

Documentation for STREUSEL Python Package

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1 Overview

The Surface Topology REcovery Using Sampling of ELeetric field (STREUSEL) software package is a comprehensive, generalized data analysis software suite used to assess atomic and molecular volumes, pore volumes and surface areas of porous materials, and interaction energetics.

2 Installation and Configuration

2.1 Installation

Download the source code from [GitHub](https://github.com/hmsoregon/STREUSEL) or clone the repository using

```
$ git clone http://www.github.com/hmsoregon/STREUSEL
```

To ensure that all package version dependancies are met, we suggest STREUSEL is configured within a virtual environment *i.e.* Anaconda. To do this, download and configure Anaconda, as described [here](#). Then create and activate a new environment using

```
$ conda create --name streusel python=3
$ conda activate streusel
```

Configure and install STREUSEL by running

```
$ python setup.py install
```

from within the STREUSEL directory.

2.2 Setting up .py files

Regardless of the system type (*i.e.* solid-state vs. molecular, VASP vs. Gaussian), the import section of the python file must reference the location of the STREUSEL package. To accomplish this, add the following import statements to your .py file

```
import sys
sys.path.insert(0, '/path/to/STREUSEL/directory')
from vasp_object import * # use for VASP models
from gaussian_cube import * # use for Gaussian models
```

The `'/path/to/STREUSEL/directory'` must be changed to the directory on your local machine. To determine this, run the following command from within the STREUSEL source code directory

```
$ pwd
```

Copy and paste the output into the `sys.path.insert` line of your python file.

3 Gaussian Calculation Functionalities

3.1 Molecular Volume

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