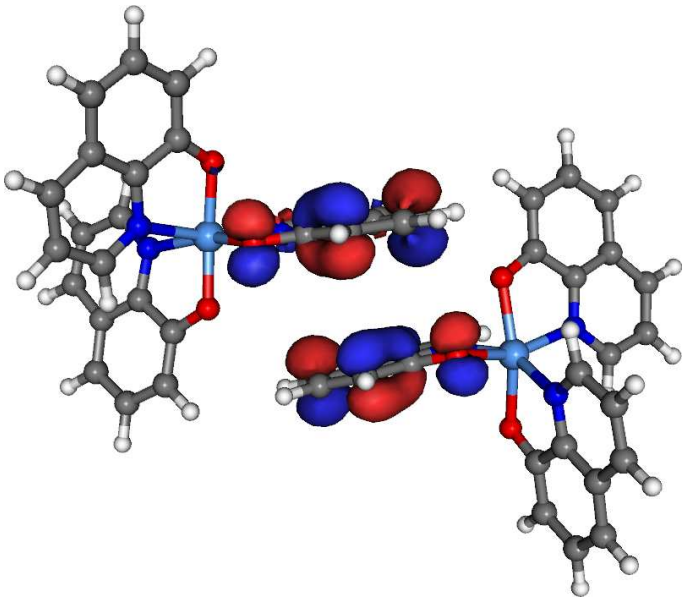
VOTCA-XTP

EXCITON TRANSPORT SIMULATIONS

USER MANUAL



compiled from: 1.5-dev (fa7077f)

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www.votca.org

Disclamer

This manual is not complete. The best way to start using the software is to look at provided tutorials. The reference section is generated automatically from the source code, so please make sure that your software and manual versions match.

Citations

Development of this software depends on academic research grants. If you are using the package, please cite the following papers

[1] Microscopic simulations of charge transport in disordered organic semiconductors,
Victor Rühle, Alexander Lukyanov, Falk May, Manuel Schrader, Thorsten Vehoff, James Kirkpatrick, Björn Baumeier and Denis Andrienko
J. Chem. Theor. Comp. 7, 3335, 2011

[2] Versatile Object-oriented Toolkit for Coarse-graining Applications
Victor Rühle, Christoph Junghans, Alexander Lukyanov, Kurt Kremer and Denis Andrienko
J. Chem. Theor. Comp. 5, 3211, 2009

Development

The core development is currently taking place at the Max Planck Institute for Polymer Research, Mainz, Germany and TU/e Eindhoven.

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Chapter 1

Introduction

VOTCA-XTP is an extension library to VOTCA-CTP. It provides internal support for quantum-chemical calculations on DFT level, including a module for excited state calculations within the GW-BSE approach.
This manual is currently being written.

Chapter 2

Input and output files

sec:io

2.1 DFT transfer integrals

list:TI_xml

Listing 2.1: Example `TI.xml` file created as the output of a `DIPRO` calculation. Due to slightly different implementations, the orbitals indices refer to monomer indices in a `Gaussian` run but to indices in the merged dimer guess in a `Turbomole` run.

```
<pair name="pair_100_155">
   <parameters>
      <HOMO_A>162</HOMO_A>
      <NoccA>1</NoccA>
      <LUMO_A>164</LUMO_A>
      <NvirtA>1</NvirtA>
      <HOMO_B>161</HOMO_B>
      <NoccB>1</NoccB>
      <LUMO_B>163</LUMO_B>
      <NvirtB>1</NvirtB>
   </parameters>
    <transport name="hole">
        <channel name="single">
            <J>1.546400416750696E-003</J>
            <e_A>-6.30726450715697</e_A>
            <e_B>-6.36775613794166</e_B>
        </channel>
        <channel name="multi">
           <molecule name="A">
               <e_HOMOm0>-6.30726450715697</e_HOMOm0>
           </molecule>
           <molecule name="B">
               <e_HOMOm0>-6.36775613794166</e_HOMOm0>
           </molecule>
               <dimer name="integrals">
                    <T_00>1.546400416750696E-003</T_00>
                    <J_sq_degen>2.391354248926727E-006</J_sq_degen>
                    <J_sq_boltz>2.391354248926727E-006</J_sq_boltz>
               </dimer>
        </channel>
    </transport>
    <transport name="electron">
        <channel name="single">
            <J>-2.797473760331286E-003</J>
            <e_A>-4.50318366770689</e_A>
            <e_B>-4.53143397059021</e_B>
```

```
        </channel>
        <channel name="multi">
               <molecule name="A">
                    <e_LUMOp0>-4.50318366770689</e_LUMOp0>
               </molecule>
               <molecule name="B">
                    <e_LUMOp0>-4.53143397059021</e_LUMOp0>
               </molecule>
               <dimer name="integrals">
                    <T_00>-2.797473760331286E-003</T_00>
                    <J_sq_degen>7.825859439742066E-006</J_sq_degen>
                    <J_sq_boltz>7.825859439742066E-006</J_sq_boltz>
               </dimer>
        </channel>
    </transport>
</pair>
```

