

Ogre



Ogre is written in Python and interfaces with the FHI-aims code to calculate surface energies at the level of density functional theory (DFT). The input of Ogre is the geometry of the bulk molecular crystal. The surface is cleaved from the bulk structure with the molecules on the surface kept intact. A slab model is constructed according to the user specifications for the number of molecular layers and the length of the vacuum region. Ogre automatically identifies all symmetrically unique surfaces for the user-specified Miller indices and detects all possible surface terminations. Ogre includes utilities, OgreSWAMP, to analyze the surface energy convergence and Wulff shape of the molecular crystal.

Installation

```
1 conda create -n ogre python=3.6
2 conda activate ogre
3 python setup.py install
```

This code might crash if you use the newest version of pymatgen, so please use the version specified in [setup.py](#)

Example

All configurations are stored in the .config file.

Ogre is for cleaving the surfaces, ogreSWAMP is for plotting surface energy convergence plots and Wulff diagram.

ogre.config:

```
1 [io]
2 structure_path = ./structures/relaxed_structures/TETCEN.cif
3 structure_name = TETCEN_test
4 format = FHI
5 ; Format can be FHI, VASP or CIF
6 [methods]
7 cleave_option = 1
8 ;0: cleave a single surface, 1: cleave surfaces for surface energy calculations
```

```

9 [parameters]
10 layers = 1-6
11 ; Layers could be specified as combination of start-end or separate numbers by space
12 vacuum_size = 40
13 highest_index = 3
14 ; Only needed in cleave_option = 1, ignored in cleave_option = 0
15 supercell_size = None
16 miller_index = 3 3 3
17 ; Only needed in cleave_option = 0, ignored in cleave_option = 1
18 desired_num_of_molecules_oneLayer = 0
19 ; Set to 0 if you don't want to change one layer structure. Default is 0 (highly
    recommended)

```

ogreSWAMP.config:

```

1 [io]
2 scf_path = example/SCF
3 structure_path = structures/relaxed_structures/ASPIRIN.cif
4 structure_name = aspirin
5 [methods]
6 fitting_method = 0
7 ; 0: linear method, 1: Boettger method.
8 [Wulff]
9 Wulff_plot = True
10 ; Whether to plot the Wulff diagram
11 projected_direction = 1 1 1
12 ; projected_direction for Wulff diagram
13 [convergence]
14 threshold = 0.35
15 consecutive_step = 2
16 ; If for N consecutive steps, the difference is smaller than threshold, then it is
    converged.

```

To run ogre

```
1 python runOgre.py --filename ogre.config
```

To launch DFT calculations, use scripts under scripts/

```

1 #Launch PBE+TS, please modify the setting in the script, same for the following scripts.
2 python AimsBatchCalc.py
3
4 #Extract the data from PBE+TS and store in .json file
5 python AimsExtractor.py
6
7 #Launch PBE+MBD
8 python MBDBatchCalc.py
9
10 #Store data in .json file
11 python MBDExtract.py

```

To run ogreSWAMP

```
1 python run0greSWAMP.py --filename ogreSWAMP.config
```