

MAGUS:

Machine learning And Graph theory assisted Universal structure Searcher

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Manual

Version 1.6.0, February 21, 2023.

<https://gitlab.com/bigd4/magus>

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Chapter 1

Installation

1.1 Dependency

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

```
numpy
scipy
scikit-learn
pyyaml $\geq$ 6.0
ase $\geq$ 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**:

```
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

*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 conda 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**: GAssearch of fixed composition Al (12 atoms per cell) by EMT.
- **03--2-Al-fix-VASP**: GAssearch of fixed composition Al (12 atoms per cell) by VASP.
- **03--3-TiO2-fix-VASP**: GAssearch of fixed composition TiO_2 (12 atoms per cell).
- **03--4-MgAlO-fix-GULP**: GAssearch of fixed composition MgAlO under high pressure by GULP.
- **03--5-Si-fix-Castep**: GAssearch of fixed composition Si by Castep.
- **03--6-ZnOH-var-GULP**: GAssearch of variable composition $\text{Zn}_x(\text{OH})_y$.

2.2.4 Molecule crystal search

- **04--1-CH4-fix-VASP**: GAssearch of molecule crystal CH_4 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**: GAssearch of 2D carbon (graphene) by VASP.

Chapter 3

Parameters

3.1 HELP FOR INPUTS

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 recommend first taking a look at examples which are easier to follow.

3.1.1 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:

3.1.2 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)

```

3.1.3 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}

```

3.1.4 clean

```
$ magus clean -h
```

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

```
optional arguments:
```

```

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

```

3.1.5 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)
```

3.1.6 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)

```

3.1.7 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)

```

3.1.8 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)
```

3.1.9 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
```

3.1.10 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)
```

3.1.11 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/layerlices.traj' of slab
                        model and
                        'results' for analyze results.
                        (default: )
  -s SLABFILE, --slabfile SLABFILE
                        slab file (default: slab.vasp)
```

3.1.12 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)
```

```
\end{tcolorbox}
```

```
\section{parameter input files}
```

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

```
\begin{tcolorbox}[breakable, enhanced]
```

```
  \begin{minted}[breaklines, breaksymbolleft={},,]{bash}
  $ 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'>
+++++^^IDefault parameters^^I+++++
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 and mutation : whether to add symmetry before crossover
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 duplicates : energy difference to determin structure
default value: 0.01

diffV duplicates : volume difference to determin structure
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'>
+++++^^IRequirement parameters^^I+++++
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
+++++^^IDefault parameters^^I+++++
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'>
+++++^^IRequirement parameters^^I+++++
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
+++++^^IDefault parameters^^I+++++

```



```
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 component structures to
generate to decide hull boundaries 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'>
+++++^^IRequirement parameters^^I+++++
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
+++++^^IDefault parameters^^I+++++
vacuum_thickness: vacuum thickness
                    default value: 10

```

```

parameter information for <class
'magus.generators.random.SPGGenerator'>
+++++^^IRequirement parameters^^I+++++
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
+++++^^IDefault parameters^^I+++++
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 component structures to
generate to decide hull boundaries 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'>
+++++^^IRequirement parameters^^I+++++
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
+++++^^IDefault parameters^^I+++++
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
+++++^^Islabinfo parameters^^I+++++
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
+++++^^Imodification parameters^^I+++++
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'>
+++++^^IRequirement parameters^^I+++++
symprec        : tolerance for symmetry finding
+++++^^IDefault parameters^^I+++++
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'>
+++++^^IRequirement parameters^^I+++++
symprec      : tolerance for symmetry finding
+++++^^IDefault parameters^^I+++++
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'>
+++++^^IRequirement parameters^^I+++++
symprec          : tolerance for symmetry finding
+++++^^IDefault parameters^^I+++++
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,
5.0, 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'>
+++++^^IRequirement parameters^^I+++++
symprec         : tolerance for symmetry finding
+++++^^IDefault parameters^^I+++++
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'>

```

```
+++++^^IRequirement parameters^^I+++++
symprec      : tolerance for symmetry finding
+++++^^IDefault parameters^^I+++++
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'>
+++++^^IRequirement parameters^^I+++++
symprec       : tolerance for symmetry finding
+++++^^IDefault parameters^^I+++++
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'>
+++++^^IRequirement parameters^^I+++++
results_dir   : path for results
pop_size      : population size
symbols       : symbols
formula       : formula
+++++^^IDefault parameters^^I+++++
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'>
+++++^^IRequirement parameters^^I+++++
results_dir   : path for results
pop_size      : population size
symbols       : symbols

```

```

formula          : formula
+++++^^IDefault parameters^^I+++++
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'>
+++++^^IDefault parameters^^I+++++
results_dir      : path for results
pop_size         : population size
symbols          : symbols
formula          : formula
+++++^^IDefault parameters^^I+++++
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'>
+++++^^IDefault parameters^^I+++++
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'>
+++++^^IDefault parameters^^I+++++
tryNum           : try attempts
                    default value: 50
cut_range        : cut range
                    default value: [1, 2]

```

```

-----
parameter information for <class
'magus.operations.mutations.SoftMutation'>
+++++^^IDefault parameters^^I+++++
tryNum           : tryNum
                    default value: 50