Chapter 3

Reference

sec:reference

3.1 Programs

sec:programs

Programs execute specific tasks (calculators).

3.1.1 xtp_testsuite

prog:xtp_testsuite

Performs tests en suite + optional arguments:

`-h, --help` show this help message and exit

`-e [ [ ...]], --execute [ [ ...]]` Tests to perform, accepts regex (def=".*")

`-l, --listonly` List all tests available, then quit.

`-x , --xml` Test-suite file (def="$VOTCASHARE/xtp/xml/testsuite.xml")

`-s , --source` Test source input directory (def="source")

`-td , --testdirectory` Test run directory (def="suite")

`-t , --target` Directory where to store targets (def="targets")

`-r , --reference` Folder with reference data to compare to (def="reference")

`-g, --generate` Generate reference from targets (def=False)

`-cmp, --compareonly` Only compare existing targets to reference (def=False)

`-v, --verbose` The wordy version (def=False)

`-sh, --showoutput` Display VOTCA::XTP exec. output (def=False)

`-c, --clean` To clean or not to clean test dir. (def=False)

`-m , --mailto` Mail the result. (def=False)

3.1.2 xtp_update

prog:xtp_update

Updates the state file + optional arguments:

`-h, --help` show this help message and exit

`-f SQLFILE, --file SQLFILE` State file to update.

3.1.3 xtp_update_exciton

prog:xtp_update_exciton

Updates the state file for singlets and triplets + optional arguments:

`-h, --help` show this help message and exit

`-f SQLFILE, --file SQLFILE` State file to update.

3.1.4 xtp_basisset

prog:xtp_basisset

xtp_update, version 1.5-dev gitid: fa7077f Creates votca xml basissetfiles from NWCHEM basissetfiles optional arguments:

`-h, --help` show this help message and exit
`-f NWCHEM, --inputnw NWCHEM` NWchem file containing the basisset.
`-o OUTPUTFILE, --outputvotca OUTPUTFILE` Path of votca outputfile

3.1.5 xtp_map

prog:xtp_map

Generates QM|MD topology
`-h [ --help ]` display this help and exit
`-v [ --verbose ]` be loud and noisy
`-t [ --topology ] arg` topology
`-c [ --coordinates ] arg` coordinates or trajectory
`-s [ --segments ] arg` definition of segments and fragments
`-f [ --file ] arg` state file

3.1.6 xtp_run

prog:xtp_run

Runs excitation/charge transport calculators
`-h [ --help ]` display this help and exit
`-v [ --verbose ]` be loud and noisy
`-o [ --options ] arg` calculator options
`-f [ --file ] arg` sqlight state file, *.sql
`-i [ --first-frame ] arg (=1)` start from this frame
`-n [ --nframes ] arg (=1)` number of frames to process
`-t [ --nthreads ] arg (=1)` number of threads to create
`-s [ --save ] arg (=1)` whether or not to save changes to state file
`-e [ --execute ] arg` List of calculators separated by ',' or ' '
`-l [ --list ]` Lists all available calculators -d [--description] arg Short description of a calculator

