corresponds to the gradient criterion to converge the transition state (default = 1E-5 Hartree).

DUPDWN=

In the case of TSOPT,to help the minmax TS optimizationi, one freeze one direction optimization if the gradoents become too differents. Default criterion ratio is 2.5.

FIFTOL=

Optimization convergence criterion for the TSOPT FIRE. Default is 1.10E-4 Hartree.

FIGRDTOL=

In the case of TSOPT it corresponds to the gradient criterion (default = 5E-5 Hartree).

FITER=

Set convergence threshold for TSOPT Gradient (default is 1E-8)

MONTECARLO

Perform Monte Carlo simulation

MAX=

Indicates the number of steps after "="

SEED=

indicates value of the SEED if Monte Carlo simulation is intended

WALL=

Refuses any displacement leading to structure not entering in a sphere of radius specified after '=' in a0. If it is set to zero, there is no distance check. Defaults is 0.

BASINHOP

Perform basin hopping simulation

MCTEMP

Additional information about for Monte Carlo simulation. Should appear after the MONTEC keyword.

TMC=

Temperature for MC simulation (no parallel tempering)

NTEMP=

Number of temperatures, defines a parallel tempering MONTE CARLO scheme

LIST

The set of temperatures is readen from a list. After the MCTEMP line are the NTEMP lines. Each line contain : the trajectory number, the temperature, the initial center of mass displacment step, the initial quaternion displacement step

GEOM

The set of temperatures follows a geometric pattern

LINEAR

The set of temperatures follows a linear pattern

TEMPMIN=

The smallest temperature

TEMPMAX=

The largest temperature

X=

inital displacement for smallest temperature

Q=

initial displacement for lowest temperature quaternion displacement

XMIN=

inital displacement for the smallest temperature (not compatible with NTEMP=1 and LIST keyword)

XMAX=

initial displacement for largest temperature (not compatible with NTEMP=1 and LIST keyword)

QMIN=

initial displacement for the lowest temperature quaternion displacement (not compatible with NTEMP=1 and LIST keyword)

QMAX=

initial displacement for the largest temperature quaternion displacement (not compatible with NTEMP=1 and LIST keyword)

RESCALE=

Frequency to rescale displacement steps

SWAP=

Kind of swap, it can be NO (no exchange), SE(exchange only between successive temperatures, AE (all exchange-exchange MC, ie possible between all temperatures, this is all exchange)

SMOD=

number of steps without trying any swap

SPERCENT=

probability to try a swap each "SWAP" step

SDBG

print some information (mostly to debug)

OUT=

frequency for molden

SOUT=

frequency for output

MSTATS

MultiPoints statistics options

DOS

compute densities of states

PATHS

perform paths over the PES, only works with quaternion apporach. A deMon.pth.inp file contain the points defined with CHKPTS NAME=PT1 followed by a line per subsystem defined with quaternions (see quaternions keyword for this general input) like for instance :" 1 0.0 0.0 0.0 1.0 0.0 0.0 0.0"

NPTS=

number of points

NPTHS=

number of paths

FREQUENCY

This keyword activates frequency analysis.

VIB=

Scaling factor for the numerical step size

DIPOLE

This keyword activates the calculation of molecular electrostatic moments.

OUTFILE

writes the dipole in an output file

DIPBIN

Dipole file is a binary file

MDYNAMICS

This keyword activates the Born-Oppenheimer molecular dynamic (BOMD) simulation

RESTA

Restart previous molecular dynamics simulation using information of deMon.qmd file

ZERO

Start a trajectory with initial velocities of the nuclei set to zero. This is the default.

DELAY=

the readen velocities are added to the velocities of the system after this number of steps

RANDOM=

Start a trajectory using random initial velocities, which have no net momentum or angular momentum and give the requested temperature specified after =.

RAN

Start a trajectory using random initial velocities, which have no net momentum or angular momentum and give the initial temperature of MDTEMP keyword.

READ

Start a new MD trajectory. Velocities of the nuclei are given in Cartesian form in the input file, immediately following the MDYNAMICS keyword.

RESET

This option resets all averages and the MD step of the trajectory. It only makes sense with the RESTART option, otherwise it has no effect.

WALL=

This option imposes a spherical potential around the system during an MD simulation. It only makes sense for a finite size system. The radius of the wall has to be provided in angstrom. The definition of the wall is ENER*(r-WALL)**EXP. WARNING: the wall is centered at the c.o.m. of the system which has to be in (0,0,0). The calculation will stop if not KEEPCOM=.true. or if OUT_PBC=.true.

ENER=

the ENER parameter in the definition of the wall. Value is in Hartree

EXP=

the EXP parameter in the definition of the wall.

QUATERNION

Keyword allowing input with quaternions. After this line, their is one line per molecule that should look like : 1 1.0 0.0 .0 1.0 0.0 0.0 0.0 (unit number, coordinates of center of mass, 4 quaternions numbers) This should be associated with the MOLECULE keyword.

BOHR

Coordinates or bond distances are given in atomic

ANGST

Coordinates or bond distances are given in Angstrom.

RANDOM

Random quaternions will be associated to these

MDSTEPS

This keyword controls the steps of the molecular dynamic (MD) simulation

MAX=

Maximum number of MD steps. The default is 1.

OUT=

Step interval to update the deMon.mol file. The default is 10.

