MAGUS:

Machine learning And Graph theory assisted Universal structure Searcher

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Manual

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https://gitlab.com/bigd4/magus

Contents

Chapter 1

Installation

1.1 Dependency

MAGUS needs python>=3.6 and gcc>=4.8. You should install pip before using it to install other packages. The following python packages are required:

numpy
scipy
scikit-learn
pyyaml>=6.0
ase>=3.18
networkx
spglib
pandas
prettytable
packaging

The following python packages are optional:

beautifulreport
plotly
dscribe
networkx
pymatgen

If you want to use MTP, you need to install mlip.

1.2 Preparation

1.2.1 Set up the ASE API with Vasp

MAGUS does VASP calculation based on ASE API. Hence, you need to do the following preparations first.

1) Make a new file **run_vasp.py**:

```python
import subprocess
exitcode = subprocess.call("mpiexec.hydra vasp_std",
shell=True)
```

ase manual.

2) Make a new **mypps** dir to store vasp pseudopotentials. You can also use soft links:

```
mypps/
├── potpaw
├── potpaw_GGA
└── potpaw_PBE
```

```
$ ln -s /your/path/PBE-5.4 mypps/potpaw_PBE
```

Three sub directories correspond to LDA, PW91 and PBE, respectively. It is allowed to leave some of them nonexistent if you do use these potentials. It is also allowed to add other pseudopotentials.

3) Set environment variables:

```
$ export VASP_SCRIPT=/your/path/run_vasp.py
$ export VASP_PP_PATH=/your/path/mypps
```

More information in: ase manual for vasp calculator.

Notice: **run_vasp.py** and **mypps** should not be under **magus** dir.

1.2.2 Set up Job System

MAGUS is developed under LSF job system, which is the default setting. But we also add support to SLURM and PBS job systems. You need to set an environment variable if you are not using the default LSF job system:

```
$ export JOB_SYSTEM=<your-job-system>
```

Add this line into your **bashrc** to make the setting work every time you log in.

1.2.3 Machine Learning Package Installation (Optional)

MLIP is a software for Machine Learning Interatomic Potentials. It has been developed at Skoltech (Moscow) by Alexander Shapeev, Evgeny Podryabinkin, Konstantin Gubaev, and Ivan Novikov.[*] According to the license, MLIP is not allowed to be published and otherwise distributed. You need to register in **https://mlip.skoltech. ru/download/** and follow the instructions.

1.2.4 Build a Virtual Environment (Optional)

And we highly recommend that you use Anaconda to build a virtual environment and install MAGUS in an isolated environment to avoid conflicts. After installing anaconda, it will automatically write several lines in your **bashrc** which is used to initialize anaconda environment. You should source **bashrc** or re-login to make anaconda activated. If you do the jobs correctly, your shell prompt should be modified to be started as **(base)**, which means you are now in base environment of anaconda. Then, create a new virtual environment with

```
$ conda create -n <your-env-name> python=<python-version>
```

<your-env-name> is the name of the environment that you can define as you will, and <python-version> should be not less than 3.6. When you want to activate this environment, use

```
$ conda activate <your-env-name>
```

1.3 Install with pip

It is convenient to install with pip. It will automatically download the source code and install the required python packages.The install command is

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[*]Novikov, Ivan S., et al. "The MLIP package: moment tensor potentials with MPI and active learning." Machine Learning: Science and Technology 2.2 (2020): 025002.

```
$ pip install git+https://gitlab.com/bigd4/magus.git
```

You may need to type in your username and password of your gitlab account because the project is not public. If you want to install in a virtual environment, do not forget to activate the environment first. If you works in a cluster and do not have permission to install in the default location, you may add **--user** parameter.

1.4 Install with Source Code

1.4.1 Download Code

1.4.1.1 Use git

Clone the project and submodules to local file system:

```
$ git clone --recursive https://gitlab.com:bigd4/magus.git
```

1.4.1.2 From Website

If you have problem downloading with git, you have the alternative choose to download the zipped package on our gitlab website. Notice that the submodules such as pybind11 will not be downloaded at the same time. You should download and extract them and replace the empty folders in the source code, respectively.

1.4.2 Use pip to Install the Source Code

After downloading the code, go into the directory and install with:

```
$ pip install -e .
```

pip will read **setup.py** in your current directory and install. The **-e** option means python will import the module from the current path, but not copy the codes to the default lib path and import the module there, which is convenient for modifying in the future. If you do not have the need, you can remove the option.

1.5 Install Offline

If you have no access to Internet and your cluster does not have a python pypi mirror, which means you cannot use pip to install packages. You have the alternative choose to download with our pre-built offline installation package. You can download it from here. Install with

```
$ ./magus-<version-number>.sh
```

Follow the instructions. It will build an isolated conda environment with all required packages. You should go into your install path. Then, add **bin** into PATH and add condalib into PYTHONPATH. Notice that this method will build a new conda. If have already installed a conda in your system, the new one will not merge into the old one, which may cause difficulties to switch conda environments. As a result, it is not recommended to install with this method if your pip works normally.

1.6 Other Settings

1.6.1 Set up Environment Variables

To run MAGUS in your console, you need to add PATH in **bashrc**.

```
$ export PATH=$PATH:/your_path_to_magus
$ export PYTHONPATH=$PYTHONPATH:/your_path_to_magus
```

1.6.2 Set up Auto Completion (Optional)

We have prepared a shell completion script for MAGUS. Add the following line into **bashrc**:

```
$ source your_path_to_magus/auto_complete.sh
```

1.7 Check Installation

If MAGUS is properly installed, you can see the version number by the following command in console:

```
$ magus -v
```
```
1.0.5
```

If you have installed other optional packages, you can check if they are properly installed using:

```
$ magus checkpack
```

Chapter 2

Examples

2.1 Example List

number	target
01	Generate structures
02	Relax structures
03	3D bulk search
04	Molecule crystal search
05	Cluster search
06	Surface reconstruct
07	Machine learning search
08	2D bulk search

2.2 Example Introductions

2.2.1 Generate structures

- **01--1-B12**: Generate 3d periodic crystal structures of boron with 12 atoms per unit cell by symmetry.

- **01--2-NH4NO3**: Generate 3d periodic crystal structures of molecule crystal with 8 NH4 and NO3 molecules per unit cell by symmetry Pccn (56).

2.2.2 Relax structures

- **02--1-C8-VASP**: Structure relaxation of diamond by vasp interface.

- **02--2-B12-MTP**: Relax 2000 structures with MTP and VASP.

2.2.3 3D bulk search

- **03--1-Al-fix-EMT**: GAsearch of fixed composition Al (12 atoms per cell) by EMT.

- **03--2-Al-fix-VASP**: GAsearch of fixed composition Al (12 atoms per cell) by VASP.

