DPTI

DeepModeling

Apr 13, 2024

CONTENTS:

DPTI is a Python package to automate thermodynamic integration (TI) calculations for free energy.

CHAPTER

ONE

INSTALL DPTI

DPTI can installed by `pip`:

```
pip install dpti
```

CHAPTER

TWO

GETTING STARTED

DPTI: A Thermodynamic Integration Automization Package for Free Energy Calculation

TODO

CHAPTER

THREE

COMMAND LINE INTERFACE

DPTI: An Automatic Workflow Software for Thermodynamic Integration Calculations

```
usage: dpti [-h] {equi,hti,hti_liq,hti_ice,hti_water,ti,ti_water,gdi,mti} ...
```

3.1 modules

the subcommands of dpti

module Possible choices: equi, hti, hti_liq, hti_ice, hti_water, ti, ti_water, gdi, mti

module-level help

3.2 Sub-commands

3.2.1 equi

equilibration simulations

```
dpti equi [-h] {gen,extract,stat-bond,compute,run} ...
```

Positional Arguments

command Possible choices: gen, extract, stat-bond, compute, run

commands for equilibration simulations

Sub-commands

gen

generate a job

```
dpti equi gen [-h] [-e ENSEMBLE] [-t TEMPERATURE] [-p PRESSURE] [-a]
              [-c CONF_NPT] [-o OUTPUT]
              PARAM
```

Positional Arguments

PARAM json parameter file

Named Arguments

-e, --ensemble the ensemble of the simulation

-t, --temperature the temperature of the system

-p, --pressure the pressure of the system

-a, --avg-posi dump the average position of atoms

Default: False

-c, --conf-npt use conf computed from NPT simulation

-o, --output the output folder for the job

Default: “new_job”

extract

extract the conf

```
dpti equi extract [-h] [-o OUTPUT] JOB
```

Positional Arguments

JOB folder of the job

Named Arguments

-o, --output output conf file name

Default: “conf.lmp”

stat-bond

Statistic of the bonds

```
dpti equi stat-bond [-h] [-s SKIP] JOB
```

Positional Arguments

JOB folder of the job

Named Arguments

-s, --skip skip this number of frames

Default: 1

compute

Compute thermodynamics

```
dpti equi compute [-h] JOB
```

Positional Arguments

JOB folder of the job

run

run the job

```
dpti equi run [-h] JOB machine
```

Positional Arguments

JOB folder of the job

machine machine.json file for the job

3.2.2 hti

Hamiltonian thermodynamic integration for atomic solid

```
dpti hti [-h] {gen,compute,run} ...
```

Positional Arguments

command Possible choices: gen, compute, run

commands of Hamiltonian thermodynamic integration for atomic solid

Sub-commands

gen

generate a job

```
dpti hti gen [-h] [-o OUTPUT] [-s {one-step,two-step,three-step}] [-z] PARAM
```

Positional Arguments

PARAM json parameter file

Named Arguments

-o, --output the output folder for the job

Default: "new_job"

-s, --switch Possible choices: one-step, two-step, three-step

one-step: switching on DP and switching off spring simultanenously. two-step: 1 switching on DP, 2 switching off spring. three-step: 1 switching on soft LJ, 2 switching on DP, 3 switching off spring and soft LJ.

Default: "one-step"

-z, --meam whether use meam instead of dp

Default: False

compute

Compute the result of a job

```
dpti hti compute [-h] [-t {helmholtz,gibbs}] [-m {inte,mbar}] [-s SCHEME]
                 [-g PV] [-G PV_ERR]
                 JOB
```

Positional Arguments

JOB folder of the job

Named Arguments

-t, --type Possible choices: helmholtz, gibbs
the type of free energy
Default: "helmholtz"

-m, --inte-method Possible choices: inte, mbar
the method of thermodynamic integration
Default: "inte"

-s, --scheme the numeric integration scheme
Default: "simpson"

-g, --pv press*vol value override to calculate Gibbs free energy

-G, --pv-err press*vol error

run

run the job

```
dpti hti run [-h] [--no-dp] JOB machine task_name
```

Positional Arguments

JOB folder of the job

machine machine.json file for the job

task_name task name, can be 00, 01, or 02

Named Arguments

--no-dp whether to use Deep Potential or not
Default: False

3.2.3 hti_liq

Hamiltonian thermodynamic integration for atomic liquid

```
dpti hti_liq [-h] {gen,compute,run} ...
```

