

VOTCA-XTP

EXCITON TRANSPORT SIMULATIONS

USER MANUAL



compiled from: 1.5-dev (fa7077f)

March 11, 2017

www.votca.org

Disclaimer

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

VOTCA-XTP is free software. The entire package is available under the Apache License. For details, check the LICENSE file in the source code. The VOTCA-XTP source code is available on our homepage, www.votca.org.

Contents

| | | |
|----------|----------------------------------|----------|
| 1 | Introduction | 1 |
| 2 | Input and output files | 3 |
| 2.1 | DFT transfer integrals | 3 |
| 3 | Reference | 5 |
| 3.1 | Programs | 5 |
| 3.1.1 | xtp_testsuite | 5 |
| 3.1.2 | xtp_update | 5 |
| 3.1.3 | xtp_update_exciton | 5 |
| 3.1.4 | xtp_basisset | 5 |
| 3.1.5 | xtp_map | 6 |
| 3.1.6 | xtp_run | 6 |
| 3.1.7 | xtp_tools | 6 |
| 3.1.8 | xtp_parallel | 6 |
| 3.1.9 | xtp_dump | 7 |
| 3.2 | Calculators | 7 |
| 3.2.1 | dft | 7 |
| 3.2.2 | exciton | 8 |
| 3.2.3 | excitoniccoupling | 8 |
| 3.2.4 | gencube | 8 |
| 3.2.5 | partialcharges | 9 |
| 3.2.6 | qmanalyze | 9 |
| 3.2.7 | spectrum | 9 |
| 3.2.8 | coupling | 9 |
| 3.2.9 | log2mps | 10 |
| 3.2.10 | molpol | 10 |
| 3.2.11 | pdb2map | 11 |
| 3.2.12 | pdb2top | 11 |
| 3.2.13 | ptopreader | 11 |
| 3.2.14 | xneighborlist | 11 |
| 3.2.15 | eanalyze | 11 |
| 3.2.16 | eimport | 12 |
| 3.2.17 | einternal | 12 |
| 3.2.18 | emultipole | 12 |
| 3.2.19 | eoutersphere | 13 |
| 3.2.20 | ianalyze | 13 |
| 3.2.21 | iimport | 13 |
| 3.2.22 | izindo | 14 |
| 3.2.23 | jobwriter | 14 |
| 3.2.24 | neighborlist | 14 |
| 3.2.25 | pairedump | 14 |

| | | |
|---------------------|-----------------|-----------|
| 3.2.26 | profile | 14 |
| 3.2.27 | rates | 15 |
| 3.2.28 | sandbox | 15 |
| 3.2.29 | stateserver | 15 |
| 3.2.30 | tdump | 16 |
| 3.2.31 | vaverage | 16 |
| 3.2.32 | zmultipole | 16 |
| 3.2.33 | edft | 17 |
| 3.2.34 | idft | 17 |
| 3.2.35 | qmmm | 17 |
| 3.2.36 | xqmultipole | 18 |
| 3.2.37 | energy2xml | 19 |
| 3.2.38 | integrals2xml | 19 |
| 3.2.39 | occupations2xml | 19 |
| 3.2.40 | pairs2xml | 19 |
| 3.2.41 | rates2xml | 19 |
| 3.2.42 | segments2xml | 19 |
| 3.2.43 | trajectory2pdb | 19 |
| 3.3 | Common options | 20 |
| Bibliography | | 21 |

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.

```
10 <pair name="pair_100_155">
11   <parameters>
12     <HOMO_A>162</HOMO_A>
13     <NoccA>1</NoccA>
14     <LUMO_A>164</LUMO_A>
15     <NvirtA>1</NvirtA>
16     <HOMO_B>161</HOMO_B>
17     <NoccB>1</NoccB>
18     <LUMO_B>163</LUMO_B>
19     <NvirtB>1</NvirtB>
20   </parameters>
21   <transport name="hole">
22     <channel name="single">
23       <J>1.546400416750696E-003</J>
24       <e_A>-6.30726450715697</e_A>
25       <e_B>-6.36775613794166</e_B>
26     </channel>
27     <channel name="multi">
28       <molecule name="A">
29         <e_HOMOm0>-6.30726450715697</e_HOMOm0>
30       </molecule>
31       <molecule name="B">
32         <e_HOMOm0>-6.36775613794166</e_HOMOm0>
33       </molecule>
34       <dimer name="integrals">
35         <T_00>1.546400416750696E-003</T_00>
36         <J_sq_degen>2.391354248926727E-006</J_sq_degen>
37         <J_sq_boltz>2.391354248926727E-006</J_sq_boltz>
38       </dimer>
39     </channel>
40   </transport>
41   <transport name="electron">
42     <channel name="single">
43       <J>-2.797473760331286E-003</J>
44       <e_A>-4.50318366770689</e_A>
45       <e_B>-4.53143397059021</e_B>
```

```
47     </channel>
48     <channel name="multi">
49         <molecule name="A">
50             <e_LUMOp0>-4.50318366770689</e_LUMOp0>
51         </molecule>
52         <molecule name="B">
53             <e_LUMOp0>-4.53143397059021</e_LUMOp0>
54         </molecule>
55         <dimer name="integrals">
56             <T_00>-2.797473760331286E-003</T_00>
57             <J_sq_degen>7.825859439742066E-006</J_sq_degen>
58             <J_sq_boltz>7.825859439742066E-006</J_sq_boltz>
59         </dimer>
60     </channel>
61 </transport>
62 </pair>
63
```