- **03--3-TiO2-fix-VASP**: GAsearch of fixed composition TiO_2 (12 atoms per cell).

- **03--4-MgAlO-fix-GULP**: GAsearch of fixed composition MgAlO under high pressure by GULP.

- **03--5-Si-fix-Castep**: GAsearch of fixed composition Si by Castep.

- **03--6-ZnOH-var-GULP**: GAsearch of variable composition $Zn_x(OH)_y$.

2.2.4 Molecule crystal search

- **04--1-CH4-fix-VASP**: GAsearch of molecule crystal CH4 with 4 molecules per unit cell.

2.2.5 Cluster search

- **05--1-LJ26**: Ground state of Lennard-Jones cluster of 26 atoms.

2.2.6 Surface reconstruct

- **06--1-C_2x1_100**: Surface reconstruction of diamond (100)-2×1.

- **06--2-SnO2_4x1_110**: Surface reconstruction of SnO_2 (110)-4×1.

2.2.7 Machine learning search

- **07--1-MgSiO3-MTP**: Use mtp to search $MgSiO_3$ under high pressure.

- **07--2-Na-NEP**: A toy example for use NEP to search sodium.

2.2.8 2D bulk search

- **08--1-graphene**: GAsearch of 2D carbon (graphene) by VASP.

Chapter 3

Input parameters

In magus we use inputs including command lines and parameter input file (in yaml format) to control programs.

If you are a new user of MAGUS (AND SINCERELY THANKS VERY MUCH FOR USING OUR PROGRAM!), before you read the full description about all inputs below, we recommand first taking a look at examples which are easier to follow.

3.1 Command lines

You can simply type

```
$ magus -h
```

to see which commands are supported for magus. You will see

```
usage: magus [-h] [-v]
             {search,summary,clean,prepare,calculate,
             generate,checkpack,test,update,getslabtool,
             mutate,parmhelp}
             ...

Magus: Machine learning And Graph theory assisted
Universal structure Searcher

optional arguments:
  -h, --help              show this help message and exit
  -v, --version           print version
```

```
Valid subcommands:
  {search,summary,clean,prepare,calculate,generate,
  checkpack,test,update,getslabtool,mutate,parmhelp}
    search              search structures
    summary             summary the results
    clean               clean the path
    prepare             generate InputFold etc to prepare
    for the search
    calculate           calculate many structures
    generate            generate many structures
    checkpack           check full
    test                do unit test of magus
    update              update magus
    getslabtool         tools to getslab in surface search
    mode
    mutate              mutation test
```

which prints valid subcommands. You can also helps for each command line:

3.1.1 search

```
$ magus search -h
- - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
usage: magus search [-h] [-ll {DEBUG,INFO,WARNING,ERROR}]
[-lp LOG_PATH]
                    [-i INPUT_FILE] [-m] [-r]

optional arguments:
  -h, --help              show this help message and exit
  -ll {DEBUG,INFO,WARNING,ERROR}, --log-level
  {DEBUG,INFO,WARNING,ERROR}
                          set verbosity level by strings:
                          ERROR, WARNING, INFO
                          and DEBUG (default: INFO)
  -lp LOG_PATH, --log-path LOG_PATH
                          set log file to log messages to
                          disk (default:
                          log.txt)
  -i INPUT_FILE, --input-file INPUT_FILE
```

```
                                the input parameter file in yaml
                                format (default:
                                input.yaml)
  -m, --use-ml                  use ml to accelerate(?) the search
  (default: False)
  -r, --restart                 Restart the searching. (default:
  False)
```

3.1.2 summary

```
$ magus summary -h
------------------------------------------------------------------
usage: magus summary [-h] [-p PREC] [-r] [-s]
[--need-sort] [-o OUTDIR]
                        [-n SHOW_NUMBER] [-sb SORTED_BY
                        [SORTED_BY ...]]
                        [-rm REMOVE_FEATURES [REMOVE_FEATURES
                        ...]]
                        [-a ADD_FEATURES [ADD_FEATURES ...]]
                        [-v]
                        [-b BOUNDARY [BOUNDARY ...]] [-t
                        {bulk,cluster}]
                        filenames [filenames ...]

positional arguments:
  filenames             file (or files) to summary

optional arguments:
  -h, --help            show this help message and exit
  -p PREC, --prec PREC  tolerance for symmetry finding
  (default: 0.1)
  -r, --reverse         whether to reverse sort (default:
  False)
  -s, --save            whether to save POSCARS (default:
  False)
  --need-sort           whether to sort (default: False)
  -o OUTDIR, --outdir OUTDIR
                        where to save POSCARS (default: .)
  -n SHOW_NUMBER, --show-number SHOW_NUMBER
```

```
                                    number of show in screen (default:
                                    100)
  -sb SORTED_BY [SORTED_BY ...], --sorted-by SORTED_BY
  [SORTED_BY ...]
                                    sorted by which arg (default:
                                    Default)
  -rm REMOVE_FEATURES [REMOVE_FEATURES ...],
  --remove-features REMOVE_FEATURES [REMOVE_FEATURES ...]
                                    the features to be removed from
                                    the show features
                                    (default: [])
  -a ADD_FEATURES [ADD_FEATURES ...], --add-features
  ADD_FEATURES [ADD_FEATURES ...]
                                    the features to be added to the
                                    show features
                                    (default: [])
  -v, --var                         use variable composition mode
  (default: False)
  -b BOUNDARY [BOUNDARY ...], --boundary BOUNDARY
  [BOUNDARY ...]
                                    in variable composition mode: add
                                    boundary (default:
                                    [])
  -t {bulk,cluster}, --atoms-type {bulk,cluster}
```

3.1.3 clean

```
$ magus clean -h
------------------------------------------------------------------
usage: magus clean [-h] [-f]

optional arguments:
  -h, --help   show this help message and exit
  -f, --force  rua!!!! (default: False)
```

3.1.4 prepare

```
$ magus prepare -h
usage: magus prepare [-h] [-v] [-m]

optional arguments:
  -h, --help  show this help message and exit
  -v, --var   variable composition search (default: False)
  -m, --mol   molecule crystal search (default: False)
```

3.1.5 calculate

```
$ magus calculate -h
```
```
usage: magus calculate [-h] [-ll
{DEBUG,INFO,WARNING,ERROR}] [-lp LOG_PATH]
                       [-m {scf,relax}] [-i INPUT_FILE]
                       [-o OUTPUT_FILE]
                       [-p PRESSURE]
                       filename

positional arguments:
  filename                structures to relax

optional arguments:
  -h, --help              show this help message and exit
  -ll {DEBUG,INFO,WARNING,ERROR}, --log-level
  {DEBUG,INFO,WARNING,ERROR}
                          set verbosity level by strings:
                          ERROR, WARNING, INFO
                          and DEBUG (default: INFO)
  -lp LOG_PATH, --log-path LOG_PATH
                          set log file to log messages to
                          disk (default:
                          log.txt)
  -m {scf,relax}, --mode {scf,relax}
                          scf or relax (default: relax)
  -i INPUT_FILE, --input-file INPUT_FILE
```

```
                                the input parameter file in yaml
                                format (default:
                                input.yaml)
      -o OUTPUT_FILE, --output-file OUTPUT_FILE
                                output traj file (default:
                                out.traj)
      -p PRESSURE, --pressure PRESSURE
                                add pressure (default: None)
```