Positional Arguments

command Possible choices: gen, compute, run

commands of Hamiltonian thermodynamic integration for atomic liquid

Sub-commands

gen

Generate a job

```
dpti hti_liq gen [-h] [-o OUTPUT] [-z] PARAM
```

Positional Arguments

PARAM json parameter file

Named Arguments

-o, --output the output folder for the job

Default: "new_job"

-z, --meam whether use meam instead of dp

Default: False

compute

Compute the result of a job

```
dpti hti_liq compute [-h] [-t {helmholtz,gibbs}] [-g PV] [-G PV_ERR] JOB
```

Positional Arguments

JOB folder of the job

Named Arguments

-t, --type	Possible choices: helmholtz, gibbs the type of free energy Default: "helmholtz"
-g, --pv	press*vol value override to calculate Gibbs free energy
-G, --pv-err	press*vol error

run

run the job

```
dpti hti_liq run [-h] [--no-dp] JOB machine task_name
```

Positional Arguments

JOB	folder of the job
machine	machine.json file for the job
task_name	task name, can be 00, 01, or 02

Named Arguments

--no-dp	whether to use Deep Potential or not Default: False

3.2.4 hti_ice

Hamiltonian thermodynamic integration for ice

```
dpti hti_ice [-h] {gen,compute,refine,run} ...
```

Positional Arguments

command	Possible choices: gen, compute, refine, run commands of Hamiltonian thermodynamic integration for ice

Sub-commands

gen

Generate a job

```
dpti hti_ice gen [-h] [-o OUTPUT] [-s {one-step,two-step,three-step}] PARAM
```

Positional Arguments

PARAM json parameter file

Named Arguments

-o, --output the output folder for the job

Default: "new_job"

-s, --switch Possible choices: one-step, two-step, three-step

one-step: switching on DP and switching off spring simultanenously.
two-step: 1 switching on DP, 2 switching off spring.
three-step: 1 switching on soft LJ, 2 switching on DP, 3 switching off spring and soft LJ.

Default: "one-step"

compute

Compute the result of a job

```
dpti hti_ice compute [-h] [-t {helmholtz,gibbs}] [-m {inte,mbar}] [-d]
                     [-p {3,5}] [-s SCHEME] [-S SHIFT] [-g PV] [-G PV_ERR]
                     [--npt NPT]
                     JOB
```

Positional Arguments

JOB folder of the job

Named Arguments

-t, --type Possible choices: helmholtz, gibbs

the type of free energy

Default: "helmholtz"

-m, --inte-method Possible choices: inte, mbar

the method of thermodynamic integration

Default: "inte"

-d, --disorder-corr	apply disorder correction for ice Default: True
-p, --partial-disorder	Possible choices: 3, 5 apply partial disorder correction for ice
-s, --scheme	the numeric integration scheme Default: “simpson”
-S, --shift	a constant shift in the energy/mole computation, will be removed from FE Default: 0.0
-g, --pv	press*vol value override to calculate Gibbs free energy
-G, --pv-err	press*vol error
--npt	directory of the npt task; will use PV from npt result, where P is the control variable and V varies.

refine

Refine the grid of a job

```
dpti hti_ice refine [-h] -i INPUT -o OUTPUT -e ERROR [-p]
```

Named Arguments

-i, --input	input job
-o, --output	output job
-e, --error	the error required
-p, --print	print the refinement and exit Default: False

run

run the job

```
dpti hti_ice run [-h] [--no-dp] JOB machine task_name
```

Positional Arguments

JOB	folder of the job
machine	machine.json file for the job
task_name	task name, can be 00, 01, or 02

Named Arguments

--no-dp whether to use Deep Potential or not

Default: False

3.2.5 hti_water

Hamiltonian thermodynamic integration for liquid water

```
dpti hti_water [-h] {gen,compute,refine,run} ...
```