SOUT=

Step interval to update the deMon.out file. The default is 1.

MDRST=

Step interval to update the deMon.qmd file. The default is 1.

TSIM=

Maximum MD run time in ps.

MDTEMP

Desired MD temperature in Kelvin. The default is 300.

TIMESTEP

This keyword specifies the time step of the molecular dynamic (MD) simulation in fs (also used in NEB)

MDBATH

This keyword specifies the temperature bath used in the molecular dynamic (MD) simulation.

SCAL

The velocities are scaled in order to control the temperature. This option is only meaningful for very large systems of for the first equilibration steps of a trajectory.

BERE

Berendsen thermostat is applied to the system as a whole.

NOSE

The Nose-Hoover chain thermostat is applied

LANGE

Local Langevin thermostat is applied individually to each atom.

STOCH_R

Stochastic Velocity-Rescaling thermostat is applied to the system as a whole.

ANDERSEN

The Andersen thermostat is applied

LOCA

Berendsen thermostat is applied individually to each atom

VAL=

> if (thermostat = SCALING) : number of steps between velocity resets / if (thermostat = BERENDSEN, LOCAL, LANGEVIN or STOCH_R) = Thermostat time constant in picoseconds[ps]. Default is = 0.5 ps.

NTHER=

Specifies the size of the chain used in the Nose-Hoover thermostat (i.e. the number of thermostats). The default value is NTHER = 4.

TTHER=

Specifies the desired temperature. The default value is TTHER = 500 K.

FREQTH=

Specifies the frequence of the Nose-Hoover thermostat. The defaut value is FREQTH = 100 cm-1.

NONE

No temperature bath. This is the default

CONSERVE

The keywords requests imposition of constraints on some or all mechanical constants of the overall motion of the system.

NONE

Do not impose constraints. This is the default, except for MDYNAMICS RANDOM.

ALL

Equivalent to COM, ANG and MOM. This is the default for MDYNAMICS RANDOM

COM

Reset position of the centre of mass of the system to (0,0,0) on each MD step.

ANG

Reset overall angular momentum of the system to zero on each MD step. This constraint makes no sense, and is ignored, for periodic calculations

MOM

Reset overall momentum of motion of the system to zero on each MD step.

MDCONSTRAINTS

This keyword imposes atomic constraints during a molecular dynamics simulation (read pdf manual)

BONDPARAM

BOND PARAMETER FOR DFTB CM3 or DFTB WMUL depending on the DFTB options. The next lines define the parameters like O H 0.32 (to define the OH bond) be careful the order of atoms is important (one definition per bon type pair).

MDPRESSURE

Activates constant-pressure molecular dynamics

P=

External pressure in MPa. The default is 0.1

TAU=

Berendsen Coupling constant in ps. The default is 1.0

COMP=

Compressibility of the system in 1/MPa. The default is set to be reasonable for water.

METADYNAMICS

Perform a metadynamics calculation in combination with molecular dynamics.

PLUMED1

Perform a metadynamics simulation using PLUMED 1.2. The input file for the MetaD papameters has to be plumed.dat. Please cite: M. Bonomi, D. Branduardi, G. Bussi, C. Camilloni, D. Provasi, P. Raiteri, D. Donadio, F. Marinelli, F. Pietrucci, R.A. Broglia and M. Parrinello, PLUMED: a portable plugin for free energy calculations with molecular dynamics, Comp. Phys. Comm. C180, 1961 (2009)'

PLUMED2

Perform a metadynamics simulation using PLUMED 2.XX. The input file for the MetaD parameters has to be plumed.inpt. Please cite: Tribello, Bonomi, Branduardi, Camilloni and Bussi Comput. Phys. Commun., DOI:10.1016/j.cpc.2013.09.018 (2013) '

PRNG

Defines the pseudo random number generator (PRNG) to use for stochastic thermostats

LSFR

Uses the Linear Feedback Shift Register (LFSR) generators of L'Ecuyer. Please cite: L'Ecuyer, P. (1999) Tables of maximally equidistributed combined LFSR (Linear Feedback Shift Register) generators', Math. of Comput., 68, 261-269. This is the default.

MRG32

Uses the Multiple Recursive Random Number Generators (MRG32) of L'Ecuyer. Please cite: L'Ecuyer, P. (1999) Good parameters and implementations for combined multiple recursive random number generators. Operations Research, 47(1), 159-164.

BOXMULLER

Uses the box-Muller transformation of a uniformally distributed variable to a random Gaussian distribution centered on 0 and of unitary variance.

ICDF

Uses the inverse cumulative distribution fonction method (ICDF) to transform a uniformally distributed variable to a random Gaussian distribution centered on 0 and of unitary variance.

PARATEMP

Perform a parallel-tempering molecular dynamics simulation. WARNING: to use this approach, the code has to be compiled using OpenMPI and the preprocessing option -DMPI. WARNING: in the actual implementation, one mpi process can handle only one replica.

TMINIMUM=

Miminum temperature of the MPDT algorithm

TMAXIMUM=

Maximum temperature of the MPDT algorithm

NUMREP=

Number of replicas in the MPDT algorithm

NBREQ=

Number of points to indicate as equilibration after an MDPT exchange in the deMon.out file. These points are indicated by a 1.0 in the last column of the file.