3.1.7 xtp_tools

prog:xtp_tools

Runs excitation/charge transport tools
`-h [ --help ]` display this help and exit
`-v [ --verbose ]` be loud and noisy
`-t [ --nthreads ] arg (=1)` number of threads to create
`-o [ --options ] arg` calculator options Tools:
`-e [ --execute ] arg` List of tools separated by ',' or ' '
`-l [ --list ]` Lists all available tools -d [--description] arg Short description of a tool

3.1.8 xtp_parallel

prog:xtp_parallel

Runs job-based heavy-duty calculators
`-h [ --help ]` display this help and exit
`-v [ --verbose ]` be loud and noisy
`-o [ --options ] arg` calculator options
`-f [ --file ] arg` sqlite state file, *.sql
`-i [ --first-frame ] arg (=1)` start from this frame
`-n [ --nframes ] arg (=1)` number of frames to process
`-t [ --nthreads ] arg (=1)` number of threads to create
`-s [ --save ] arg (=1)` whether or not to save changes to state file
`-r [ --restart ] arg` restart pattern: 'host(pc1:234) stat(FAILED)'
`-c [ --cache ] arg (=8)` assigns jobs in blocks of this size
`-j [ --jobs ] arg (=run)` task(s) to perform: input, run, import
`-m [ --maxjobs ] arg (=-1)` maximum number of jobs to process (-1 = inf)

`-e [ --execute ] arg` List of calculators separated by ',' or ' '
`-l [ --list ]` Lists all available calculators -d [--description] arg Short description of a calculator

3.1.9 xtp_dump

prog:xtp_dump

Extracts information from the state file

`-h [ --help ]` display this help and exit
`-v [ --verbose ]` be loud and noisy
`-o [ --options ] arg` calculator options
`-f [ --file ] arg` sqlight state file, *.sql
`-i [ --first-frame ] arg (=1)` start from this frame
`-n [ --nframes ] arg (=1)` number of frames to process
`-t [ --nthreads ] arg (=1)` number of threads to create
`-s [ --save ] arg (=1)` whether or not to save changes to state file Extractors:
`-e [ --extract ] arg` List of extractors separated by ',' or ' '
`-l [ --list ]` Lists all available extractors -d [--description] arg Short description of an extractor

3.2 Calculators

sec:calculators

Calculator is a piece of code which computes specific system properties, such as site energies, transfer integrals, etc. `xtp_run`, `xtp_kmc_run` are wrapper programs which executes such calculators. The generic syntax is

```
xtp_run -e "calc1, calc2, ..." -o options.xml
```

File `options.xml` lists all options needed to run a specific calculator. The format of this file is explained in listing 3.1. A complete list of calculators is given in the calculators reference section.

list:calc

Listing 3.1: A part of the `options.xml` file with options for the `calculator_name{1,2}` calculators.

```
<calculator_name1>
          <option1>value1</option1>
          <option2>value2</option2>
          ...
</calculator_name1>

<calculator_name2>
          <option1>value1</option1>
          <option2>value2</option2>
          ...
</calculator_name2>
...
```

A list of all calculators and their short descriptions can be obtain using

```
xtp_run --list
```

A detailed description of all options of a specific calculator(s) is available via

```
xtp_run --desc calc1,calc2,...
```

3.2.1 dft

calc:dft

Standalone DFT calculator (experimental)

option	default	unit	description

package			
tasks			
output			
reporting			
xyz			
dftengine			
archive			

Return to the description of `dft`.

3.2.2 exciton

calc:exciton

Standalone GW-BSE calculator

option	default	unit	description
dftpackage			
tasks			
reporting			
output			
molecule			
log			
orbitals			
xyz			
levels			
gwbse_options			
optimize			
state			
spintype			
displacement			
convergence			
archive			

Return to the description of `exciton`.