Positional Arguments

command Possible choices: gen, compute, refine, run

commands of Hamiltonian thermodynamic integration for liquid water

Sub-commands

gen

Generate a job

```
dpti hti_water gen [-h] [-o OUTPUT] PARAM
```

Positional Arguments

PARAM json parameter file

Named Arguments

-o, --output the output folder for the job

Default: “new_job”

compute

Compute the result of a job

```
dpti hti_water compute [-h] [-t {helmholtz,gibbs}] [-m {inte,mbar}]
                       [-s SCHEME] [-g PV] [-G PV_ERR] [--npt NPT]
                       JOB
```

Positional Arguments

JOB	folder of the job

Named Arguments

-t, --type	Possible choices: helmholtz, gibbs
	the type of free energy
	Default: "helmholtz"
-m, --inte-method	Possible choices: inte, mbar
	the method of thermodynamic integration
	Default: "inte"
-s, --scheme	the numeric integration scheme
	Default: "simpson"
-g, --pv	press*vol value override to calculate Gibbs free energy
-G, --pv-err	press*vol error
--npt	directory of the npt task; will use PV from npt result, where P is the control variable and V varies.

refine

Refine the grid of a job

```
dpti hti_water refine [-h] -i INPUT -o OUTPUT -e ERROR
```

Named Arguments

-i, --input	input job
-o, --output	output job
-e, --error	the error required

run

run the job

```
dpti hti_water run [-h] [--no-dp] JOB machine task_name
```

Positional Arguments

JOB	folder of the job
machine	machine.json file for the job
task_name	task name, can be 00, 01, or 02

Named Arguments

--no-dp	whether to use Deep Potential or not Default: False

3.2.6 ti

thermodynamic integration along isothermal or isobaric paths

```
dpti ti [-h] {gen,compute,refine,run} ...
```

Positional Arguments

command	Possible choices: gen, compute, refine, run commands of thermodynamic integration along isothermal or isobaric paths

Sub-commands

gen

Generate a job

```
dpti ti gen [-h] [-o OUTPUT] [-z] PARAM
```

Positional Arguments

PARAM	json parameter file

Named Arguments

-o, --output	the output folder for the job Default: “new_job”
-z, --meam	whether use meam instead of dp Default: False

compute

Compute the result of a job

```
dpti ti compute [-h] [-m {inte,mbar}] [-e E0] [-E E0_ERR] [-t T0] [-s SCHEME]
                [-H HTI]
                JOB
```

Positional Arguments

JOB folder of the job

Named Arguments

-m, --inte-method Possible choices: inte, mbar

the method of thermodynamic integration

Default: "inte"

-e, --Eo free energy of starting point

Default: 0

-E, --Eo-err The statistical error of the starting free energy

Default: 0

-t, --To the starting thermodynamic position

-s, --scheme the numerical integration scheme

Default: "simpson"

-H, --hti the HTI job folder; will extract the free energy of the starting point as from the result.json file in this folder

refine

Refine the grid of a job

```
dpti ti refine [-h] -i INPUT -o OUTPUT -e ERROR
```

Named Arguments

-i, --input input job

-o, --output output job

-e, --error the error required

run

run the job

```
dpti ti run [-h] JOB machine
```

Positional Arguments

JOB folder of the job

machine machine.json file for the job

3.2.7 ti_water

thermodynamic integration along isothermal or isobaric paths for water

```
dpti ti_water [-h] {gen,compute,refine,run} ...
```

Positional Arguments

command Possible choices: gen, compute, refine, run

commands of thermodynamic integration along isothermal or isobaric paths for water

Sub-commands

gen

Generate a job

```
dpti ti_water gen [-h] [-o OUTPUT] PARAM
```

Positional Arguments

PARAM json parameter file

Named Arguments

-o, --output the output folder for the job

Default: “new_job”

compute

Compute the result of a job

```
dpti ti_water compute [-h] [-m {inte,mbar}] [-e EO] [-E EO_ERR] [-t TO]
                      [-s SCHEME] [-S SHIFT] [-H HTI]
                      JOB
```

Positional Arguments

JOB folder of the job

Named Arguments

-m, --inte-method Possible choices: inte, mbar

the method of thermodynamic integration

Default: "inte"

-e, --Eo free energy of starting point

-E, --Eo-err the statistical error of the starting free energy

-t, --To the starting thermodynamic position

-s, --scheme the numerical integration scheme

Default: "simpson"

-S, --shift a constant shift in the energy/mole computation, will be removed from FE