Chapter 3

Reference

3.1 Programs

Programs execute specific tasks (calculators).

3.1.1 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

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

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

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

```

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

```

98 3.1.5 xtp_map

prog:xtp_map

```

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

```

106 3.1.6 xtp_run

prog:xtp_run

```

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

```

119 3.1.7 xtp_tools

prog:xtp_tools

```

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

```

127 3.1.8 xtp_parallel

prog:xtp_parallel

```

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

```

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

3.1.9 xtp_dump

prog:xtp_dump

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

3.2 Calculators

std:calculators

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

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

162 File options.xml lists all options needed to run a specific calculator. The format of this file is
163 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.

```
164 <calculator_name1>
165     <option1>value1</option1>
166     <option2>value2</option2>
167     ...
168 </calculator_name1>
169
170
171 <calculator_name2>
172     <option1>value1</option1>
173     <option2>value2</option2>
174     ...
175 </calculator_name2>
176 ...
177
```

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

```
179 xtp_run --list
```

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

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

3.2.1 dft

calc:dft

183 Standalone DFT calculator (experimental)

| option | default | unit | description |
|--------|---------|------|-------------|
|--------|---------|------|-------------|

| | | | |
|-----------|--|--|--|
| package | | | |
| tasks | | | |
| output | | | |
| reporting | | | |
| xyz | | | |
| dftengine | | | |
| archive | | | |

184 Return to the description of [dft](#).

185 3.2.2 exciton

calc:exciton

186 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 | | | |

187 Return to the description of [exciton](#).

188 3.2.3 excitoncoupling

calc:excitoniccoupling

189 Exciton couplings from serialized orbital files

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

190 Return to the description of [excitoniccoupling](#).

191 3.2.4 gencube

calc:gencube

192 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/excitedstate density / density excited-ground state |
| mode | new | | new: generate new cube file, subtract: subtract to cube files specified below |
| infile1 | | | Cubefile to subtract infile2 from |
| infile2 | | | Cubefile to subtract 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 | | | additional 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 serIALIZED 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.xml | eV | Output file |
| degeneracy | 0 | | Criterion 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 |

205 Return to the description of [coupling](#).

206 3.2.9 log2mps

calc:log2mps

207 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 |

208 Return to the description of [log2mps](#).

209 3.2.10 molpol

calc:molpol

210 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 |

211 Return to the description of [molpol](#).

212 3.2.11 **pdb2map**

calc:pdb2map

213 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 |

214 Return to the description of [pdb2map](#).

215 3.2.12 **pdb2top**

calc:pdb2top

216 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 |

217 Return to the description of [pdb2top](#).

218 3.2.13 **ptopreader**

calc:ptopreader

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

| option | default | unit | description |
|-----------|---------|------|---------------------------|
| ptop_file | | | Binary archive .ptop-file |

220 Return to the description of [ptopreader](#).

221 3.2.14 **xneighborlist**

calc:xneighborlist

222 Evaluates neighborlist, including long-range neighbors for energy transfer

| option | default | unit | description |
|----------------|---------|------|-------------|
| segments | | | |
| type | | | |
| cutoff | | | |
| constant | | | |
| exciton_cutoff | | | |

223 Return to the description of [xneighborlist](#).

224 3.2.15 **eanalyze**

calc:eanalyze

225 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 | | | ? |

226 Return to the description of [eanalyze](#).

227 3.2.16 eimport

calc:eimport

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

| option | default | unit | description |
|--------|---------|------|-------------|
|--------|---------|------|-------------|

229 Return to the description of [eimport](#).

230 3.2.17 einternal

calc:einternal

231 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 |

232 Return to the description of [einternal](#).

233 3.2.18 emultipole

calc:emultipole

234 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 |

235 Return to the description of [emultipole](#).

236 3.2.19 eoutersphere

calc:eoutersphere

237 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 |

238 Return to the description of [eoutersphere](#).

239 3.2.20 ianalyze

calc:ianalyze

240 Evaluates a histogram of a logarithm of squared couplings

| option | default | unit | description |
|------------------|---------|------|--|
| resolution_logJ2 | | | Bin size of histogram $\log(J^2)$ |
| resolution_space | | nm | Bin size for r in $\log(J^2(r))$ |
| states | | | States for which to calculate the histogram. Example: 1 -1 |

