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

Introduction

1.1 Overview

MAGUS is the abbreviation for Machine learning And Graph theory assisted Universal structure Searcher. It is a machine learning and graph theory assisted crystal structure prediction method developed by Prof. Jian Sun's group at the School of Physics at Nanjing University. The programming languages are mainly Python and C++ and it is built as a pip installable package. Users can use just a few commands to install the package. MAGUS has also the advantage of high modularity and extensibility. All source codes are transparent to users after installation, and users can modify particular parts according to their needs.

MAGUS has been used to study multiple systems. Several designed new materials have been synthesized experimentally, and a number of high-profile academic papers have been published. (Publications using MAGUS)

1.2 Current Features

- Generation of atomic structures for a given symmetry, support cluster, surface, 2D and 3D crystals including molecules, confined systems, etc
- Geometry optimization of a large number of structures with DFT or active learning machine learning potential
- Multi-target search for structures with fixed or variationally component
- API for VASP, CASTEP, Quantum ESPRESSO, ORCA, MTP, NEP, DeepMD, gulp, lammps, XTB, ASE, etc. Easy for extension.

1.3 Interface

MAGUS now supports the following packages to calculate the energy of structures, some of them are commercial or need registration to get the permission to use.

- VASP
- CASTEP
- Quantum ESPRESSO
- ORCA
- ASE built-in EMT & LJ
- MTP
- NEP
- DeepMD
- gulp
- lammps
- XTB
- siesta
- QUIP via ASE
- OpenKim via ASE

You can also write interfaces to connect MAGUS and other codes by add them in the `/magus/calculators` directory.

1.4 How to Get Access

MAGUS is free for non-commercial academic use. To get access to the source code, you need to register at the following link (`https://www.wjx.top/vm/m5eWS0X.aspx`). We will invite you into our gitlab project as soon as possible. Then you can see the whole project after logging in. Please contact us by email (magus@nju.edu.cn) if you have any questions concerning MAGUS.

1.5 How to Cite

Reference	Cite for What
1, 2	for any work that used MAGUS
3, 4	Graph theory
5	Surface reconstruction
6	Structure searching in confined space

1. Junjie Wang, Hao Gao, Yu Han, Chi Ding, Shuning Pan, Yong Wang, Qiuhan Jia, Hui-Tian Wang, Dingyu Xing, and Jian Sun, "MAGUS: machine learning and graph theory assisted universal structure searcher", Natl. Sci. Rev. 10, nwad128, (2023).

2. Kang Xia, Hao Gao, Cong Liu, Jianan Yuan, Jian Sun, Hui-Tian Wang, Dingyu Xing, "A novel superhard tungsten nitride predicted by machine-learning accelerated crystal structure search", Sci. Bull. 63, 817 (2018).

3. Hao Gao, Junjie Wang, Yu Han, Jian Sun, "Enhancing Crystal Structure Prediction by Decomposition and Evolution Schemes Based on Graph Theory", Fundamental Research 1, 466 (2021).

4. Hao Gao, Junjie Wang, Zhaopeng Guo, Jian Sun, "Determining dimensionalities and multiplicities of crystal nets" npj Comput. Mater. 6, 143 (2020).

5. Yu Han, Junjie Wang, Chi Ding, Hao Gao, Shuning Pan, Qiuhan Jia, and Jian Sun, "Prediction of surface reconstructions using MAGUS", J. Chem. Phys. 158, 174109 (2023).

6. Chi Ding, Junjie Wang, Yu Han, Jianan Yuan, Hao Gao, and Jian Sun, "High Energy Density Polymeric Nitrogen Nanotubes inside Carbon Nanotubes", Chin. Phys. Lett. 39, 036101 (2022). (Express Letter)

1.6 Publications Using MAGUS

See the full publication list here.

Chapter 2

Installation

2.1 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.

2.2 Preparation

2.2.1 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("<Your_vasp_command>",
shell=True)
```

<Your_vasp_command> is the command to run VASP on your cluster, e.g. `mpirun vasp_std` .

Notice: remember to load the corresponding environment, such as ips or openmpi, if you want to run vasp in parallel (run a single vasp job with multiple cores). If you want to use parallel mode (run several vasp jobs at the same time), you also need to load environment in child jobs by adding control lines after "preProcessing" option, see details in Sec. 5.1.

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-to>/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 not use these potentials. It is also allowed to add other pseudopotentials.

3) Set environment variables:

```
$ export VASP_SCRIPT=<your-path-to>/run_vasp.py
$ export VASP_PP_PATH=<your-path-to>/mypps
```

More information in: ase manual for vasp calculator.

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

2.2.2 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>
```

<your-job-system> should be one of LSF, SLURM and PBS. Add this line into your `bashrc` to make the setting work every time you log in.

Notice: in some PBS job system, "qsub" commond may not be under system path in compute nodes. See section 5.3 for solution.

2.2.3 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.* You can follow the instructions in https://mlip.skoltech.ru/download/.

2.2.4 Build a Virtual Environment (Optional)

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 are 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>
```

*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.

2.3 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

```
$ 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. Your git version should not be too low, or https connection may fail. And there should be gcc in your environment. If you want to install in a virtual environment, do not forget to activate the environment first. If you work in a cluster and do not have permission to install in the default location, you may add `--user` parameter.

2.4 Install with Source Code

2.4.1 Download Code

2.4.1.1 Use git

Clone the project and submodules to local file system:

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

2.4.1.2 From Website

If you have problem downloading with git, you have the alternative choice 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.