Default: 0.0

-H, --hti the HTI job folder; will extract the free energy of the starting point as from the result.json file in this folder

refine

Refine the grid of a job

```
dpti ti_water refine [-h] -i INPUT -o OUTPUT -e ERROR
```

Named Arguments

-i, --input input job

-o, --output output job

-e, --error the error required

run

run the job

```
dpti ti_water run [-h] JOB machine
```

Positional Arguments

JOB	folder of the job
machine	machine.json file for the job

3.2.8 gdi

compute the phase boundary via Gibbs-Duhem integration

```
dpti gdi [-h] [-g GDIDATA_JSON] [-b BEGIN] [-e END] [-d {t,p}]
         [-i INITIAL_VALUE] [-s STEP_VALUE [STEP_VALUE ...]] [-a ABS_TOL]
         [-r REL_TOL] [-w] [-o OUTPUT] [-f FIRST_STEP] [-S SHIFT SHIFT] [-v]
         [-z]
         PARAM MACHINE
```

Positional Arguments

PARAM	json parameter file
MACHINE	json machine file

Named Arguments

-g, --gdidata-json	json gdi integration file
-b, --begin	start of the integration
-e, --end	end of the integration
-d, --direction	Possible choices: t, p direction of the integration, along T or P
-i, --initial-value	the initial value of T (direction=p) or P (direction=t)
-s, --step-value	the T (direction=t) or P (direction=p) values must be evaluated
-a, --abs-tol	the absolute tolerance of the integration Default: 10
-r, --rel-tol	the relative tolerance of the integration Default: 0.01
-w, --if-water	assumes water molecules: nmols = natoms//3 Default: False

-o, --output	the output folder for the job Default: "new_job"
-f, --first-step	the first step size of the integrator
-S, --shift	the output folder for the job Default: [0.0, 0.0]
-v, --verbose	print detailed infomation Default: False
-z, --if-meam	whether use meam instead of dp Default: False

3.2.9 mti

mass thermodynamic integration: quantum free energy calculation using PIMD

```
dpti mti [-h] {gen,run,compute} ...
```

Positional Arguments

command	Possible choices: gen, run, compute commands of mass thermodynamic integration

Sub-commands

gen

Generate a job

```
dpti mti gen [-h] [-o OUTPUT] PARAM
```

Positional Arguments

PARAM	json parameter file

Named Arguments

-o, --output	the output folder for the job Default: "new_job"

run

run the job

```
dpti mti run [-h] JOB PARAM machine
```

Positional Arguments

JOB	folder of the job
PARAM	json parameter file
machine	machine.json file for the job

compute

Compute the result of a job

```
dpti mti compute [-h] [--natom_mol NATOM_MOL] JOB
```

Positional Arguments

JOB	folder of the job

Named Arguments

--natom_mol	the number of atoms in the molecule

CHAPTER

FOUR

DPTI API

4.1 dpti package

4.1.1 Subpackages

dpti.dags package

Submodules

dpti.dags.dp_ti_gdi module

class dpti.dags.dp_ti_gdi.**GDIDAGFactory**(*gdi_name*, *dag_work_base*)

Bases: object

Methods

create_loop_dag
create_main_dag

create_loop_dag()

create_main_dag()

dagargs: ClassVar[Dict[str, object]] = {'default_args': {'owner': 'airflow', 'start_date': datetime.datetime(2018, 1, 1, 0, 0)}, 'schedule_interval': None}

default_args: ClassVar[Dict[str, object]] = {'owner': 'airflow', 'start_date': datetime.datetime(2018, 1, 1, 0, 0)}

class dpti.dags.dp_ti_gdi.**GDIWorkflow**(*dag_name*, *var_name*)

Bases: object

Methods

get_dag_run_state
trigger_loop
wait_until_end

get_dag_run_state()

trigger_loop(*submission*, *task_list*, *mdata*)

wait_until_end()

dpti.dags.utils module

dpti.dags.utils.**get_empty_submission**(*job_work_dir*, *context*)

dpti.lib package

Submodules

dpti.lib.RemoteJob module

class dpti.lib.RemoteJob.**CloudMachineJob**(*ssh_session*, *local_root*)

