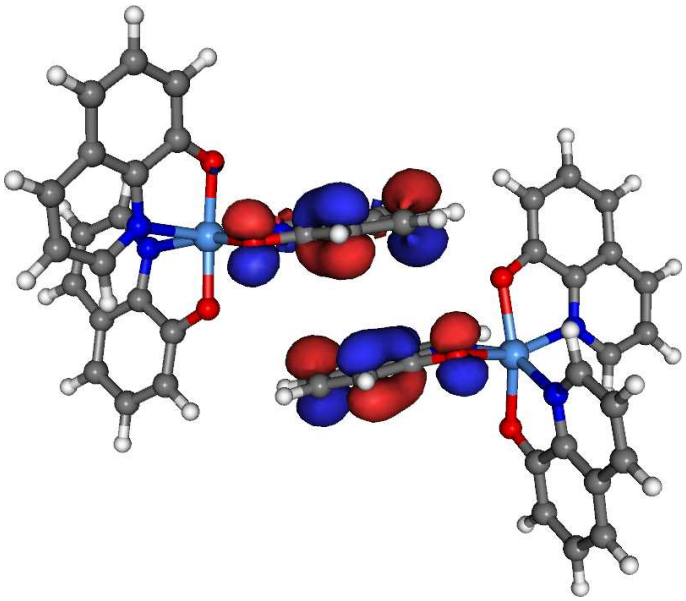
# VOTCA-XTP

## EXCITON TRANSPORT SIMULATIONS

USER MANUAL



compiled from: 1.5-dev (fa7077f)

March 2, 2017

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.

## Copyright

# Contents

# 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