3.2.3 excitoncoupling

calc:excitoncoupling

Exciton couplings from serialized orbital files

option	default	unit	description
classical			
output	excitoncoupling		Output file
bsecoupling_options			
orbitalsA	A.orb		Serialized orbitals file
orbitalsB	B.orb		Serialized orbitals file
orbitalsAB	AB.orb		Serialized orbitals file

Return to the description of `excitoncoupling`.

3.2.4 gencube

calc:gencube

Tool to generate cube files from .orb file

option	default	unit	description
output	state.cube		Output file
input	system.orb		Input file
padding	6.5		How far the grid should start from the molecule

xsteps	25		Gridpoints in x-direction
ysteps	25		Gridpoints in y-direction
zsteps	25		Gridpoints in z-direction
state	1		State to generate cube file for
spin			Singlet or Triplet
type	ground		qp:quasiparticle,ground:groundstate,transition:transitionstate,excited/exc gs:excitedstate density/density excited-ground state
mode	new		new: generate new cube file, substract: substract to cube files specified below
infile1			Cubefile to substract infile2 from
infile2			Cubefile to substract from infile1

193 Return to the description of `gencube`.

194 3.2.5 partialcharges

calc:partialcharges

195 Tool to derive partial charges from QM results stores in serialized file

option	default	unit	description
output	Moleculecharge		Output file either .mps or .pdb
input	molecule.orb		Serialized file
esp_options			options for the method

196 Return to the description of `partialcharges`.

197 3.2.6 qmanalyze

calc:qmanalyze

198 Analysis tool for QM results stores in serialized file

option	default	unit	description
output	qmanalyze.out		Output file
BSE			additonal info about BSE results
input	molecule.orb		Serialized file

199 Return to the description of `qmanalyze`.

200 3.2.7 spectrum

calc:spectrum

201 Calculate optical spectrum from serizalized orb file

option	default	unit	description
input			
output			
fwhm			
lower			
upper			
points			

202 Return to the description of `spectrum`.

203 3.2.8 coupling

calc:coupling

204 Electronic couplings from log and orbital files (GAUSSAIN, TURBOMOLE, NWChem)

option	default	unit	description

dftpackage			First-principles package
output	coupling.out.xm		Output file
degeneracy	0	eV	Criterium for the degeneracy of two levels
moleculeA			
log	A.log		Log file of molecule A
orbitals	A.orb		Orbitals file
levels	3		Output HOMO, ..., HOMO-levels; LUMO, ..., LUMO+levels
trim	2		
moleculeB			
log	B.log		Log file of molecule B
orbitals	B.orb		Orbitals file
levels	3		Output HOMO, ..., HOMO-levels; LUMO, ..., LUMO+levels
trim	2		
dimerAB			
log	AB.log		Log file of dimer AB
orbitals	A.orb		Orbitals file

Return to the description of `coupling`.

3.2.9 log2mps

calc:log2mps

Generates an mps-file (with polar-site definitions) from a QM log-file

option	default	unit	description
package			QM package
logfile			Log-file generated by QM package, with population/esp-fit data

Return to the description of `log2mps`.

3.2.10 molpol

calc:molpol

Molecular polarizability calculator (and optimizer)

option	default	unit	description
mpsfiles			
input			mps input file
output			mps output file
polar			xml file with infos on polarizability tensor
induction			
expdamp			Thole sharpness parameter
wSOR			mixing factor for convergence
maxiter			maximum number of iterations
tolerance			rel. tolerance for induced moments
target			
optimize			if 'true', refine atomic polarizabilities to match molecular polarizable volume specified in target.molpol
molpol			target polarizability tensor in format xx xy xz yy yz zz (this should be in the eigen-frame, hence xy = xz = yz = 0), if optimize=true the associated polarizable volume will be matched iteratively and the resulting set of polar sites written to mpsfiles.output
tolerance			relative tolerance when optimizing the polarizable volume

Return to the description of `molpol`.