EXSTEP=

Numbef MD STEPS between MDPT exchanges

SHORT

If activited, this option avoids to write the average properties along the MDPT run in the deMon.out files

LINEAR

Linear distribution of temperatures between TMINIMUM and TMAXIMUM. The default is an exponential distribution.

VISUALIZATION

This keyword activates the interface to the visualization programs MOLDEN and MOLEKEL

MOLDE

The MOLDEN interface is activated. The MOLDEN input is written to the file deMon.mol. This is the default

MOLEK

The MOLEKEL interface is activated. The MOLEKEL input is written to the file deMon.mkl.

FULL

A full MOLDEN or MOLEKEL input is written. This is the default if the option MOLDEN or MOLEKEL is set.

FORCEFIELD

Set different forcefield characteristics. Two options are possible UFF (Universal Force-Field) or FFDS (reading forcefields paramenter from independet input file. The type of each atom should be specified on the corresponding line.

FF=

Specify the type of force field. It can be equal to either UFF or directly set the Forcefield type within the FFDS Forcefields options. Same name for Forcefield include in FFDS file has to be written. For instance, OPLS-AA, AMBER99SB, etc. Look up in FFDS file and copy same name in FF=.

QMMM

Set type of QM/MM calculations want to be run. Possibilities are QM fora pure QM calculation. MM for a pure Moleculare Mechanics calculation. Or QM/MM for a hybrid calculations with QM and MM methods. Default QM. If QMMM is on, the type of each atom should be specified on the corresponding line.

COUPLING=

Set the type of QM/MM coupling. It can be MECHANICAL coupling. Neglected external charges interactions between MM atoms and QM atoms or ELECTROSTATIC coupling. Including external charges interactions between MM atoms and QM atoms.

QM/MM

To perform QM/MM calculation

QM

To perform only QM calculation

MM

To perform only MM calculation

CHR=

> Set type of reading charges. Two options are possible, input (CHR=INPUT) reading charges from input file (in geometry Q=). Other possibility is to read MM charges from FFDS parameters file (CHR=FFDS).

DFTB

Perform a DFTB calculation

SCC

The self-consistent charge variant of DFTB. The default is non-SCC.

MEMOSCC

use previous atomic charges to restart the SCC process at a new geometry. This keyword automatically set SCC calculation (even without SCC keyword)

TOL=

The SCC convergence criterion in electron charges. The default is 1.0E-8.

DIAG=

User-specified diagonalisation routine for the generalised Eigen value systems. The method is specified after the '='. Legal options are DSYGVD, DSYGV, DSYGVR, SOM.

ETOL=

Requested energy tolerance for iterative solvers of the total energy (used for CPBO, see CARPAR section)

MAX=

Maximum number of SCC cycles. The default is 100

MIX=

Mixing value for simple and Broyden mixing. The default is 0.2. This value is independent from the DFT mixing value

SIMPLE

Simple mixing instead of Broyden convergence acceleration is performed for SCC. This is per default switched off

L-DEP

> Angular momentum resolved SCC. Here, the self-consistent charge procedure is applied to Mulliken shell charges rather than to Mul- liken atomic charges.By default, this option is deactivated.

FERMI=

As FERMI, but with used-specified Fermi temperature (in K) following the keyword.

FERMI

The electron occupation follows a Fermi distribution

THIRD

Third order DFTB; The running directory should contain a file names 3ord_param for 3rd order derivatives parameters, each line being like H -0.1857, recomended to be used with GCOR (reference Gauss et al. JCTC, 011, 7, 931

GCOR=

Correction for gamma function for short range; value for Zeta provided after GCOR= (reference Gauss et al. JCTC, 011, 7, 931

DISP=

London dispersion with a damping function. By default this option is switched off. DISP=1 Zhechkov et al., JCTC 2005 DISP=2 : Rapacioli et al., JCP, 2009

DISP

Equivalent to DISP=1. By default this option is switched off.

CONST=

Perform charge constrained DFTB calculation, the number after "=" specifies the subsystem on which the charge is localised

QCONS=

Specify the charge to be localized on a subsystel (if different from the total charge

CDIFF=

Specify that a second part of the subsystem, constrained is for the difference between charges

CONS2=

Specify that a second part of the subsystem will have the opposite charge of the first one with two constaraints search

CONST

Perform charge constrained DFTB calculation.

CI

Perform DFTB+CI calculation (to be used with CONST and SIZECI keywords). By default of diagonal terms are computed with the overlaps between SLATER determinents (not using the HOMO approximation).

NOSLAT

Compute CI matrices assuming that only the HOMO orbitals are involved instead of computing matrices elements with slater determinants.

SIZECI=

Specifies the size of the CI matrix for DFTB-CI calculation.

LEV_S=

Use level-shift for the SCC convergency

CM3INTER

Use CM3 charges instead of Mulliken charges for intermolecular interactions. CM3 parameter defined by BONDPARAM keyword

CM3POT

Use CM3 charges instead of Mulliken charge for all the system. CM3 parameter defined by BONDPARAM keyword

WMUL

Weight the Mulliken distribution, the weights are fixed by parameters defined byu BONDPARAM keyword

EPSMUL

Weight the Mulliken distribution, the weight is epsii/(epsii+epsjj)

LRESP

Perform a TDDFTB calculation (Linear response)

PRINT

This keyword controls optional printing.

MOE

Print molecular orbital energies and occupations

ASE

Print energies and forces for ASE

MOS=

Print molecular orbital energies, occupations and coefficients.