3.1.6 generate

```
$ magus generate -h
------------------------------------------------------------------
usage: magus generate [-h] [-ll
{DEBUG,INFO,WARNING,ERROR}] [-lp LOG_PATH]
                        [-i INPUT_FILE] [-o OUTPUT_FILE] [-n
                        NUMBER]

optional arguments:
  -h, --help              show this help message and exit
  -ll {DEBUG,INFO,WARNING,ERROR}, --log-level
  {DEBUG,INFO,WARNING,ERROR}
                          set verbosity level by strings:
                          ERROR, WARNING, INFO
                          and DEBUG (default: INFO)
  -lp LOG_PATH, --log-path LOG_PATH
                          set log file to log messages to
                          disk (default:
                          log.txt)
  -i INPUT_FILE, --input-file INPUT_FILE
                          the input parameter file in yaml
                          format (default:
                          input.yaml)
  -o OUTPUT_FILE, --output-file OUTPUT_FILE
                          where to save generated traj
                          (default: gen.traj)
  -n NUMBER, --number NUMBER
                          generate number (default: 10)
```

3.1.7 checkpack

```
$ magus checkpack -h

usage: magus checkpack [-h] [-ll
{DEBUG,INFO,WARNING,ERROR}] [-lp LOG_PATH]

                       [{all,calculators,comparators,fingerprints}]

positional arguments:
  {all,calculators,comparators,fingerprints}
                        the package to check (default:
                        all)

optional arguments:
  -h, --help            show this help message and exit
  -ll {DEBUG,INFO,WARNING,ERROR}, --log-level
  {DEBUG,INFO,WARNING,ERROR}
                        set verbosity level by strings:
                        ERROR, WARNING, INFO
                        and DEBUG (default: INFO)
  -lp LOG_PATH, --log-path LOG_PATH
                        set log file to log messages to
                        disk (default:
                        log.txt)
```

3.1.8 test

```
$ magus test -h

usage: magus test [-h] [totest]

positional arguments:
  totest      the package to test (default: *)

optional arguments:
  -h, --help  show this help message and exit
```

3.1.9   update

```
$ magus update -h

usage: magus update [-h] [-u] [-f]
optional arguments:
  -h, --help   show this help message and exit
  -u, --user   add --user to pip install (default: False)
  -f, --force  add --force-reinstall to pip install
  (default: False)
```

3.1.10   getslabtool

```
$ magus getslabtool -h

usage: magus getslabtool [-h] [-f FILENAME] [-s SLABFILE]

optional arguments:
  -h, --help            show this help message and exit
  -f FILENAME, --filename FILENAME
                        defaults is
                        './Ref/layerslices.traj' of slab
                        model and
                        'results' for analyze results.
                        (default: )
  -s SLABFILE, --slabfile SLABFILE
                        slab file (default: slab.vasp)
```

3.1.11   mutate

```
$ magus mutate -h

usage: magus mutate [-h] [-i INPUT_FILE] [-s SEED_FILE]
[-o OUTPUT_FILE]
                        [--cutandsplice] [--replaceball]
                        [--soft] [--perm]
```

```
                        [--lattice] [--ripple] [--slip]
                        [--rotate] [--rattle]
                        [--formula] [--lyrslip] [--shell]
                        [--lyrsym] [--clusym]

optional arguments:
  -h, --help            show this help message and exit
  -i INPUT_FILE, --input_file INPUT_FILE
                        input_file (default: input.yaml)
  -s SEED_FILE, --seed_file SEED_FILE
                        seed_file (default: seed.traj)
  -o OUTPUT_FILE, --output_file OUTPUT_FILE
                        output_file (default: result)
  --cutandsplice        add option to use operation!
  (default: False)
  --replaceball         add option to use operation!
  (default: False)
  --soft                add option to use operation!
  (default: False)
  --perm                add option to use operation!
  (default: False)
  --lattice             add option to use operation!
  (default: False)
  --ripple              add option to use operation!
  (default: False)
  --slip                add option to use operation!
  (default: False)
  --rotate              add option to use operation!
  (default: False)
  --rattle              add option to use operation!
  (default: False)
  --formula             add option to use operation!
  (default: False)
  --lyrslip             add option to use operation!
  (default: False)
  --shell               add option to use operation!
  (default: False)
  --lyrsym              add option to use operation!
  (default: False)
  --clusym              add option to use operation!
  (default: False)
```

3.2   Parameter inputs

A yaml format parameter file is also necessary. By default is 'input.yaml'. IN THE FUTURE we will add command line to easily export notes and default values by

```
$ magus parmhelp
```