Bases: *RemoteJob*

Methods

block_call
block_checkcall
check_status
clean
download
get_job_root
submit
upload

check_status()

submit(*job_dirs*, *cmd*, *args=None*, *resources=None*)

class dpti.lib.RemoteJob.**JobStatus**(*value*)

Bases: Enum

An enumeration.

finished = 5

running = 3

terminated = 4

unknow = 100

unsubmitted = 1

waiting = 2

class dpti.lib.RemoteJob.**PBSJob**(*ssh_session*, *local_root*)

Bases: *RemoteJob*

Methods

block_call
block_checkcall
check_status
clean
download
get_job_root
submit
upload

check_status()

submit(*job_dirs*, *cmd*, *args=None*, *resources=None*)

class dpti.lib.RemoteJob.**RemoteJob**(*ssh_session*, *local_root*)

Bases: object

Methods

block_call
block_checkcall
clean
download
get_job_root
upload

block_call(*cmd*)

block_checkcall(*cmd*)

clean()

download(*job_dirs*, *remote_down_files*)

get_job_root()

upload(*job_dirs*, *local_up_files*, *dereference=True*)

class dpti.lib.RemoteJob.**SSHSession**(*jdata*)

Bases: object

Methods

close
get_session_root
get_ssh_client

close()

get_session_root()

get_ssh_client()

class dpti.lib.RemoteJob.**SlurmJob**(*ssh_session*, *local_root*)

Bases: *RemoteJob*

Methods

block_call
block_checkcall
check_status
clean
download
get_job_root
submit
upload

check_status()

submit(*job_dirs*, *cmd*, *args=None*, *resources=None*)

dpti.lib.dump module

dpti.lib.dump.**box2dumpbox**(*orig*, *box*)

dpti.lib.dump.**dumpbox2box**(*bounds*, *tilt*)

dpti.lib.dump.**get_atype**(*lines*)

dpti.lib.dump.**get_dumpbox**(*lines*)

dpti.lib.dump.**get_natoms**(*lines*)

dpti.lib.dump.**get_natoms_vec**(*lines*)

dpti.lib.dump.**get_natomtypes**(*lines*)

dpti.lib.dump.**get_posi**(*lines*)

dpti.lib.dump.**split_traj**(*dump_lines*)

dpti.lib.dump.**system_data**(*lines*)

dpti.lib.lammps module

dpti.lib.lammps.**get_last_dump**(*dump*)

dpti.lib.lammps.**get_natoms**(*filename*)

dpti.lib.lammps.**get_thermo**(*filename*)

dpti.lib.lammps.**get_thermo_old**(*filename*)

dpti.lib.lmp module

dpti.lib.lmp.**box2lmpbox**(*orig*, *box*)

dpti.lib.lmp.**from_system_data**(*system*)

dpti.lib.lmp.**get_atoms**(*lines*)

dpti.lib.lmp.**get_atype**(*lines*)

dpti.lib.lmp.**get_id**(*lines*)

dpti.lib.lmp.**get_lmpbox**(*lines*)

dpti.lib.lmp.**get_natoms**(*lines*)

dpti.lib.lmp.**get_natoms_vec**(*lines*)

dpti.lib.lmp.**get_natomtypes**(*lines*)

dpti.lib.lmp.**get_posi**(*lines*)

dpti.lib.lmp.**lmpbox2box**(*lohi*, *tilt*)

dpti.lib.lmp.**system_data**(*lines*)

dpti.lib.lmp.**to_system_data**(*lines*)

dpti.lib.ovito_file_convert module

dpti.lib.utils module

dpti.lib.utils.**block_avg**(*inp*, *skip=0*, *block_size=10*)

dpti.lib.utils.**compute_nrefine**(*all_t*, *integrand*, *err*, *error_scale=None*)

dpti.lib.utils.**copy_file_list**(*file_list*, *from_path*, *to_path*)

dpti.lib.utils.**create_dict_not_empty_key**(***kwargs*)

dpti.lib.utils.**create_path**(*path*)

dpti.lib.utils.**cvt_conf**(*fin*, *fout*, *ofmt='vasp'*)

Format convert from fin to fout, specify the output format by ofmt.