DE2

Print Hessian matrix.

MC

Print a lot of MC information. Type MC=X to print the energy informations every X steps.

DEBUG

Generate debug output

CARPAR

Activates a Car-Parrinello Molecular Dynamics simulation. This option is only available for DFTB. By default, this option is off.

FOM=

Ficticious orbital mass for Car-Parrinello DFTB (in atomic units).

LGTOL=

The requested tolerance to ensure orthonormality of the orbitals using a Lagrange multiplier. The default is 10*-10 in atomic units.

BO

The Car-Parrinello approach is used to reach the Born Oppenheimer surface at each point

DELMO=

Multiplier for MO energy gradient for the MO optimisation using the Car-Parrinello approach in conjunction with the steepest descent technique (requires CARPAR BO). The default is 0.1.

MOMD=

Same as the MOMD keyword, but specifying the friction parameter. The default is 10*10-2.

MOMD

Requests a molecular dynamics-like optimisation of the molecular orbitals: A Car-Parrinello MD is carried out. Whenever gradient and velocity of an orbital have opposite signs an additional friction term is added to the equations of motion.

BAND

BAND STRUCTURE CALCULATION

NK1=

Number of kpoints in 1st vector

NK2=

Number of kpoints in 2st vector

NK3=

Number of kpoints in 3st vector

MOLECULES

Keyword to defines MOLECULES. After this line, their is one line per molecules with the unit numer and the molecule type like : 1 WAT except if MOLTYPE is used (see below). This keyword should appear in the input file at the very end. The running directory should contain a file named MOLECULES with for each molecule type a line like WAT NAT=3 (3 letters for the molecule name and the number of atoms). The NAT next lines are standard atom name plus xyz inputs (C 0.071715 0.071715 0.000000).

NMOL=

number of subsystems

RIGID

In the case of Monte Carlo exploration, these subsystems

ALLATOMS

The subsystems will never be treated as rigid

MOLTYPE=

all units are of the same type of molecule defined after MOLTYPE=

CUTSYS

Separate the system in subsystems (not necessary if MOLECULES keyword is used)

NMOL=

number of subsystems

RIGID

In the case of Monte Carlo exploration, these subsystems will be treated as rigid

ALLATOMS

The subsystems will never be treated as rigid

NATMOL=

number of atoms per subsystem (all molecules have the

PARAM

The path to the DFTB parameters folder will be written

PTYPE=

specifies the parameter : NSC for non SCC, MAT or BIO for SCC, OWN for personal file

CHARGE

This keyword specifies the charge of the system. for instance : CHARGE 3

GEOMETRY

This keyword It specifies the molecular geometry and should be placed at the end of the input file. It is followed by the molecular geometry

BOHR

Coordinates or bond distances are given in atomic units

ANGST

Coordinates or bond distances are given in Angstrom. (This is the default

CARTE

The molecular structure is given in Cartesian coordinates. This is the default.

MIXED

The first atoms of the molecular structure are defined by Cartesian coordinates and the following ones are defined by a Z-Matrix.

ZMATR

The molecular structure is defined by a Z-Matrix

MULTIPLICITY

This keyword specifies the multiplicity of the system, integer following MULTIPLICITY 3

OPTIMIZATION

This keyword controls the geometry optimization

MAX=

Maximum number of optimisation steps. The default is 100.

TOL=

Optimization convergence criterion for the energy. Default is 3E-4 Hartree.

GRADTOL=

Optimization convergence criterion for the gradients. Default is 4E-6 Hartree in general.

STEP=

Maximum step size in optimization (Bohr). Default is 0.3 Bohr.

CGRAD

Uses the conjugate gradient method. This is the default.

NUCFRIC=

Perform optimisation via MD with additional friction term with a user-defined mulitplier to the dissipative term.

NUCFRIC

Perform geometry optimisation via MD with additional friction term for degrees of freedom where velocity and gradient have opposite sign. The multiplier of the dissipative term is by default 0.6

SDC=

Uses the steepest descent method for geometry optimisation with specified multipler of the gradient. The default is 0.1

SDC

Uses the steepest descent method for geometry optimisation

NUCFRIC=

Perform optimisation via MD with additional friction term with a user-defined mulitplier to the dissipative term.

NUCFRIC

Perform geometry optimisation via MD with additional friction term for degrees of freedom where velocity and gradient have opposite sign. The multiplier of the dissipative term is by default 0.6

OUT=

Interval to output structure during optmimisation

NEB

This keyword controls the NEB search of transition states. If no option, a default calculation was made (NEB PTITR=13 OPT=COMB TYPROT=SVD NODEBUG).

PTITR=

Number of intermediate image in NEB strings between initial points

PTMAX=

Maximum number of image for NEB, at the end of FIRE OPTIMIZATION if this number is not reach, add two new images around each maximum and make a new OPTIMIZATION.

TYPROT=

Specify the type of rotation (SVD only at the moment)

TYPROT

Perform rotation of images to match with each others at each step of NEB. It takes default rotation to position the 3 first atoms allways in the same plan.

KNEB=

Set de spring constant. Default is 0.0972 Hartree/Bohr

NDEBUG=

For NEB. Write information in debug files and set interval.

NODEBUG

For NEB. No information file.