to see help for which parameters you can set in 'input.yaml'. For current version they are:

```
parameter information for <class
'magus.parameters.magusParameters'>
+++++  Default parameters  +++++
formulaType    : type of formula, choose from fix or var
                  default value: fix
structureType  : structure type, choose from bulk, layer,
confined_bulk, cluster, surface
                  default value: bulk
spacegroup     : spacegroup to generate random structures
                  default value: [1-230]
DFTRelax       : DFTRelax
                  default value: False
initSize       : size of first population
                  default value: =popSize
goodSize       : number of good indivials per generation
                  default value: =popSize
molMode        : search molecule clusters
                  default value: False
mlRelax        : use Machine learning relaxation
                  default value: False
symprec        : tolerance for symmetry finding
                  default value: 0.1
bondRatio      : limitation to detect clusters
                  default value: 1.15
eleSize        : used in variable composition mode,
control how many boundary structures are generated
                  default value: 0
volRatio       : cell_volume/SUM(atom_ball_volume) when
generating structures (around this number)
                  default value: 2
dRatio         : distance between each pair of two atoms
in the structure is
```

```
                    not less than (radius1+radius2)*d_ratio
                     default value: 0.7
molDetector     : methods to detect mol, choose from 1 and
2. See
                    Hao Gao, Junjie Wang, Zhaopeng Guo, Jian
                    Sun, "Determining dimensionalities and
                    multiplicities
                    of crystal nets" npj Comput. Mater. 6,
                    143 (2020)
                    [doi.org/10.1016/j.fmre.2021.06.005]
                    for more details.
                     default value: 0
addSym          : whether to add symmetry before crossover
and mutation
                     default value: True
randRatio       : ratio of new generated random structures
in next generation
                     default value: 0.2
chkMol          : use mol dectector
                     default value: False
chkSeed         : check seeds
                     default value: True
diffE           : energy difference to determin structure
duplicates
                     default value: 0.01
diffV           : volume difference to determin structure
duplicates
                     default value: 0.05
comparator      : comparator, type magus checkpack to see
which comparators you have.
                     default value: nepdes
fp_calc         : fingerprints, type magus checkpack to see
which fingerprint method you have.
                     default value: nepdes
n_cluster       : number of good individuals per generation
                     default value: =saveGood
autoOpRatio     : automantic GA operation ratio
                     default value: False
autoRandomRatio: automantic random structure generation
ratio
                     default value: False
```

```
----------------------------------------------------------------
parameter information for <class
'magus.generators.random.MoleculeSPGGenerator'>
+++++  Requirement parameters  +++++
input_mols      : input molecules
formula_type    : type of formula, choose from fix or var
symbols         : atom symbols
formula         : formula
min_n_atoms     : minimum number of atoms per unit cell
max_n_atoms     : maximum number of atoms per unit cell
+++++  Default parameters  +++++
symprec         : tolerance for symmetry finding for
molucule
                  default value: 0.1
threshold_mol   : distance between each pair of two
molecules in the structure is
                  not less than
                  (mol_radius1+mol_radius2)*threshold_mol
                   default value: 1.0
max_attempts    : max attempts to generate a random
structure
                  default value: 50
p_pri           : probability of generate primitive cell
                  default value: 0.0
volume_ratio    : cell_volume/SUM(atom_ball_volume) when
generating structures (around this number)
                  default value: 1.5
n_split         : split cell into n_split parts
                  default value: [1]
dimension       : dimension
                  default value: 3
ele_size        : number of single compontent structures to
                  generate to decide hull boundarys in
                  variable composition mode
                  default value: 0
min_lattice     : min lattice
                  default value: [-1, -1, -1, -1, -1, -1]
max_lattice     : max lattice
                  default value: [-1, -1, -1, -1, -1, -1]
min_volume      : min volume
                  default value: -1
```

```
max_volume      : max volume
                  default value: -1
min_n_formula  : minimum formula
                  default value: None
max_n_formula  : maximum formula
                  default value: None
d_ratio         : distance between each pair of two atoms
in the structure is
                  not less than (radius1+radius2)*d_ratio
                  default value: 1.0
distance_matrix: distance between each pair of two atoms
in the structure is
                  not less than
                  (radius1+radius2)*distance_matrix[1][2]
                  default value: None
spacegroup      : spacegroup to generate random structures
                  default value: [1-230]
max_ratio       :  max formula ratio in variable
composition mode, for example set 10 and Zn11(OH) is not
allowed
                  default value: 1000
full_ele        : only generate structures with full
elements
                  default value: True
----------------------------------------------------------------
parameter information for <class
'magus.generators.random.LayerSPGGenerator'>
+++++  Requirement parameters  +++++
min_thickness  : minimum thickness
max_thickness  : maximum thickness
formula_type   : type of formula, choose from fix or var
symbols         : atom symbols
formula         : formula
min_n_atoms     : minimum number of atoms per unit cell
max_n_atoms     : maximum number of atoms per unit cell
+++++  Default parameters  +++++
symprec         : symprec
                  default value: 0.1
threshold_mol  : threshold_mol
                  default value: 1.0
spg_type        : spg_type
```

```
                     default value: layer
vacuum_thickness: vacuum_thickness
                     default value: 10
max_attempts    : max attempts to generate a random
structure
                     default value: 50
p_pri           : probability of generate primitive cell
                     default value: 0.0
volume_ratio    : cell_volume/SUM(atom_ball_volume) when
generating structures (around this number)
                     default value: 1.5
n_split         : split cell into n_split parts
                     default value: [1]
dimension       : dimension
                     default value: 3
ele_size        : number of single compontent structures to
                   generate to decide hull boundarys in
                   variable composition mode
                     default value: 0
min_lattice     : min lattice
                     default value: [-1, -1, -1, -1, -1, -1]
max_lattice     : max lattice
                     default value: [-1, -1, -1, -1, -1, -1]
min_volume      : min volume
                     default value: -1
max_volume      : max volume
                     default value: -1
min_n_formula   : minimum formula
                     default value: None
max_n_formula   : maximum formula
                     default value: None
d_ratio         : distance between each pair of two atoms
in the structure is
                   not less than (radius1+radius2)*d_ratio
                     default value: 1.0
distance_matrix: distance between each pair of two atoms
in the structure is
                   not less than
                   (radius1+radius2)*distance_matrix[1][2]
                     default value: None
spacegroup      : spacegroup to generate random structures
```

```
                    default value: [1-230]
max_ratio      :   max formula ratio in variable
composition mode, for example set 10 and Zn11(OH) is not
allowed
                    default value: 1000
full_ele       : only generate structures with full
elements
                    default value: True
------------------------------------------------------------
parameter information for <class
'magus.reconstruct.generator.ClusterSPGGenerator'>
+++++  Requirement parameters  +++++
formula_type   : type of formula, choose from fix or var
symbols        : atom symbols
formula        : formula
min_n_atoms    : minimum number of atoms per unit cell
max_n_atoms    : maximum number of atoms per unit cell
+++++  Default parameters  +++++
vacuum_thickness: vacuum thickness
                    default value: 10
------------------------------------------------------------