3.2.11 pdb2map

calc:pdb2map

Converts MD + QM files to VOTCA mapping. Combinations: pdb+xyz,gro+xyz,pdb

option	default	unit	description
pdb	conf.pdb		Input pdb file
gro	conf.gro		Input gro file
xyz	conf.xyz		Input xyz file
xml	conf.xml		Resulting xml file

Return to the description of `pdb2map`.

3.2.12 pdb2top

calc:pdb2top

Generates fake Gromacs topology file .top

option	default	unit	description
num	1		Num of mols in the box
pdb	conf.pdb		Input pdb file
gro	conf.gro		Input gro file

Return to the description of `pdb2top`.

3.2.13 ptopreader

calc:ptopreader

Reads binary .ptop-files (serialized from ewdbgpol) and processes them into something readable

option	default	unit	description
ptop_file			Binary archive .ptop-file

Return to the description of `ptopreader`.

3.2.14 xneighborlist

calc:xneighborlist

Evaluates neighborlist, including long-range neighbors for energy transfer

option	default	unit	description
segments			
type			
cutoff			
constant			
exciton_cutoff			

Return to the description of `xneighborlist`.

3.2.15 eanalyze

calc:eanalyze

Histogram and correlation function of site energies and pair energy differences

option	default	unit	description
resolution_sites		eV	Bin size for site energy histogram
resolution_pairs		eV	Bin size for pair energy histogram
resolution_space		eV	Bin size for site energy correlation
states			?

Return to the description of `eanalyze`.

3.2.16 eimport

calc:eimport

Imports site energies from the output file of emultipole and writes them to the state file

option	default	unit	description

Return to the description of `eimport`.

3.2.17 einternal

calc:einternal

Reads in site and reorganosation energies and writes them to the state file

option	default	unit	description
energiesXML			XML input file with vacuum site, reorganization (charging, discharging) energies

Return to the description of `einternal`.

3.2.18 emultipole

calc:emultipole

Evaluates polarization contribution based on the Thole model

option	default	unit	description
multipoles			Polar Site Definitions in GDMA punch-file format
control			Control options for induction computation
induce	1		Enter '1' / '0' to toggle induction on / off
first			First segment for which to compute site energies
last			Last segment for which to compute site energies
output			File to write site energies to. Site energies are also stored in the state file
check			Check mapping of polar sites to fragment
tholeparam			Thole parameters required for charge-smearing
cutoff		nm	Cut-off beyond which all interactions are neglected
cutoff2		nm	Cut-off beyond which polarization is neglected
expdamp			Damping exponent used in exponential damping function
scaling			1-n interaction scaling, currently not in use
esp			Control options for potential calculation
calcESP			Enter '1' / '0' to toggle on / off. If '1', site energies will not be evaluated
cube			
grid			XYZ file specifying grid points for potential evaluation
output			File to write grid-point potential to
esf			Control options for field calculation
calcESF			Enter '1' / '0' to toggle on / off. If '1', site energies will not be evaluated
grid			XYZ file specifying grid points for field evaluation
output			File to write grid-point field to
alphamol			Control options for molecular-polarizability calculation
calcAlpha			Enter '1' / '0' to toggle on / off. If '1', site energies will not be evaluated
output			File to write polarizability tensor in global frame and in diagonal form to
convparam			Convergence parameters for self-consistent field calculation

wSOR_N			Mixing factor for successive overrelaxation of neutral system, usually between 0.3 and 0.5
wSOR_C			Mixing factor for successive overrelaxation of charged system, usually between 0.3 and 0.5
tolerance			Convergence criterion, fulfilled if relative change smaller than tolerance
maxiter			Maximum number of iterations in the convergence loop

Return to the description of `emultipole`.