OPT=

Select one of the 3 types of NEB OPTIMIZATION of standard NEB (OPT=GRAD, FIRE, COMB(FIRE+GRAD)). OPT=DELR skip standard NEB, in TSNEB= (mandatory in this case) create a new rope with TS fixed point

FTOL=

Optimization energetic convergence criterion for the OPT FIRE. Default is 5.10E-3 Hartree.

MAX=

It corresponds to maximum displacement for FIRE search (default is 0.188 Bohr)

GRADTOL=

It corresponds to the gradient convergency criterion (default = 1e-3 Hartree).

TOLITER=

Set convergence threshold for OPT Gradient (default is 1E-6)

STEP=

> The default is 100. Number of maximal steps for gradient convergency below threshold

TSOPT=

Same as TSOPT followed with a NEB optimization select one of the 3 types of NEB OPTIMIZATION implemented (TSOPT=GRAD, FIRE, COMB(FIRE+GRAD)

TSOPT

Optimize the different transistion states using frequency analysis (following one negative frequency)

TSTOL=

In the case of TSOPT it corresponds to the gradient criterion to converge the transition state (default = 1E-5 Hartree).

DUPDWN=

In the case of TSOPT,to help the minmax TS optimizationi, one freeze one direction optimization if the gradoents become too differents. Default criterion ratio is 2.5.

FIFTOL=

Optimization convergence criterion for the TSOPT FIRE. Default is 1.10E-4 Hartree.

FIGRDTOL=

In the case of TSOPT it corresponds to the gradient criterion (default = 5E-5 Hartree).

FITER=

Set convergence threshold for TSOPT Gradient (default is 1E-8)

NMIN=

For NEB-FIRE. Set the number of steps before acceleration (rescale velocity + timestep). Default is 5.

INC=

For NEB-FIRE. Set the time step increment if the system is accelerating. Default is 1.1.

DEC=

For NEB-FIRE. Set the deceleration multipîcation factor for time step. Default is 0.5.

ALPHAS=

For NEB-FIRE. Set the reference value of alpha (see FIRE method). Default is 0.1.

FALPHA=

For NEB-FIRE. Set the multiplication of alpha (see FIRE methode). Default is 0.99.

MONTECARLO

Perform Monte Carlo simulation

MAX=

Indicates the number of steps after "="

SEED=

indicates value of the SEED if Monte Carlo simulation is intended

WALL=

Refuses any displacement leading to structure not entering in a sphere of radius specified after '=' in a0. If it is set to zero, there is no distance check. Defaults is 0.

BASINHOP

Perform basin hopping simulation

MCTEMP

Additional information about for Monte Carlo simulation. Should appear after the MONTEC keyword.

TMC=

Temperature for MC simulation (no parallel tempering)

NTEMP=

Number of temperatures, defines a parallel tempering MONTE CARLO scheme

LIST

The set of temperatures is readen from a list. After the MCTEMP line are the NTEMP lines. Each line contain : the trajectory number, the temperature, the initial center of mass displacment step, the initial quaternion displacement step

GEOM

The set of temperatures follows a geometric pattern

LINEAR

The set of temperatures follows a linear pattern

TEMPMIN=

The smallest temperature

TEMPMAX=

The largest temperature

X=

inital displacement for smallest temperature

Q=

initial displacement for lowest temperature quaternion displacement

XMIN=

inital displacement for the smallest temperature (not compatible with NTEMP=1 and LIST keyword)

XMAX=

initial displacement for largest temperature (not compatible with NTEMP=1 and LIST keyword)

QMIN=

initial displacement for the lowest temperature quaternion displacement (not compatible with NTEMP=1 and LIST keyword)

QMAX=

initial displacement for the largest temperature quaternion displacement (not compatible with NTEMP=1 and LIST keyword)

RESCALE=

Frequency to rescale displacement steps

SWAP=

Kind of swap, it can be NO (no exchange), SE(exchange only between successive temperatures, AE (all exchange-exchange MC, ie possible between all temperatures, this is all exchange)

SMOD=

number of steps without trying any swap

SPERCENT=

probability to try a swap each "SWAP" step

SDBG

print some information (mostly to debug)

OUT=

frequency for molden

SOUT=

frequency for output

MSTATS

MultiPoints statistics options

DOS

compute densities of states

PATHS

perform paths over the PES, only works with quaternion apporach. A deMon.pth.inp file contain the points defined with CHKPTS NAME=PT1 followed by a line per subsystem defined with quaternions (see quaternions keyword for this general input) like for instance :" 1 0.0 0.0 0.0 1.0 0.0 0.0 0.0"

NPTS=

number of points

NPTHS=

number of paths

FREQUENCY

This keyword activates frequency analysis.

VIB=

Scaling factor for the numerical step size

NOIC

Put zero in the Hessian matrix for intermolecular-cross terms (use cutsys) contributions

DIPOLE

This keyword activates the calculation of molecular electrostatic moments.

OUTFILE

writes the dipole in an output file

QCM3

Dipole is computed with CM3 charges

QMULL

Dipole is computed with Mulliken charges

QALL

Dipole with CM3 and Mulliken charges are printed

DIPBIN

Dipole file is a binary file

TSH

This keyword activates the non-adiabatic molecular dynamics simulation with the trajectory-surface hopping approach

CISCASIDA

Use Casida ansatz for the CIS coefficients in TSH

DECOH

Activates the decoherence correction for Ehrenfest coefficients within TSH

NSTATES=

Number of excited states to be considered in TSH=.