parameter information for <class
'magus.generators.random.SPGGenerator'>
+++++  Requirement parameters  +++++
formula_type   : type of formula, choose from fix or var
symbols        : atom symbols
formula        : formula
min_n_atoms    : minimum number of atoms per unit cell
max_n_atoms    : maximum number of atoms per unit cell
+++++  Default parameters  +++++
max_attempts   : max attempts to generate a random
structure
                    default value: 50
p_pri          : probability of generate primitive cell
                    default value: 0.0
volume_ratio   : cell_volume/SUM(atom_ball_volume) when
generating structures (around this number)
                    default value: 1.5
n_split        : split cell into n_split parts
                    default value: [1]
dimension      : dimension
```

```
                        default value: 3
 ele_size       : number of single compontent structures to
                        generate to decide hull boundarys in
                        variable composition mode
                        default value: 0
 min_lattice    : min lattice
                        default value: [-1, -1, -1, -1, -1, -1]
 max_lattice    : max lattice
                        default value: [-1, -1, -1, -1, -1, -1]
 min_volume     : min volume
                        default value: -1
 max_volume     : max volume
                        default value: -1
 min_n_formula  : minimum formula
                        default value: None
 max_n_formula  : maximum formula
                        default value: None
 d_ratio        : distance between each pair of two atoms
 in the structure is
                        not less than (radius1+radius2)*d_ratio
                        default value: 1.0
 distance_matrix: distance between each pair of two atoms
 in the structure is
                        not less than
                        (radius1+radius2)*distance_matrix[1][2]
                        default value: None
 spacegroup     : spacegroup to generate random structures
                        default value: [1-230]
 max_ratio      :  max formula ratio in variable
 composition mode, for example set 10 and Zn11(OH) is not
 allowed
                        default value: 1000
 full_ele       : only generate structures with full
 elements
                        default value: True
 ------------------------------------------------------------
 parameter information for <class
 'magus.reconstruct.generator.SurfaceGenerator'>
 +++++  Requirement parameters  +++++
 formula_type   : type of formula, choose from fix or var
 symbols        : atom symbols
```

```
formula         : formula
min_n_atoms     : minimum number of atoms per unit cell
max_n_atoms     : maximum number of atoms per unit cell
+++++  Default parameters  +++++
randwalk_range  : maximum range of random walk
                      default value: 0.5
randwalk_ratio  : ratio of random walk atoms
                      default value: 0.3
rcs_x           : size[x] of reconstruction
                      default value: [1]
rcs_y           : size[y] of reconstruction
                      default value: [1]
buffer          : use buffer layer
                      default value: True
rcs_formula     : formula of surface region
                      default value: None
spg_type        : generate with planegroup/layergroup
                      default value: plane
+++++  slabinfo parameters  +++++
bulk_file       : file of bulk structure
                      default value: None
cutslices       : bulk_file contains how many atom layers
                      default value: 2
bulk_layernum   : number of atom layers in substrate region
                      default value: 3
buffer_layernum: number of atom layers in buffer region
                      default value: 3
rcs_layernum    : number of atom layers in top surface
region
                      default value: 2
direction       : Miller indices of surface direction,
i.e.[1,0,0]
                      default value: None
rotate          : R
                      default value: 0
matrix          : matrix notation
                      default value: None
addH            : passivate bottom surface with H
                      default value: False
pcell           : use primitive cell
                      default value: True
```

```
+++++  modification parameters  +++++
adsorb          : adsorb atoms to cleaved surface
                    default value: {}
clean           : clean cleaved surface
                    default value: {}
defect          : add defect to cleaved surface
                    default value: {}
------------------------------------------------------------
parameter information for <class
'magus.populations.individuals.Bulk'>
+++++  Requirement parameters  +++++
symprec         : tolerance for symmetry finding
+++++  Default parameters  +++++
mol_detector    : methods to detect mol, choose from 1 and
2. See
                    Hao Gao, Junjie Wang, Zhaopeng Guo, Jian
                    Sun, "Determining dimensionalities and
                    multiplicities
                    of crystal nets" npj Comput. Mater. 6,
                    143 (2020)
                    [doi.org/10.1016/j.fmre.2021.06.005]
                    for more details.
                     default value: 0
n_repair_try    : attempts to repair structures when doing
GA operation
                     default value: 5
max_attempts    : maximum attempts
                     default value: 50
check_seed      : if check seeds
                     default value: False
min_lattice     : min_lattice
                     default value: [0.0, 0.0, 0.0, 45.0,
                     45.0, 45.0]
max_lattice     : max_lattice
                     default value: [99, 99, 99, 135, 135,
                     135]
d_ratio         : distance between each pair of two atoms
in the structure is
                     not less than (radius1+radius2)*d_ratio
                      default value: 1.0
```

```
distance_matrix: distance between each pair of two atoms
in the structure is
                not less than
                (radius1+radius2)*distance_matrix[1][2]
                 default value: None
radius         : radius
                default value: None
max_forces     : if forces of a structure larger is than
this number it will be deleted.
                default value: 50.0
max_enthalpy   : if enthalpy of a structure is larger than
this number it will be deleted.
                default value: 100.0
full_ele       : full_ele
                default value: True
max_length_ratio: if max-cell-length/min-cell-length of a
structure is larger than this number it will be deleted.
                default value: 8
-----------------------------------------------------------
parameter information for <class
'magus.populations.individuals.Layer'>
+++++  Requirement parameters  +++++
symprec        : tolerance for symmetry finding
+++++  Default parameters  +++++
vacuum_thickness: vacuum_thickness
                default value: 10
bond_ratio     : bond_ratio
                default value: 1.1
n_repair_try   : attempts to repair structures when doing
GA operation
                default value: 5
max_attempts   : maximum attempts
                default value: 50
check_seed     : if check seeds
                default value: False
min_lattice    : min_lattice
                default value: [0.0, 0.0, 0.0, 45.0,
                45.0, 45.0]
max_lattice    : max_lattice
                default value: [99, 99, 99, 135, 135,
                135]
```

```
d_ratio        : distance between each pair of two atoms
in the structure is
                 not less than (radius1+radius2)*d_ratio
                  default value: 1.0
distance_matrix: distance between each pair of two atoms
in the structure is
                 not less than
                 (radius1+radius2)*distance_matrix[1][2]
                  default value: None
radius         : radius
                  default value: None
max_forces     : if forces of a structure larger is than
this number it will be deleted.
                  default value: 50.0
max_enthalpy   : if enthalpy of a structure is larger than
this number it will be deleted.
                  default value: 100.0
full_ele       : full_ele
                  default value: True
max_length_ratio: if max-cell-length/min-cell-length of a
structure is larger than this number it will be deleted.
                  default value: 8
------------------------------------------------------------
parameter information for <class
'magus.populations.individuals.ConfinedBulk'>
+++++  Requirement parameters  +++++
symprec        : tolerance for symmetry finding
+++++  Default parameters  +++++
vacuum_thickness: vacuum thickness
                  default value: 10
n_repair_try   : attempts to repair structures when doing
GA operation
                  default value: 5
max_attempts   : maximum attempts
                  default value: 50
check_seed     : if check seeds
                  default value: False
min_lattice    : min_lattice