3.2.19 eoutersphere

calc:eoutersphere

Evaluates outersphere reorganization energy

option	default	unit	description
multipoles			XML allocation polar sites
method			Type of the method: **constant** - all pairs have value **lambda**. **spheres** - molecules are treated as spheres with radii **radius** and Pekar factor **pekar**. **dielectric** - with Pekar factor **pekar** and partial charges from resulting dielectric fields
lambdaconst		eV	The value for all pairs in the **constant** method
pekar			Pekar factor used for methods **spheres** and **dielectric**
segment			
type			
radius			
segment			
type			
radius			
cutoff		nm	Cutoff radius in between pair and the exterior molecule. Can be used in **spheres** and **dielectric**

Return to the description of `eoutersphere`.

3.2.20 ianalyze

calc:ianalyze

Evaluates a histogram of a logarithm of squared couplings

option	default	unit	description
resolution_logJ2			Bin size of histogram log(J2)
resolution_space		nm	Bin size for r in log(J2(r))
states			States for which to calculate the histogram. Example: 1 -1

Return to the description of `ianalyze`.

3.2.21 iimport

calc:iimport

Imports electronic couplings from xml of xtp-dipro using folders of pairdump

option	default	unit	description
idft_jobs_file			idft jobs file
probabilityfile_h	ianalyze.ispatial.out		For coarse grained simulations provide here the distance dependent means and sigmas of hole transfer integrals. This file can be created using the ianalyze calculator.

probabilityfile_e	ianalyze.ispatial e.out		For coarse grained simulations provide here the distance dependent means and sigmas of electron transfer integrals. This file can be created using the ianalyze calculator.

Return to the description of `iimport`.

3.2.22 izindo

calc:izindo

Semiempirical electronic coupling elements for all neighbor list pairs

option	default	unit	description
orbitalsXML			File with paths to .orb files

Return to the description of `izindo`.

3.2.23 jobwriter

calc:jobwriter

Writes list of jobs for a parallel execusion

option	default	unit	description
keys			job type
single_id			Segment ID as argument for mps.single
kmc_cutoff		nm	Pair-interaction cut-off as argument for mps.kmc

Return to the description of `jobwriter`.

3.2.24 neighborlist

calc:neighborlist

option	default	unit	description
segments			
type			
cutoff			
constant			
exciton_cutoff			

Return to the description of `neighborlist`.

3.2.25 pairdump

calc:pairdump

Coordinates of molecules and pairs from the neighbor list

option	default	unit	description
molecules			If **true** outputs single molecules, otherwise only pairs

Return to the description of `pairdump`.

3.2.26 profile

calc:profile

Density and site energy profiles

option	default	unit	description
axis			Axis along which to calculate density and energy profiles
direction	0 0 1		Axis direction
min		nm	Minimal projected position for manual binning

max		nm	Maximal projected position for manual binning
bin	0.1	nm	Spatial resolution of the profile
auto	1		'0' for manual binning using min and max, '1' for automated
particles			
type	segments		What centers of mass to use: 'segments' or 'atoms'
first	1		ID of the first segment
last	-1		ID of the last segment, -1 is the list end
output			
density	density.dat		Density profile file
energy	energy.dat		Energy profile file

Return to the description of `profile`.

3.2.27 rates

calc:rates

Hopping rates using classical or semi-classical expression

option	default	unit	description
field			Field in x y z direction
temperature		K	Temperature for rates
method			Method chosen to compute rates. Can either be **marcus** or **jortner**. The first is the high temperature limit of Marcus theory, the second is the rate proposed by Jortner and Bixon
nmaxvib	20		If the method of choice is **jortner**, the maximal number of excited vibrations on the molecules has to be specified as an integer for the summation
omegavib	0.2	eV	If the method of choice is **jortner**, the vibration frequency of the quantum mode has to be given in units of eV. The default value is close to the CC bond-stretch at 0.2eV

Return to the description of `rates`.

3.2.28 sandbox

calc:sandbox

Sandbox to test xtp classes

option	default	unit	description
ID			Not in use

Return to the description of `sandbox`.

3.2.29 stateserver

calc:stateserver

Export SQLite file to human readable format

option	default	unit	description
out			Output file name
pdb			PDB coordinate file name
keys			Sections to write to readable format (topology, segments, pairs, coordinates)

Return to the description of `stateserver`.