MDYNAMICS

This keyword activates the Born-Oppenheimer molecular dynamic (BOMD) simulation

RESTA

Restart previous molecular dynamics simulation using information of deMon.qmd file

ZERO

Start a trajectory with initial velocities of the nuclei set to zero. This is the default.

DELAY=

the readen velocities are added to the velocities of the system after this number of steps

RANDOM=

Start a trajectory using random initial velocities, which have no net momentum or angular momentum and give the requested temperature specified after =.

RAN

Start a trajectory using random initial velocities, which have no net momentum or angular momentum and give the initial temperature of MDTEMP keyword.

READ

Start a new MD trajectory. Velocities of the nuclei are given in Cartesian form in the input file, immediately following the MDYNAMICS keyword.

RESET

This option resets all averages and the MD step of the trajectory. It only makes sense with the RESTART option, otherwise it has no effect.

WALL=

This option imposes a spherical potential around the system during an MD simulation. It only makes sense for a finite size system. The radius of the wall has to be provided in angstrom. The definition of the wall is ENER*(r-WALL)**EXP. WARNING: the wall is centered at the c.o.m. of the system which has to be in (0,0,0). The calculation will stop if not KEEPCOM=.true. or if OUT_PBC=.true.

ENER=

the ENER parameter in the definition of the wall. Value is in Hartree

EXP=

the EXP parameter in the definition of the wall.

QUATERNION

Keyword allowing input with quaternions. After this line, their is one line per molecule that should look like : 1 1.0 0.0 .0 1.0 0.0 0.0 0.0 (unit number, coordinates of center of mass, 4 quaternions numbers) This should be associated with the MOLECULE keyword.

BOHR

Coordinates or bond distances are given in atomic

ANGST

Coordinates or bond distances are given in Angstrom.

RANDOM

Random quaternions will be associated to these

MDSTEPS

This keyword controls the steps of the molecular dynamic (MD) simulation

MAX=

Maximum number of MD steps. The default is 1.

OUT=

Step interval to update the deMon.mol file. The default is 10.

SOUT=

Step interval to update the deMon.out file. The default is 1.

MDRST=

Step interval to update the deMon.qmd file. The default is 1.

TSIM=

Maximum MD run time in ps.

MDTEMP

Desired MD temperature in Kelvin. The default is 300.

TIMESTEP

This keyword specifies the time step of the molecular dynamic (MD) simulation in fs (also used in NEB)

MDBATH

This keyword specifies the temperature bath used in the molecular dynamic (MD) simulation.

SCAL

The velocities are scaled in order to control the temperature. This option is only meaningful for very large systems of for the first equilibration steps of a trajectory.

BERE

Berendsen thermostat is applied to the system as a whole.

NOSE

The Nose-Hoover chain thermostat is applied

LANGE

Local Langevin thermostat is applied individually to each atom.

STOCH_R

Stochastic Velocity-Rescaling thermostat is applied to the system as a whole.

ANDERSEN

The Andersen thermostat is applied

LOCA

Berendsen thermostat is applied individually to each atom

VAL=

if (thermostat = SCALING) : number of steps between velocity resets / if (thermostat = BERENDSEN, LOCAL, LANGEVIN or STOCH_R) = Thermostat time constant in picoseconds[ps]. Default is = 0.5 ps.

NTHER=

Specifies the size of the chain used in the Nose-Hoover thermostat (i.e. the number of thermostats). The default value is NTHER = 4.

TTHER=

Specifies the desired temperature. The default value is TTHER = 500 K.

FREQTH=

Specifies the frequence of the Nose-Hoover thermostat. The defaut value is FREQTH = 100 cm-1.

NONE

No temperature bath. This is the default

CONSERVE

The keywords requests imposition of constraints on some or all mechanical constants of the overall motion of the system.

NONE

Do not impose constraints. This is the default, except for MDYNAMICS RANDOM.

ALL

Equivalent to COM, ANG and MOM. This is the default for MDYNAMICS RANDOM

COM

Reset position of the centre of mass of the system to (0,0,0) on each MD step.

ANG

Reset overall angular momentum of the system to zero on each MD step. This constraint makes no sense, and is ignored, for periodic calculations

MOM

Reset overall momentum of motion of the system to zero on each MD step.

MDCONSTRAINTS

This keyword imposes atomic constraints during a molecular dynamics simulation (read pdf manual)

BONDPARAM

BOND PARAMETER FOR DFTB CM3 or DFTB WMUL depending on the DFTB options. The next lines define the parameters like O H 0.32 (to define the OH bond) be careful the order of atoms is important (one definition per bon type pair).

MDPRESSURE

Activates constant-pressure molecular dynamics

P=

External pressure in MPa. The default is 0.1

TAU=

Berendsen Coupling constant in ps. The default is 1.0

COMP=

Compressibility of the system in 1/MPa. The default is set to be reasonable for water.

METADYNAMICS

Perform a metadynamics calculation in combination with molecular dynamics.