                  default value: [0.0, 0.0, 0.0, 45.0,
                  45.0, 45.0]
max_lattice    : max_lattice
```

```
                    default value: [99, 99, 99, 135, 135,
                    135]
d_ratio         : distance between each pair of two atoms
in the structure is
                    not less than (radius1+radius2)*d_ratio
                    default value: 1.0
distance_matrix: distance between each pair of two atoms
in the structure is
                    not less than
                    (radius1+radius2)*distance_matrix[1][2]
                    default value: None
radius          : radius
                    default value: None
max_forces      : if forces of a structure larger is than
this number it will be deleted.
                    default value: 50.0
max_enthalpy    : if enthalpy of a structure is larger than
this number it will be deleted.
                    default value: 100.0
full_ele        : full_ele
                    default value: True
max_length_ratio: if max-cell-length/min-cell-length of a
structure is larger than this number it will be deleted.
                    default value: 8
------------------------------------------------------------
parameter information for <class
'magus.reconstruct.individuals.Surface'>
+++++  Requirement parameters  +++++
symprec         : tolerance for symmetry finding
+++++  Default parameters  +++++
vacuum_thickness: vacuum thickness
                    default value: 10
buffer          : use buffer region
                    default value: True
fixbulk         : fix atom positions in substrate
                    default value: True
slices_file     : file name for slices_file
                    default value: Ref/layerslices.traj
n_repair_try    : attempts to repair structures when doing
GA operation
                    default value: 5
```

```
max_attempts   : maximum attempts
                   default value: 50
check_seed     : if check seeds
                   default value: False
min_lattice    : min_lattice
                   default value: [0.0, 0.0, 0.0, 45.0,
                   45.0, 45.0]
max_lattice    : max_lattice
                   default value: [99, 99, 99, 135, 135,
                   135]
d_ratio        : distance between each pair of two atoms
in the structure is
                   not less than (radius1+radius2)*d_ratio
                   default value: 1.0
distance_matrix: distance between each pair of two atoms
in the structure is
                   not less than
                   (radius1+radius2)*distance_matrix[1][2]
                   default value: None
radius         : radius
                   default value: None
max_forces     : if forces of a structure larger is than
this number it will be deleted.
                   default value: 50.0
max_enthalpy   : if enthalpy of a structure is larger than
this number it will be deleted.
                   default value: 100.0
full_ele       : full_ele
                   default value: True
max_length_ratio: if max-cell-length/min-cell-length of a
structure is larger than this number it will be deleted.
                   default value: 8
-------------------------------------------------------------
parameter information for <class
'magus.reconstruct.individuals.Cluster'>
+++++  Requirement parameters  +++++
symprec        : tolerance for symmetry finding
+++++  Default parameters  +++++
vacuum_thickness: vacuum thickness surrounding cluster to
break pbc when runing calculation
                   default value: 10
```

```
cutoff         : two atoms are "connected" if their
distance < cutoff*radius.
                  default value: 1.0
weighten       : use weighten atoms when appending or
removing atoms
                  default value: True
n_repair_try   : attempts to repair structures when doing
GA operation
                  default value: 5
max_attempts   : maximum attempts
                  default value: 50
check_seed     : if check seeds
                  default value: False
min_lattice    : min_lattice
                  default value: [0.0, 0.0, 0.0, 45.0,
                  45.0, 45.0]
max_lattice    : max_lattice
                  default value: [99, 99, 99, 135, 135,
                  135]
d_ratio        : distance between each pair of two atoms
in the structure is
                  not less than (radius1+radius2)*d_ratio
                  default value: 1.0
distance_matrix: distance between each pair of two atoms
in the structure is
                  not less than
                  (radius1+radius2)*distance_matrix[1][2]
                  default value: None
radius         : radius
                  default value: None
max_forces     : if forces of a structure larger is than
this number it will be deleted.
                  default value: 50.0
max_enthalpy   : if enthalpy of a structure is larger than
this number it will be deleted.
                  default value: 100.0
full_ele       : full_ele
                  default value: True
max_length_ratio: if max-cell-length/min-cell-length of a
structure is larger than this number it will be deleted.
                  default value: 8
```

```
----------------------------------------------------------
parameter information for <class
'magus.reconstruct.individuals.AdClus'>
+++++  Requirement parameters  +++++
symprec        : tolerance for symmetry finding
+++++  Default parameters  +++++
substrate      : substrate file name
                 default value: substrate.vasp
dist_clus2surface: distance from cluster to surface
                 default value: 2
size           : size
                 default value: [1, 1]
vacuum_thickness: vacuum thickness surrounding cluster to
break pbc when runing calculation
                 default value: 10
cutoff         : two atoms are "connected" if their
distance < cutoff*radius.
                 default value: 1.0
weighten       : use weighten atoms when appending or
removing atoms
                 default value: True
n_repair_try   : attempts to repair structures when doing
GA operation
                 default value: 5
max_attempts   : maximum attempts
                 default value: 50
check_seed     : if check seeds
                 default value: False
min_lattice    : min_lattice
                 default value: [0.0, 0.0, 0.0, 45.0,
                 45.0, 45.0]
max_lattice    : max_lattice
                 default value: [99, 99, 99, 135, 135,
                 135]
d_ratio        : distance between each pair of two atoms
in the structure is
                 not less than (radius1+radius2)*d_ratio
                 default value: 1.0
distance_matrix: distance between each pair of two atoms
in the structure is
```

```
                    not less than
                    (radius1+radius2)*distance_matrix[1][2]
                     default value: None
 radius         : radius
                     default value: None
 max_forces     : if forces of a structure larger is than
 this number it will be deleted.
                     default value: 50.0
 max_enthalpy   : if enthalpy of a structure is larger than
 this number it will be deleted.
                     default value: 100.0
 full_ele       : full_ele
                     default value: True
 max_length_ratio: if max-cell-length/min-cell-length of a
 structure is larger than this number it will be deleted.
                     default value: 8
 ----------------------------------------------------------------
 parameter information for <class
 'magus.populations.populations.FixPopulation'>
 +++++  Requirement parameters  +++++
 results_dir    : path for results
 pop_size       : population size
 symbols        : symbols
 formula        : formula
 +++++  Default parameters  +++++
 check_seed     : if check seed is turned on, we will check
 your seeds and delete those donot meet requirements
                     default value: False
 ----------------------------------------------------------------
 parameter information for <class
 'magus.populations.populations.VarPopulation'>
 +++++  Requirement parameters  +++++
 results_dir    : path for results
 pop_size       : population size
 symbols        : symbols
 formula        : formula
 +++++  Default parameters  +++++
 check_seed     : if check seed is turned on, we will check
 your seeds and delete those donot meet requirements
                     default value: False
 ----------------------------------------------------------------
```

```
parameter information for <class
'magus.reconstruct.individuals.RcsPopulation'>
+++++  Requirement parameters  +++++
results_dir    : path for results
pop_size       : population size
symbols        : symbols
formula        : formula
+++++  Default parameters  +++++
check_seed     : if check seed is turned on, we will check
your seeds and delete those donot meet requirements
                  default value: False
------------------------------------------------------------
parameter information for <class
'magus.operations.crossovers.CutAndSplicePairing'>
+++++  Default parameters  +++++
tryNum         : try attempts