dpti.lib.utils.**get_file_md5**(*file_path*)

dpti.lib.utils.**get_first_matched_key_from_dict**(*dct*, *lst*)

dpti.lib.utils.**get_task_file_abspath**(*task_name*, *file_name*)

dpti.lib.utils.**integrate**(*xx*, *yy*, *ye*, *scheme_='s'*)

dpti.lib.utils.**integrate_range**(*xx*, *yy*, *ye*, *scheme='s'*)

dpti.lib.utils.**integrate_range_hti**(*all_lambda*, *de*, *de_err*, *scheme='s'*)

dpti.lib.utils.**integrate_range_simpson**(*xx*, *yy*, *ye*)

dpti.lib.utils.**integrate_range_trapezoidal**(*xx*, *yy*, *ye*)

dpti.lib.utils.**integrate_simpson**(*xx*, *yy*, *ye*)

dpti.lib.utils.**integrate_simpson_nonuniform**(*x*, *f*, *fe*)

dpti.lib.utils.**integrate_sys_err**(*xx*, *yy*, *scheme_='s'*)

dpti.lib.utils.**integrate_sys_err_simpson**(*xx*, *yy*)

dpti.lib.utils.**integrate_sys_err_trapezoidal**(*xx*, *yy*)

dpti.lib.utils.**integrate_trapezoidal**(*xx*, *yy*, *ye*)

dpti.lib.utils.**interval_sys_err_trapezoidal**(*xx*, *yy*, *mode*)

dpti.lib.utils.**link_file_in_dict**(*dct*, *key_list*, *target_dir*)

dpti.lib.utils.**make_iter_name**(*iter_index*)

dpti.lib.utils.**parse_seq**(*in_s*, *, *protect_eps=None*)

dpti.lib.utils.**relative_link_file**(*file_path*, *target_dir*)

dpti.lib.vasp module

dpti.lib.vasp.**perturb_xz**(*poscar_in*, *poscar_out*, *pert=0.01*)

dpti.lib.vasp.**poscar_natoms**(*poscar_in*)

dpti.lib.vasp.**poscar_scale**(*poscar_in*, *poscar_out*, *scale*)

dpti.lib.vasp.**poscar_vol**(*poscar_in*)

dpti.lib.vasp.**reciprocal_box**(*box*)

dpti.lib.vasp.**regulate_poscar**(*poscar_in*, *poscar_out*)

dpti.lib.vasp.**sort_poscar**(*poscar_in*, *poscar_out*, *new_names*)

dpti.lib.water module

dpti.lib.water.**add_bonds**(*lines_*, *max_roh=1.3*)

dpti.lib.water.**compute_bonds**(*box*, *atype*, *posis*, *max_roh=1.3*, *uniq_hbond=True*)

dpti.lib.water.**dist_via_oh_list**(*box*, *posis*, *list_oh*)

dpti.lib.water.**min_ho**(*box*, *atype*, *posis*)

dpti.lib.water.**min_oh_list**(*box*, *atype*, *posis*)

dpti.lib.water.**min_oho**(*box*, *atype*, *posis*)

dpti.lib.water.**min_oo**(*box*, *atype*, *posis*)

dpti.lib.water.**posi_diff**(*box*, *r0*, *r1*)

dpti.lib.water.**posi_shift**(*box*, *r0*, *r1*)

4.1.2 Submodules

4.1.3 dpti.einstein module

dpti.einstein.**compute_lambda**(*temp*, *mass*)

dpti.einstein.**compute_spring**(*temp*, *spring_k*)

dpti.einstein.**free_energy**(*job*)

dpti.einstein.**frenkel**(*job*)

dpti.einstein.**ideal_gas_fe**(*job*)

4.1.4 dpti.equi module

dpti.equi.**add_module_subparsers**(*main_subparsers*)

dpti.equi.**add_subparsers**(*module_subparsers*)

dpti.equi.**exec_args**(*args*, *parser*)

dpti.equi.**extract**(*job_dir*, *output*)

dpti.equi.**gen_equi_dump_settings**(*if_dump_avg_posi*)

dpti.equi.**gen_equi_ensemble_settings**(*ens*)

dpti.equi.**gen_equi_force_field**(*model*, *if_meam=False*, *meam_model=None*)

dpti.equi.**gen_equi_header**(*nsteps*, *thermo_freq*, *dump_freq*, *mass_map*, *temp*, *tau_t*, *tau_p*, *equi_conf*, *pres=None*)