PLUMED1

Perform a metadynamics simulation using PLUMED 1.2. The input file for the MetaD papameters has to be plumed.dat. Please cite: M. Bonomi, D. Branduardi, G. Bussi, C. Camilloni, D. Provasi, P. Raiteri, D. Donadio, F. Marinelli, F. Pietrucci, R.A. Broglia and M. Parrinello, PLUMED: a portable plugin for free energy calculations with molecular dynamics, Comp. Phys. Comm. C180, 1961 (2009)'

PLUMED2

Perform a metadynamics simulation using PLUMED 2.XX. The input file for the MetaD parameters has to be plumed.inpt. Please cite: Tribello, Bonomi, Branduardi, Camilloni and Bussi Comput. Phys. Commun., DOI:10.1016/j.cpc.2013.09.018 (2013) '

PRNG

Defines the pseudo random number generator (PRNG) to use for stochastic thermostats

LSFR

Uses the Linear Feedback Shift Register (LFSR) generators of L'Ecuyer. Please cite: L'Ecuyer, P. (1999) Tables of maximally equidistributed combined LFSR (Linear Feedback Shift Register) generators', Math. of Comput., 68, 261-269. This is the default.

MRG32

Uses the Multiple Recursive Random Number Generators (MRG32) of L'Ecuyer. Please cite: L'Ecuyer, P. (1999) Good parameters and implementations for combined multiple recursive random number generators. Operations Research, 47(1), 159-164.

BOXMULLER

Uses the box-Muller transformation of a uniformally distributed variable to a random Gaussian distribution centered on 0 and of unitary variance.

ICDF

Uses the inverse cumulative distribution fonction method (ICDF) to transform a uniformally distributed variable to a random Gaussian distribution centered on 0 and of unitary variance.

PARATEMP

Perform a parallel-tempering molecular dynamics simulation. WARNING: to use this approach, the code has to be compiled using OpenMPI and the preprocessing option -DMPI. WARNING: in the actual implementation, one mpi process can handle only one replica.

SYNC

Make synchronous PTMD

ASYNC1

Make Asynchronous PTMD with EXTIME as the condition to perform the exchanges and MAXTIME as the condition to end the simulation. Note that the different replicas will not perform the same number of MD steps between 2 exchanges so the ensemble properties will be different compared to synchronous simulation. Should not be used for production.

ASYNC2

Same as ASYNC1 but the simulation will end when the 1st replica will have performed the MDSTEPS specified in the DYNAMICS keyword line. Same remark as ASYNC1... Should not be used for production.

ASYNC3

Make Asynchronous PTMD with EXSTEP as the condition to perform the exchanges as in Synchronous PTMD but the exchanges will occur when the 1st replica will have perform the EXSTEP since the last exchange whatever the number of MD steps the other replicas will have done. As with ASYNC2, the simulation will end when the 1st replica will have performed the MDSTEPS specified in the DYNAMICS keyword line.

EXTIME=

Wall-clock time between 2 exchange steps for PTMD with ASYNC1 or ASYNC2.

MAXTIME=

Max wall-clock time for a PTMD simulation with ASYNC1.

RANDOM=

If RANDOM is 1 than the random number used in the Metropolis-Criterion is drawn by the master MPI process (the one handling the 1st replica) and sent to all the other processes. If RANDOM = 2 than each process draws its own random number. It has no impact on the exchange rate neither the properties. Default is RANDOM = 1.

TMINIMUM=

Miminum temperature of the MPDT algorithm

TMAXIMUM=

Maximum temperature of the MPDT algorithm

NUMREP=

Number of replicas in the MPDT algorithm

NBREQ=

Number of points to indicate as equilibration after an MDPT exchange in the deMon.out file. These points are indicated by a 1.0 in the last column of the file.

EXSTEP=

Numbef MD STEPS between MDPT exchanges

SHORT

If activited, this option avoids to write the average properties along the MDPT run in the deMon.out files

LINEAR

Linear distribution of temperatures between TMINIMUM and TMAXIMUM. The default is an exponential distribution.

VISUALIZATION

This keyword activates the interface to the visualization programs MOLDEN and MOLEKEL

MOLDE

The MOLDEN interface is activated. The MOLDEN input is written to the file deMon.mol. This is the default

MOLEK

The MOLEKEL interface is activated. The MOLEKEL input is written to the file deMon.mkl.

FULL

A full MOLDEN or MOLEKEL input is written. This is the default if the option MOLDEN or MOLEKEL is set.

FORCEFIELD

Set different forcefield characteristics. Two options are possible UFF (Universal ForceField) or FFDS (reading forcefields paramenter from independet input file. The type of each atom should be specified on the corresponding line.

FF=

Specify the type of force field. It can be equal to either UFF or directly set the Forcefield type within the FFDS Forcefields options. Same name for Forcefield include in FFDS file has to be written. For instance, OPLS-AA, AMBER99SB, etc. Look up in FFDS file and copy same name in FF=.

QMMM

Set type of QM/MM calculations want to be run. Possibilities are QM fora pure QM calculation. MM for a pure Moleculare Mechanics calculation. Or QM/MM for a hybrid calculations with QM and MM methods. Default QM. If QMMM is on, the type of each atom should be specified on the corresponding line.

COUPLING=

Set the type of QM/MM coupling. It can be MECHANICAL coupling. Neglected external charges interactions between MM atoms and QM atoms or ELECTROSTATIC coupling. Including external charges interactions between MM atoms and QM atoms.

QM/MM

To perform QM/MM calculation

QM

To perform only QM calculation

MM

To perform only MM calculation

CHR=

> Set type of reading charges. Two options are possible, input (CHR=INPUT) reading charges from input file (in geometry Q=). Other possibility is to read MM charges from FFDS parameters file (CHR=FFDS).