241 Return to the description of [ianalyze](#).

242 3.2.21 iimport

calc:iimport

243 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.h.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.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. |
|-------------------|-----------------------|--|---|

244 Return to the description of `iimport`.

245 3.2.22 izindo

calc:izindo

246 Semiempirical electronic coupling elements for all neighbor list pairs

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

247 Return to the description of `izindo`.

248 3.2.23 jobwriter

calc:jobwriter

249 Writes list of jobs for a parallel execution

| 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 |

250 Return to the description of `jobwriter`.

251 3.2.24 neighborlist

calc:neighborlist

| option | default | unit | description |
|----------------|---------|------|-------------|
| segments | | | |
| type | | | |
| cutoff | | | |
| constant | | | |
| exciton_cutoff | | | |

252 Return to the description of `neighborlist`.

253 3.2.25 pairdump

calc:pairdump

254 Coordinates of molecules and pairs from the neighbor list

| option | default | unit | description |
|-----------|---------|------|---|
| molecules | | | If <code>**true**</code> outputs single molecules, otherwise only pairs |

255 Return to the description of `pairdump`.

256 3.2.26 profile

calc:profile

257 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 |

258 Return to the description of [profile](#).

259 3.2.27 rates

calc:rates

260 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 |

261 Return to the description of [rates](#).

262 3.2.28 sandbox

calc:sandbox

263 Sandbox to test xtp classes

| option | default | unit | description |
|--------|---------|------|-------------|
| ID | | | Not in use |

264 Return to the description of [sandbox](#).

265 3.2.29 stateserver

calc:stateserver

266 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) |

267 Return to the description of [stateserver](#).

3.2.30 **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**

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**

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 |

276 Return to the description of [zmultipole](#).

277 3.2.33 edft

calc:edft

278 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 |

279 Return to the description of [edft](#).

280 3.2.34 idft

calc:idft

281 Projection method for electronic couplings. Requires edft output

| 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 |

282 Return to the description of [idft](#).

283 3.2.35 qmmm

calc:qmmm

284 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: $d = q \cdot a$ |
| 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 considered |

| | | | |
|-------------------|---------|----|--|
| 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 the 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 successive overrelaxation algorithm for a neutral QM region |
| wSOR_C | | | Mixing factor for the successive 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](#).

289 **3.2.37 energy2xml**calc:energy2xml
290

Write out energies from SQL file

| option | default | unit | description |
|--------|---------|------|-------------|
|--------|---------|------|-------------|

291 Return to the description of [energy2xml](#).292 **3.2.38 integrals2xml**calc:integrals2xml
293

Write out transfer integrals from SQL file

| option | default | unit | description |
|--------|---------|------|-------------|
|--------|---------|------|-------------|

294 Return to the description of [integrals2xml](#).295 **3.2.39 occupations2xml**calc:occupations2xml
296

Write out site occupation probabilities from SQL file

| option | default | unit | description |
|--------|---------|------|-------------|
|--------|---------|------|-------------|

297 Return to the description of [occupations2xml](#).298 **3.2.40 pairs2xml**calc:pairs2xml
299

Write out neighbourlist from SQL file

| option | default | unit | description |
|--------|---------|------|-------------|
|--------|---------|------|-------------|

300 Return to the description of [pairs2xml](#).301 **3.2.41 rates2xml**

calc:rates2xml

302 Write out charge transfer rates from SQL file

| option | default | unit | description |
|--------|---------|------|-------------|
|--------|---------|------|-------------|

303 Return to the description of [rates2xml](#).304 **3.2.42 segments2xml**

calc:segments2xml

305 Write out segment data from SQL file

| option | default | unit | description |
|--------|---------|------|-------------|
|--------|---------|------|-------------|

306 Return to the description of [segments2xml](#).307 **3.2.43 trajectory2pdb**calc:trajectory2pdb
308

Generate PDB files for the mapped MD/QM topology

| option | default | unit | description |
|--------|---------|------|-------------|
|--------|---------|------|-------------|

309 Return to the description of [trajectory2pdb](#).

3.3 Common options

310
ref:options

| name | Description of the option |
|------|---------------------------|
|------|---------------------------|

Bibliography

- [ruhle_microscopic_2011](#) [1] V. RÅijhle *et al.*, J. Chem. Theory Comput. 7, 3335 (2011), bibtex: ruhle_microscopic_2011. [ii](#)
- [ruhle_versatile_2009](#) [2] V. RÅijhle *et al.*, J. Chem. Theory Comput. 5, 3211 (2009), bibtex: ruhle_versatile_2009. [ii](#)