dpti.equi.**gen_equi_lammps_input**(*nsteps*, *thermo_freq*, *dump_freq*, *mass_map*, *temp*, *tau_t*, *tau_p*, *equi_conf*, *model*, *timestep*, *if_dump_avg_posi*, *ens*, *pres=None*, *if_meam=False*, *meam_model=None*)

dpti.equi.**gen_equi_thermo_settings**(*timestep*)

dpti.equi.**handle_compute**(*args*)

dpti.equi.**handle_extract**(*args*)

dpti.equi.**handle_gen**(*args*)

dpti.equi.**handle_run**(*args*)

dpti.equi.**handle_stat_bond**(*args*)

dpti.equi.**make_task**(*iter_name*, *jdata*, *ens=None*, *temp=None*, *pres=None*, *if_dump_avg_posi=None*, *npt_dir=None*)

dpti.equi.**npt_equi_conf**(*npt_dir*)

dpti.equi.**post_task**(*iter_name*, *natoms=None*, *is_water=None*)

dpti.equi.**run_task**(*task_name*, *machine_file*)

dpti.equi.**water_bond**(*iter_name*, *skip=1*)

4.1.5 dpti.gdi module

class dpti.gdi.**GibbsDuhemFunc**(*jdata*, *mdata*, *task_path*, *inte_dir*, *pref=1.0*, *natoms=None*, *shift=[0, 0]*, *verbose=False*, *if_meam=False*, *meam_model=None*, *workflow=None*)

Bases: `object`

Methods

`__call__`(x, y)	Call self as a function.

dpti.gdi.**add_module_subparsers**(*main_subparsers*)

dpti.gdi.**gdi_main_loop**(*jdata*, *mdata*, *gdidata_dict={}*, *gdidata_cli={}*, *workflow=None*)

dpti.gdi.**handle_gdi**(*args*)

dpti.gdi.**make_dpdt**(*temp*, *pres*, *inte_dir*, *task_path*, *mdata*, *natoms=None*, *shift=[0, 0]*, *verbose=False*, *if_meam=False*, *meam_model=None*, *workflow=None*)

4.1.6 dpti.hti module

dpti.hti.**add_module_subparsers**(*main_subparsers*)

dpti.hti.**compute_task**(*job*, *free_energy_type='helmholtz'*, *method='inte'*, *scheme='simpson'*, *manual_pv=None*, *manual_pv_err=None*)

dpti.hti.**handle_compute**(*args*)

dpti.hti.**handle_gen**(*args*)

dpti.hti.**handle_run**(*args*)

dpti.hti.**hti_phase_trans_analyze**(*job*, *jdata=None*)

dpti.hti.**make_iter_name**(*iter_index*)

dpti.hti.**make_tasks**(*iter_name*, *jdata*, *ref='einstein'*, *switch='one-step'*, *if_meam=None*)

dpti.hti.**post_tasks**(*iter_name*, *jdata*, *natoms=None*, *method='inte'*, *scheme='s'*)

dpti.hti.**print_thermo_info**(*info*)

dpti.hti.**refine_task**(*from_task*, *to_task*, *err*, *print_ref=False*, *if_meam=None*, *meam_model=None*)

dpti.hti.**run_task**(*task_dir*, *machine_file*, *task_name*, *no_dp=False*)

4.1.7 dpti.hti_ice module

dpti.hti_ice.**add_module_subparsers**(*main_subparsers*)

dpti.hti_ice.**add_subparsers**(*module_subparsers*)

dpti.hti_ice.**exec_args**(*args*, *parser*)

dpti.hti_ice.**handle_compute**(*args*)

dpti.hti_ice.**handle_gen**(*args*)

dpti.hti_ice.**handle_refine**(*args*)

dpti.hti_ice.**handle_run**(*args*)

4.1.8 dpti.hti_liq module

dpti.hti_liq.**add_module_subparsers**(*main_subparsers*)

dpti.hti_liq.**compute_task**(*job*, *free_energy_type='helmholtz'*, *scheme='simpson'*, *manual_pv=None*, *manual_pv_err=None*)

dpti.hti_liq.**handle_compute**(*args*)

dpti.hti_liq.**handle_gen**(*args*)

dpti.hti_liq.**handle_run**(*args*)

dpti.hti_liq.**make_iter_name**(*iter_index*)

dpti.hti_liq.**make_tasks**(*iter_name*, *jdata*, *if_meam=None*)

dpti.hti_liq.**post_tasks**(*iter_name*, *natoms*)