DFTB

Perform a DFTB calculation

SCC

The self-consistent charge variant of DFTB. The default is non-SCC.

MEMOSCC

use previous atomic charges to restart the SCC process at a new geometry. This keyword automatically set SCC calculation (even without SCC keyword)

TOL=

The SCC convergence criterion in electron charges. The default is 1.0E-8.

DIAG=

User-specified diagonalisation routine for the generalised Eigen value systems. The method is specified after the '='. Legal options are DSYGVD, DSYGV, DSYGVR, SOM.

ETOL=

Requested energy tolerance for iterative solvers of the total energy (used for CPBO, see CARPAR section)

MAX=

Maximum number of SCC cycles. The default is 100

MIX=

Mixing value for simple and Broyden mixing. The default is 0.2. This value is independent from the DFT mixing value

SIMPLE

Simple mixing instead of Broyden convergence acceleration is performed for SCC. This is per default switched off

L-DEP

> Angular momentum resolved SCC. Here, the self-consistent charge procedure is applied to Mulliken shell charges rather than to Mul- liken atomic charges.By default, this option is deactivated.

FERMI=

As FERMI, but with used-specified Fermi temperature (in K) following the keyword.

FERMI

The electron occupation follows a Fermi distribution

THIRD

Third order DFTB; The running directory should contain a file names 3ord_param for 3rd order derivatives parameters, each line being like H -0.1857, recomended to be used with GCOR (reference Gauss et al. JCTC, 011, 7, 931

GCOR=

Correction for gamma function for short range; value for Zeta provided after GCOR= (reference Gauss et al. JCTC, 011, 7, 931

DISP=

London dispersion with a damping function. By default this option is switched off. DISP=1 Zhechkov et al., JCTC 2005 DISP=2 : Rapacioli et al., JCP, 2009

DISP

Equivalent to DISP=1. By default this option is switched off.

CONST=

Perform charge constrained DFTB calculation, the number after "=" specifies the subsystem on which the charge is localised

QCONS=

Specify the charge to be localized on a subsystel (if different from the total charge

CDIFF=

Specify that a second part of the subsystem, constrained is for the difference between charges

CONS2=

Specify that a second part of the subsystem will have the opposite charge of the first one with two constaraints search

CONST

Perform charge constrained DFTB calculation.

CI

Perform DFTB+CI calculation (to be used with CONST and SIZECI keywords). By default of diagonal terms are computed with the overlaps between SLATER determinents (not using the HOMO approximation).

NOSLAT

Compute CI matrices assuming that only the HOMO orbitals are involved instead of computing matrices elements with slater determinants.

SIZECI=

Specifies the size of the CI matrix for DFTB-CI calculation.

LEV_S=

Use level-shift for the SCC convergency

CM3INTER

Use CM3 charges instead of Mulliken charges for intermolecular interactions. CM3 parameter defined by BONDPARAM keyword

CM3POT

Use CM3 charges instead of Mulliken charge for all the system. CM3 parameter defined by BONDPARAM keyword

WMUL

Weight the Mulliken distribution, the weights are fixed by parameters defined byu BONDPARAM keyword

DWEIGHT

Weight the Mulliken distribution, the weights are obtained from the density matrix Pii/(Pii+Pjj)

EPSMUL

Weight the Mulliken distribution, the weight is epsii/(epsii+epsjj)

LRESP

Perform a TDDFTB calculation (Linear response)

PRINT

This keyword controls optional printing.

MDEXTRA

Print insanely detailed MD output

ATOMMAP

Print atom ordering maps

G42

Print G42 output

HYBRID

print HYBRIDATION (only based on bond order)

MOE

Print molecular orbital energies and occupations

ASE

Print energies and forces for ASE

MOS=

Print molecular orbital energies, occupations and coefficients.

DE2

Print Hessian matrix.

OPT

Generate full optimization output

RAM

Print RAM allocation table.

PBC

Print periodic bondary conditions information

MD

Print detailed MD output

MC

Print a lot of MC information. Type MC=X to print the energy informations every X steps.

DEBUG

Generate debug output

CARPAR

Activates a Car-Parrinello Molecular Dynamics simulation. This option is only available for DFTB. By default, this option is off.

FOM=

Ficticious orbital mass for Car-Parrinello DFTB (in atomic units).

LGTOL=

The requested tolerance to ensure orthonormality of the orbitals using a Lagrange multiplier. The default is 10*-10 in atomic units.

BO

The Car-Parrinello approach is used to reach the Born Oppenheimer surface at each point

DELMO=

Multiplier for MO energy gradient for the MO optimisation using the Car-Parrinello approach in conjunction with the steepest descent technique (requires CARPAR BO). The default is 0.1.

MOMD=

Same as the MOMD keyword, but specifying the friction parameter. The default is 10*10-2.

MOMD

Requests a molecular dynamics-like optimisation of the molecular orbitals: A Car-Parrinello MD is carried out. Whenever gradient and velocity of an orbital have opposite signs an additional friction term is added to the equations of motion.

LGPROP

propagate lagrangian coefficients

BAND

BAND STRUCTURE CALCULATION

NK1=

Number of kpoints in 1st vector

NK2=

Number of kpoints in 2st vector

NK3=

Number of kpoints in 3st vector