2.4.2 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 that python will import the module directly 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.

2.5 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.

2.6 Other Settings

2.6.1 Set up Environment Variables

To run MAGUS in your console, you need to add such path variables in `bashrc`.

```
$ export PATH=<your_path_to_magus>:$PATH
$ export PYTHONPATH=<your_path_to_magus>:$PYTHONPATH
```

If you use anaconda to manage your environment, the above actions should be unnecessary for you. When you activate your env, the path variables are automatically set.

2.6.2 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
```

2.7 Check Installation

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

```
$ magus -v
```

```
1.6.0
```

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

```
$ magus checkpack
```

Chapter 3

Examples

We have prepared a series of examples which you can find in the `examples` folder in your MAGUS installation path. In each example, there is a `README.md`. You should follow the instructions in it. The input parameters and other needed input files are almost ready, but you should modify the computing queue in both `job` and `input.yaml`. If you use virtual environment, you should also write the control lines to activate your python environment (see section 5.2 for details).

3.1 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

3.2 Example Introductions

3.2.1 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).

3.2.2 Relax Structures

- `02--1-C8-VASP`: Structure relaxation of diamond by vasp interface.
- `02--2-B12-MTP`: Relax 2000 structures with MTP and VASP.

3.2.3 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 $Zn_x(OH)_y$.

3.2.4 Molecule Crystal Search

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

3.2.5 Cluster Search

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

3.2.6 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.

3.2.7 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.

3.2.8 2D Bulk Search

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

Chapter 4

Input

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.

4.1 Input Files

A typical structure search task needs the following input files:

- **input.yaml**: the basic input file that defines the main parameters in the task. It is in standard yaml format. You should especially pay attention to the indent and the space after quotation mark.
- **inputFold:** the folder containing the extra needed input files for calculators, such as INCAR for VASP and in.lammps for LAMMPS.
- **Seeds:** the folder containing seed structures. There are two types of seed files. The first one is `POSCARS_<gen>`, which is in VASP format. The second one is `seeds_<gen>.traj`, which is in ASE traj format. <gen> stands for the generation you want to input the seeds. You can add several seed files for several generations. Generally, you need only put `POSCAR_1` or `seeds_1.traj` in the folder to add the seeds in the initial generation.

4.2 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,tool,
             mutate,parmhelp}
             ...

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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
    tool                some tools
    mutate              mutation test
```

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

4.2.1 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)
  -p, --use-parallel    use parallel mode. (default:
  False)
```

4.2.2 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}
```

4.2.3 clean

```
$ magus clean -h
```

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

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

4.2.4 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)
```

4.2.5 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)
```

4.2.6 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)
```

4.2.7 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)
```

4.2.8 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
```

4.2.9 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)
```

4.2.10 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)
```

4.3 Input Parameters

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 for random symmetric structure
generation
                  default value: -1
max_volume     : max volume for random symmetric structure
generation
                  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 for random symmetric structure
generation
                  default value: -1
max_volume     : max volume for random symmetric structure
generation
                  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 for random symmetric structure
generation
                  default value: -1
max_volume     : max volume for random symmetric structure
generation
                  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
-------------------------------------------------------------
```

Chapter 5

FAQ

5.1 How to Set Environment Variables

There are two modes in MAGUS: serial mode and parallel mode, controlled by "mode" option.

In serial mode ("mode: serial"), only one parent job runs. All sub calculations (such as vasp relaxations) will run under the computing resource you apply for the parent job. Hence, you can modify environment variables in the parent job and they will be effective to all calculations.

In parallel mode ("mode: parallel"), the parent job only works for some simple calculations and submitting child jobs into job system to do more time-consuming calculations, which means child jobs take different environment variables from the parent job. Generally, child job submission scripts are generated automatically by MAGUS, but you should add some environment variables to make the scripts fit for your system. The most convenient way to do that is to add "preprocessing" option in `input.yaml` under each Calculator category. For example:

```yaml
# general parameters
formulaType: fix
...
# calcultor parameters
MainCalculator:
  jobPrefix: Vasp
  ...
  preProcessing: |
    #BSUB -gpu "num=1"
    module purge
    module load ips/xxxx cuda/xxxx
```

```
export PATH=$PATH:xxxx
```

or you can just write in a single line if your code is short:

```
preProcessing: module load ips; source activate myenv
```

MAGUS will concatenate these codes after preProcessing into the submission script.

TIPS: There is a trick that most job systems run a new submission job with a new shell which will execute your bashrc at first. As a result, you can add the frequently used codes, such as `module load ips` , into bashrc and then you need not add such codes in preProcessing.

5.2 How to Use Python Virtual Environment

If you install MAGUS in your default env and you can directly run MAGUS in your console and `import magus` in python, you need do nothing and it will all work fine. If you install MAGUS in another env, you should modify the input files to activate the env in jobs. Add

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

in the submission job and add

```
preProcessing: source activate <your-env-name>
```

in the `input.yaml` under each Calculator category such as MainCalculator.

5.3 PBS Job System Parallel Mode "qsub" Command Not Found

In some PBS system, "qsub" command can only be found in login nodes but cannot be found in compute nodes. That is because "qsub" command is not under system path in compute nodes. To fix "qsub command not found" error, you need to add the path of "qsub" in your parent batch job. You can use

```
which qsub
```

to get the path. You will get the output <your-pbs-lib-dir>/qsub. Then add such line in your batch file before MAGUS commands:

```
export PATH=<your-pbs-lib-dir>:$PATH
```

NOTICE: only add the directory path. Do not add “qsub”.