3.2.30 tdump

calc:tdump

Coarse-grained and back-mapped (using rigid fragments) trajectories

option	default	unit	description
md	MD.pdb		Name of the coarse-grained trajectory
qm	QM.pdb		Name of the trajectory with back-substituted rigid fragments
frames	1		Number of frames to output

Return to the description of `tdump`.

3.2.31 vaverage

calc:vaverage

Computes site-centered velocity averages from site occupancies

option	default	unit	description
carriers			Carrier types for which to compute velocity averages
tabulate			Tabulate 'atoms' or 'segments'

Return to the description of `vaverage`.

3.2.32 zmultipole

calc:zmultipole

Evaluates polarization contribution based on the Thole model

option	default	unit	description
multipoles			Polar Site Definitions in GDMA punch-file format
control			Control options for induction computation
induce	1		Enter '1' / '0' to toggle induction on / off
first			First segment for which to compute site energies
last			Last segment for which to compute site energies
output			File to write site energies to. Site energies are also stored in the state file
check			Check mapping of polar sites to fragment
tholeparam			Thole parameters required for charge-smearing
cutoff		nm	Cut-off beyond which all interactions are neglected
cutoff2		nm	Cut-off beyond which polarization is neglected
expdamp			Damping exponent used in exponential damping function
scaling			1-n interaction scaling, currently not in use
esp			Control options for potential calculation
calcESP			Enter '1' / '0' to toggle on / off. If '1', site energies will not be evaluated
cube			
grid			XYZ file specifying grid points for potential evaluation
output			File to write grid-point potential to
esf			Control options for field calculation
calcESF			Enter '1' / '0' to toggle on / off. If '1', site energies will not be evaluated
grid			XYZ file specifying grid points for field evaluation
output			File to write grid-point field to
alphamol			Control options for molecular-polarizability calculation
calcAlpha			Enter '1' / '0' to toggle on / off. If '1', site energies will not be evaluated
output			File to write polarizability tensor in global frame and in diagonal form to

convparam			Convergence parameters for self-consistent field calculation
wSOR_N			Mixing factor for successive overrelaxation of neutral system, usually between 0.3 and 0.5
wSOR_C			Mixing factor for successive overrelaxation of charged system, usually between 0.3 and 0.5
tolerance			Convergence criterion, fulfilled if relative change smaller than tolerance
maxiter			Maximum number of iterations in the convergence loop

Return to the description of `zmultipole`.

3.2.33 edft

calc:edft

A wrapper for first principles based single site calculations

option	default	unit	description
tasks	input,run,parse		What to run
store	orbitals		What to store

Return to the description of `edft`.

3.2.34 idft

calc:idft

Projection method for electronic couplings. Requires edft otput

option	default	unit	description
tasks	input,run,parse,		What to do
store	orbitals,overlap		What to store
degeneracy	0	eV	Criterium for the degeneracy of two levels
levels	3		Output between HOMO, ..., HOMO-levels; LUMO, ..., LUMO+levels
trim	2		Use trim*occupied of virtual orbitals

Return to the description of `idft`.

3.2.35 qmmm

calc:qmmm

QM/MM with the Thole MM model

option	default	unit	description
pdb_check			PDB file of polar sites
write_chk	dipoles.xyz		XYZ file with dipoles split onto point charges
format_chk	xyz		format, gaussian or xyz
split_dpl	1		'0' do not split dipoles onto point charges, '1' do split
dpl_spacing	1e-3	nm	Spacing to be used when splitting dipole onto point charges: d = q * a
dftpackage			DFT package to use for the QM region
gwbse			Specify if GW/BSE excited state calculation ist needed
gwbse_options			GW/BSE options file
state			Number of excited state, which is to be calculated
type			Character of the excited state to be calculated
filter			Filter with which to find the excited state after each calculation
oscillator_strength			Oscillator strength filter, only states with higher oscillator strength are considered
charge_transfer			Charge transfer filter , only states with charge transfer above threshold are consdered