4.1.9 dpti.hti_water module

dpti.hti_water.**add_module_subparsers**(*main_subparsers*)

dpti.hti_water.**add_subparsers**(*module_subparsers*)

dpti.hti_water.**compute_ideal_mol**(*iter_name*)

dpti.hti_water.**exec_args**(*args*, *parser*)

dpti.hti_water.**handle_compute**(*args*)

dpti.hti_water.**handle_gen**(*args*)

dpti.hti_water.**handle_refine**(*args*)

dpti.hti_water.**handle_run**(*args*)

dpti.hti_water.**make_tasks**(*iter_name*, *jdata*)

dpti.hti_water.**post_tasks**(*iter_name*, *natoms*, *method='inte'*, *scheme='s'*)

dpti.hti_water.**refine_tasks**(*from_task*, *to_task*, *err*)

dpti.hti_water.**spring_inte**(*temp*, *kk*, *r0*)

4.1.10 dpti.main module

dpti.main.**create_parser**()

dpti.main.**main**()

4.1.11 dpti.mti module

dpti.mti.**add_module_subparsers**(*main_subparsers*)

dpti.mti.**add_subparsers**(*module_subparsers*)

dpti.mti.**exec_args**(*args*, *parser*)

dpti.mti.**handle_compute**(*args*)

dpti.mti.**handle_gen**(*args*)

dpti.mti.**handle_run**(*args*)

dpti.mti.**make_tasks**(*iter_name*, *jdata*)

dpti.mti.**post_tasks**(*iter_name*, *jdata*, *natoms_mol=None*)

dpti.mti.**run_task**(*task_name*, *jdata*, *machine_file*)

4.1.12 dpti.old_equi module

dpti.old_equi.**extract**(*job_dir*, *output*)

dpti.old_equi.**make_task**(*iter_name*, *jdata*, *ens=None*, *temp=None*, *pres=None*, *avg_posi=None*, *npt_conf=None*, *if_meam=None*)

dpti.old_equi.**npt_equi_conf**(*npt_name*)

dpti.old_equi.**post_task**(*iter_name*, *natoms=None*, *is_water=False*)

dpti.old_equi.**water_bond**(*iter_name*, *skip=1*)

4.1.13 dpti.relax module

4.1.14 dpti.ti module

dpti.ti.**add_module_subparsers**(*main_subparsers*)

dpti.ti.**compute_task**(*job*, *inte_method*, *Eo*, *Eo_err*, *To*, *scheme='simpson'*)

dpti.ti.**handle_compute**(*args*)

dpti.ti.**handle_gen**(*args*)

dpti.ti.**handle_refine**(*args*)

dpti.ti.**handle_run**(*args*)

dpti.ti.**make_iter_name**(*iter_index*)

dpti.ti.**make_tasks**(*iter_name*, *jdata*, *if_meam=None*)

dpti.ti.**parse_seq_ginv**(*seq*)

dpti.ti.**post_tasks**(*iter_name*, *jdata*, *Eo*, *Eo_err=0*, *To=None*, *natoms=None*, *scheme='simpson'*, *shift=0.0*)

dpti.ti.**post_tasks_mbar**(*iter_name*, *jdata*, *Eo*, *natoms=None*)

dpti.ti.**refine_task**(*from_task*, *to_task*, *err*)

dpti.ti.**run_task**(*task_name*, *machine_file*)

4.1.15 dpti.ti_water module

dpti.ti_water.**add_module_subparsers**(*main_subparsers*)

dpti.ti_water.**add_subparsers**(*module_subparsers*)

dpti.ti_water.**exec_args**(*args*, *parser*)

dpti.ti_water.**handle_compute**(*args*)

dpti.ti_water.**handle_gen**(*args*)

dpti.ti_water.**handle_refine**(*args*)

dpti.ti_water.**handle_run**(*args*)

CHAPTER

FIVE

PHASE DIAGRAM OF WATER

This example describes how to calculate the phase diagram of water.

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SIX

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