```

```

-----
parameter information for <class
'magus.operations.mutations.PermMutation'>
+++++^^IDefault parameters^^I++++
tryNum          : try attempts
                  default value: 50
frac_swaps      : possibility to swap
                  default value: 0.5
-----

parameter information for <class
'magus.operations.mutations.LatticeMutation'>
+++++^^IDefault parameters^^I++++
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'>
+++++^^IDefault parameters^^I++++
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'>
+++++^^IDefault parameters^^I++++
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'>

```

```

+++++^^IDefault parameters^^I+++++

```

```

tryNum         : try attempts
                  default value: 50
p              : possibility
                  default value: 1

```

```

-----
parameter information for <class
'magus.operations.mutations.RattleMutation'>

```

```

+++++^^IDefault parameters^^I+++++

```

```

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'>

```

```

+++++^^IDefault parameters^^I+++++

```

```

tryNum         : try attempts
                  default value: 10
n_candidate    : number of candidates
                  default value: 5

```

```

-----
parameter information for <class
'magus.reconstruct.ga.LyrSlipMutation'>

```

```

+++++^^IDefault parameters^^I+++++

```

```

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'>
+++++^^IDefault parameters^^I+++++
tryNum         : tryNum
                default value: 10
d              : d
                default value: 0.23
-----
parameter information for <class
'magus.reconstruct.ga.LyrSymMutation'>
+++++^^IDefault parameters^^I+++++
tryNum         : tryNum
                default value: 10
symprec        : symprec
                default value: 0.0001
-----
parameter information for <class
'magus.reconstruct.ga.CluSymMutation'>
+++++^^IDefault parameters^^I+++++
tryNum         : tryNum
                default value: 10
symprec        : symprec
                default value: 0.0001
-----
parameter information for <class
'magus.calculators.emt.EMTCalculator'>
+++++^^IRequirement parameters^^I+++++
work_dir       : work dictionary
job_prefix     : calculation dictionary
+++++^^IDefault parameters^^I+++++
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'>
+++++^^^IDefault parameters^^^I+++++
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
+++++^^^IRequirement_parallel parameters^^^I+++++
queue_name    : queue name
num_core      : num_core
work_dir      : work dictionary
job_prefix    : calculation dictionary
+++++^^^IDefault_parallel parameters^^^I+++++
pre_processing : serves to add any sentence you wish when
submitting 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'>
+++++^^IDefault parameters^^I+++++
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
+++++^^IRequirement_parallel parameters^^I+++++
queue_name     : queue name
num_core       : num_core
work_dir       : work dictionary
job_prefix     : calculation dictionary
+++++^^IDefault_parallel parameters^^I+++++
pre_processing : serves to add any sentence you wish when
submitting 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'>
+++++^^IDefault parameters^^I+++++
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
+++++^^IRequirement_parallel parameters^^I+++++
queue_name     : queue name
num_core       : num_core
work_dir       : work dictionary
job_prefix     : calculation dictionary
+++++^^IDefault_parallel parameters^^I+++++
pre_processing : serves to add any sentence you wish when
submitting 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'>
+++++^^IDefault parameters^^I+++++
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
+++++^^IRequirement_parallel parameters^^I+++++
queue_name     : queue name
num_core       : num_core
work_dir       : work dictionary
job_prefix     : calculation dictionary
+++++^^IDefault_parallel parameters^^I+++++

```

pre_processing : serves to add any sentence you wish when submitting 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'>

+++++^^IRequirement parameters^^I+++++

work_dir : work dictionary

job_prefix : calculation dictionary

+++++^^IDefault parameters^^I+++++

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'>

+++++^^IDefault parameters^^I+++++

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
+++++^^IRequirement_parallel parameters^^I++++
queue_name                      : queue name
num_core                        : num_core
work_dir                       : work dictionary
job_prefix                     : calculation dictionary
+++++^^IDefault_parallel parameters^^I++++
pre_processing : serves to add any sentence you wish when
submitting 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.cstep.CastepCalculator'>
+++++^^IDefault parameters^^I++++
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
+++++^^IRequirement_parallel parameters^^I+++++
queue_name      : queue name
num_core        : num_core
work_dir        : work dictionary
job_prefix      : calculation dictionary
+++++^^IDefault_parallel parameters^^I+++++
pre_processing  : serves to add any sentence you wish when
                  submitting 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'>
+++++^^IRequirement parameters^^I+++++
work_dir        : work dictionary
job_prefix      : calculation dictionary
+++++^^IDefault parameters^^I+++++
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'>
+++++^^IDefault parameters^^I+++++
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
+++++^^IRequirement_parallel parameters^^I+++++
queue_name     : queue name
num_core       : num_core
work_dir       : work dictionary
job_prefix     : calculation dictionary
+++++^^IDefault_parallel parameters^^I+++++
pre_processing : serves to add any sentence you wish when
submitting 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'>  
+++++^^IRequirement parameters^^I+++++  
work_dir      : work dictionary  
job_prefix    : calculation dictionary  
+++++^^IDefault parameters^^I+++++  
pressure      : pressure  
                default value: 0.0  
-----  
parameter information for <class  
'magus.calculators.mtp.TwoShareMTPCalculator'>  
+++++^^IRequirement parameters^^I+++++  
work_dir      : work dictionary  
job_prefix    : calculation dictionary  
+++++^^IDefault parameters^^I+++++  
pressure      : pressure  
                default value: 0.0  
-----
```