qmmmconvg			convergence criteria for the QM/MM
dR	0.001	nm	RMS of coordinates
dQ	0.001	e	RMS of charges
dE_QM	0.0001	eV	Energy change of the QM region
dE_MM	0.0001	eV	Energy change of the MM region
max_iter	10		Number of iterations
coulombmethod			Options for the MM embedding
method	cut-off		Method for evaluation of electrostatics
cutoff1			Cut-off for the polarizable MM1 shell
cutoff2			Cut-off for the static MM2 shell
tholemodel			Parameters for teh Thole model
induce			'1' - induce '0' - no induction
induce_intra_pair			'1' - include mutual interaction of induced dipoles in the QM region. '0' - do not
exp_damp	0.39		Sharpness parameter
scaling			Bond scaling factors
convergence			Convergence parameters for the MM1 (polarizable) region
wSOR_N			Mixing factor for the succesive overrelaxation algorithm for a neutral QM region
wSOR_C			Mixing factor for the succesive overrelaxation algorithm for a charged QM region
max_iter	512		Maximal number of iterations to converge induced dipoles
tolerance			Maximum RMS change allowed in induced dipoles

285 Return to the description of `qmmm`.

286 ### 3.2.36 xqmultipole

calc:xqmultipole

287 Electrostatic interaction and induction energy of charged molecular clusters

option	default	unit	description
mapping			Polar-site mapping definition
job_file			Job file
emp_file			Polar-background definition, allocation of mps-files to segments
pdb_check			Whether or not to output a pdb-file of the mapped polar sites
format_chk			Format for check-file: 'xyz' or 'gaussian'
split_dpl			Split dipoles onto point charges in check-file
dpl_spacing		nm	Spacing between point charges for check-file output
coulombmethod			
method			Currently only cut-off supported
cutoff1		nm	Full-interaction radius cut-off
cutoff2		nm	Radius of electrostatic buffer
tholemodel			
induce			Induce - or not
induce_intra_pair			Induce mutually within the charged cluster
exp_damp			Thole sharpness parameter
scaling			Bond scaling parameters, currently not used
convergence			
wSOR_N			SOR mixing factor for overall neutral clusters
wSOR_C			SOR mixing factor for overall charged clusters
max_iter			Maximum number of iterations
tolerance			Relative tolerance as convergence criterion

288 Return to the description of `xqmultipole`.

3.2.37 energy2xml

calc:energy2xml

Write out energies from SQL file

option	default	unit	description

Return to the description of `energy2xml`.

3.2.38 integrals2xml

calc:integrals2xml

Write out transfer integrals from SQL file

option	default	unit	description

Return to the description of `integrals2xml`.

3.2.39 occupations2xml

calc:occupations2xml

Write out site occupation probabilities from SQL file

option	default	unit	description

Return to the description of `occupations2xml`.

3.2.40 pairs2xml

calc:pairs2xml

Write out neighbourlist from SQL file

option	default	unit	description

Return to the description of `pairs2xml`.

3.2.41 rates2xml

calc:rates2xml

Write out charge transfer rates from SQL file

option	default	unit	description

Return to the description of `rates2xml`.

3.2.42 segments2xml

calc:segments2xml

Write out segment data from SQL file

option	default	unit	description

Return to the description of `segments2xml`.

3.2.43 trajectory2pdb

calc:trajectory2pdb

Generate PDB files for the mapped MD/QM topology

option	default	unit	description

Return to the description of `trajectory2pdb`.

3.3 Common options

ref:options

name	Description of the option

Bibliography

ruhle_microscopic_2011 [1] V. RÃijhle *et al.*, J. Chem. Theory Comput. **7**, 3335 (2011), bibtex: ruhle_microscopic_2011. ii

ruhle_versatile_2009 [2] V. RÃijhle *et al.*, J. Chem. Theory Comput. **5**, 3211 (2009), bibtex: ruhle_versatile_2009. ii