                  default value: 50
cut_disp       : cut displacement
                  default value: 0
best_match     : choose best match
                  default value: False
------------------------------------------------------------
parameter information for <class
'magus.operations.crossovers.ReplaceBallPairing'>
+++++  Default parameters  +++++
tryNum         : try attempts
                  default value: 50
cut_range      : cut range
                  default value: [1, 2]
------------------------------------------------------------
parameter information for <class
'magus.operations.mutations.SoftMutation'>
+++++  Default parameters  +++++
tryNum         : tryNum
                  default value: 50
------------------------------------------------------------
parameter information for <class
'magus.operations.mutations.PermMutation'>
+++++  Default parameters  +++++
tryNum         : try attempts
                  default value: 50
```

```
frac_swaps      : possibility to swap
                    default value: 0.5
-----------------------------------------------------------
parameter information for <class
'magus.operations.mutations.LatticeMutation'>
+++++  Default parameters  +++++
tryNum          : try attempts
                    default value: 50
sigma           : Gauss distribution standard deviation
                    default value: 0.1
cell_cut        : coefficient of gauss distribution in cell
mutation
                    default value: 1
keep_volume     : whether to keep the volume unchange
                    default value: True
-----------------------------------------------------------
parameter information for <class
'magus.operations.mutations.RippleMutation'>
+++++  Default parameters  +++++
tryNum          : try attempts
                    default value: 50
rho             : rho
                    default value: 0.3
mu              : mu
                    default value: 2
eta             : eta
                    default value: 1
-----------------------------------------------------------
parameter information for <class
'magus.operations.mutations.SlipMutation'>
+++++  Default parameters  +++++
tryNum          : try attempts
                    default value: 50
cut             : cut position
                    default value: 0.5
randRange       : range of movement
                    default value: [0.5, 2]
-----------------------------------------------------------
parameter information for <class
'magus.operations.mutations.RotateMutation'>
+++++  Default parameters  +++++
```

```
tryNum          : try attempts
                    default value: 50
p               : possibility
                    default value: 1
--------------------------------------------------------------
parameter information for <class
'magus.operations.mutations.RattleMutation'>
+++++  Default parameters  +++++
tryNum          : try attempts
                    default value: 50
p               : possibility
                    default value: 0.25
rattle_range    : range of rattle
                    default value: 4
d_ratio         : d_ratio
                    default value: 0.7
keep_sym        : if keeps symmetry when rattles
                    default value: None
symprec         : tolerance for symmetry finding
                    default value: 0.1
--------------------------------------------------------------
parameter information for <class
'magus.operations.mutations.FormulaMutation'>
+++++  Default parameters  +++++
tryNum          : try attempts
                    default value: 10
n_candidate     : number of candidates
                    default value: 5
--------------------------------------------------------------
parameter information for <class
'magus.reconstruct.ga.LyrSlipMutation'>
+++++  Default parameters  +++++
tryNum          : tryNum
                    default value: 10
cut             : cut
                    default value: 0.2
randRange       : randRange
                    default value: [0, 1]
--------------------------------------------------------------
parameter information for <class
'magus.reconstruct.ga.ShellMutation'>
```

```
+++++  Default parameters  +++++
tryNum          : tryNum
                   default value: 10
d               : d
                   default value: 0.23
------------------------------------------------------------
parameter information for <class
'magus.reconstruct.ga.LyrSymMutation'>
+++++  Default parameters  +++++
tryNum          : tryNum
                   default value: 10
symprec         : symprec
                   default value: 0.0001
------------------------------------------------------------
parameter information for <class
'magus.reconstruct.ga.CluSymMutation'>
+++++  Default parameters  +++++
tryNum          : tryNum
                   default value: 10
symprec         : symprec
                   default value: 0.0001
------------------------------------------------------------
parameter information for <class
'magus.calculators.emt.EMTCalculator'>
+++++  Requirement parameters  +++++
work_dir        : work dictionary
job_prefix      : calculation dictionary
+++++  Default parameters  +++++
eps             : convergence energy
                   default value: 0.05
max_step        : maximum number of relax steps
                   default value: 100
optimizer       : optimizer method, choose from bfgs, fire,
lbfgs
                   default value: bfgs
max_move        : max range of movement
                   default value: 0.1
relax_lattice   : if to relax lattice
                   default value: True
pressure        : pressure
                   default value: 0.0
```

```
--------------------------------------------------------------
parameter information for <class
'magus.calculators.lammps.LammpsCalculator'>
+++++  Default parameters  +++++
mode           : choose from parallel or serial
                  default value: parallel
pressure       : pressure
                  default value: 0.0
exe_cmd        : command line to run lammps
                  default value:
save_traj      : save_traj
                  default value: False
atomStyle      : atomStyle
                  default value: atomic
job_prefix     : job_prefix
                  default value: Lammps
+++++  Requirement_parallel parameters  +++++
queue_name     : quene name
num_core       : num_core
work_dir       : work dictionary
job_prefix     : calculation dictionary
+++++  Default_parallel parameters  +++++
pre_processing : serves to add any sentence you wish when
submiting the job to change system variables, load modules
etc.
                  default value:
wait_time      : wait_time
                  default value: 200
verbose        : verbose
                  default value: False
kill_time      : kill_time
                  default value: 100000
num_parallel   : num_parallel
                  default value: 1
pressure       : pressure
                  default value: 0.0
--------------------------------------------------------------
parameter information for <class
'magus.calculators.mtp.MTPNoSelectCalculator'>
+++++  Default parameters  +++++
mode           : choose from parallel or serial
```

```
                        default value: parallel
pressure        : pressure
                        default value: 0.0
force_tolerance: force_tolerance
                        default value: 0.05
stress_tolerance: stress_tolerance
                        default value: 1.0
min_dist        : min_dist
                        default value: 0.5
n_epoch         : n_epoch
                        default value: 200
job_prefix      : job_prefix
                        default value: MTP
+++++  Requirement_parallel parameters  +++++
queue_name      : quene name
num_core        : num_core
work_dir        : work dictionary
job_prefix      : calculation dictionary
+++++  Default_parallel parameters  +++++
pre_processing : serves to add any sentence you wish when
submiting the job to change system variables, load modules
etc.
                        default value:
wait_time       : wait_time
                        default value: 200
verbose         : verbose
                        default value: False
kill_time       : kill_time
                        default value: 100000
num_parallel    : num_parallel
                        default value: 1
pressure        : pressure
                        default value: 0.0
-------------------------------------------------------------
parameter information for <class
'magus.calculators.mtp.MTPSelectCalculator'>
+++++  Default parameters  +++++
mode            : choose from parallel or serial
                        default value: parallel
pressure        : pressure
                        default value: 0.0
```

```
xc             : xc
                 default value: PBE
weights        : weights
                 default value: [1.0, 0.01, 0.001]
scaled_by_force: scaled_by_force
                 default value: 0.0
force_tolerance: force_tolerance
                 default value: 0.05
stress_tolerance: stress_tolerance
                 default value: 1.0
min_dist       : min_dist
                 default value: 0.5
n_epoch        : n_epoch
                 default value: 200
ignore_weights : ignore_weights
                 default value: True
job_prefix     : job_prefix
                 default value: MTP
n_fail         : n_fail
                 default value: 0
+++++  Requirement_parallel parameters  +++++
queue_name     : quene name
num_core       : num_core
work_dir       : work dictionary
job_prefix     : calculation dictionary
+++++  Default_parallel parameters  +++++
pre_processing : serves to add any sentence you wish when
submiting the job to change system variables, load modules
etc.
                 default value:
wait_time      : wait_time
                 default value: 200
verbose        : verbose
                 default value: False
kill_time      : kill_time
                 default value: 100000
num_parallel   : num_parallel
                 default value: 1
pressure       : pressure
                 default value: 0.0
--------------------------------------------------------------
```

```
parameter information for <class
'magus.calculators.mtp.MTPLammpsCalculator'>
+++++  Default parameters  +++++
mode           : choose from parallel or serial
                   default value: parallel
pressure       : pressure
                   default value: 0.0
xc             : xc
                   default value: PBE
weights        : weights
                   default value: [1.0, 0.01, 0.001]
scaled_by_force: scaled_by_force
                   default value: 0.0
force_tolerance: force_tolerance
                   default value: 0.05
stress_tolerance: stress_tolerance
                   default value: 1.0
min_dist       : min_dist
                   default value: 0.5
n_epoch        : n_epoch
                   default value: 200
ignore_weights : ignore_weights
                   default value: True
job_prefix     : job_prefix
                   default value: MTP
n_fail         : n_fail
                   default value: 0
+++++  Requirement_parallel parameters  +++++
queue_name     : quene name
num_core       : num_core
work_dir       : work dictionary
job_prefix     : calculation dictionary
+++++  Default_parallel parameters  +++++
pre_processing : serves to add any sentence you wish when
submiting the job to change system variables, load modules
etc.
                   default value:
wait_time      : wait_time
                   default value: 200
verbose        : verbose
                   default value: False
```

```
kill_time       : kill_time
                    default value: 100000
num_parallel   : num_parallel
                    default value: 1
pressure        : pressure
                    default value: 0.0
-----------------------------------------------------------------
parameter information for <class
'magus.calculators.quip.QUIPCalculator'>
+++++  Requirement parameters  +++++
work_dir        : work dictionary
job_prefix      : calculation dictionary
+++++  Default parameters  +++++
eps             : convergence energy
                    default value: 0.05
max_step        : maximum number of relax steps
                    default value: 100
optimizer       : optimizer method, choose from bfgs, fire,
lbfgs
                    default value: bfgs
max_move        : max range of movement
                    default value: 0.1
relax_lattice  : if to relax lattice
                    default value: True
pressure        : pressure
                    default value: 0.0
-----------------------------------------------------------------
parameter information for <class
'magus.calculators.vasp.VaspCalculator'>
+++++  Default parameters  +++++
mode            : choose from parallel or serial
                    default value: parallel
pressure        : pressure
                    default value: 0.0
xc              : xc
                    default value: PBE
pp_label        : pp_label
                    default value: None
job_prefix      : job_prefix
                    default value: Vasp
+++++  Requirement_parallel parameters  +++++
```

```
queue_name      : quene name
num_core        : num_core
work_dir        : work dictionary
job_prefix      : calculation dictionary
+++++  Default_parallel parameters  +++++
pre_processing : serves to add any sentence you wish when
submiting the job to change system variables, load modules
etc.
                  default value:
wait_time       : wait_time
                  default value: 200
verbose         : verbose
                  default value: False
kill_time       : kill_time
                  default value: 100000
num_parallel    : num_parallel
                  default value: 1
pressure        : pressure
                  default value: 0.0
---------------------------------------------------------------
parameter information for <class
'magus.calculators.castep.CastepCalculator'>
+++++  Default parameters  +++++
mode            : choose from parallel or serial
                  default value: parallel
pressure        : pressure
                  default value: 0.0
xc_functional  : xc_functional
                  default value: PBE
pspot           : pspot
                  default value: 00PBE
suffix          : suffix
                  default value: usp
job_prefix      : job_prefix
                  default value: Castep
kpts            : kpts
                  default value: {'density': 10, 'gamma':
                  True, 'even': False}
castep_command : castep_command
                  default value: castep
castep_pp_path : castep_pp_path
```

```
                    default value: None
+++++  Requirement_parallel parameters  +++++
queue_name      : quene name
num_core        : num_core
work_dir        : work dictionary
job_prefix      : calculation dictionary
+++++  Default_parallel parameters  +++++
pre_processing : serves to add any sentence you wish when
submiting the job to change system variables, load modules
etc.
                    default value:
wait_time       : wait_time
                    default value: 200
verbose         : verbose
                    default value: False
kill_time       : kill_time
                    default value: 100000
num_parallel    : num_parallel
                    default value: 1
pressure        : pressure
                    default value: 0.0
-----------------------------------------------------------
parameter information for <class
'magus.calculators.lj.LJCalculator'>
+++++  Requirement parameters  +++++
work_dir        : work dictionary
job_prefix      : calculation dictionary
+++++  Default parameters  +++++
eps             : convergence energy
                    default value: 0.05
max_step        : maximum number of relax steps
                    default value: 100
optimizer       : optimizer method, choose from bfgs, fire,
lbfgs
                    default value: bfgs
max_move        : max range of movement
                    default value: 0.1
relax_lattice   : if to relax lattice
                    default value: True
pressure        : pressure
                    default value: 0.0
```

```
--------------------------------------------------------
parameter information for <class
'magus.calculators.gulp.GulpCalculator'>
+++++  Default parameters  +++++
mode            : choose from parallel or serial
                    default value: parallel
pressure        : pressure
                    default value: 0.0
exe_cmd         : command line to run gulp
                    default value: gulp < input > output
job_prefix      : job_prefix
                    default value: Gulp
+++++  Requirement_parallel parameters  +++++
queue_name      : quene name
num_core        : num_core
work_dir        : work dictionary
job_prefix      : calculation dictionary
+++++  Default_parallel parameters  +++++
pre_processing : serves to add any sentence you wish when
submiting the job to change system variables, load modules
etc.
                    default value:
wait_time       : wait_time
                    default value: 200
verbose         : verbose
                    default value: False
kill_time       : kill_time
                    default value: 100000
num_parallel    : num_parallel
                    default value: 1
pressure        : pressure
                    default value: 0.0
--------------------------------------------------------
parameter information for <class
'magus.calculators.base.AdjointCalculator'>
+++++  Requirement parameters  +++++
work_dir        : work dictionary
job_prefix      : calculation dictionary
+++++  Default parameters  +++++
pressure        : pressure
                    default value: 0.0
```

```
-----------------------------------------------------------
parameter information for <class
'magus.calculators.mtp.TwoShareMTPCalculator'>
+++++  Requirement parameters  +++++
work_dir        : work dictionary
job_prefix      : calculation dictionary
+++++  Default parameters  +++++
pressure        : pressure
                    default value: 0.0
-----------------------------------------------------------
```