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# **Molsystem Documentation**

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**Paul Saxe**

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Contents:



## **MOLSYSTEM**

Molsystem provides a general class for handling molecular and periodic systems

- Free software: GNU Lesser General Public License v3+
- Documentation: <https://molsystem.readthedocs.io>.

### **1.1 Features**

- Complete the initial version!
  - Remove the coordinates from the `Atoms` class and allow for multiple sets of coordinates – conformers, trajectories, etc.
  - Provide a concept of the ‘current’ system

### **1.2 Credits**

This package was created with [Cookiecutter](#) and the [audreyr/cookiecutter-pypackage](#) project template.





## INSTALLATION

### 2.1 Stable release

To install MolSystem, run this command in your terminal:

```
$ pip install molssystem
```

This is the preferred method to install Molsystem, as it will always install the most recent stable release.

If you don't have `pip` installed, this [Python installation guide](#) can guide you through the process.

### 2.2 From sources

The sources for Molsystem can be downloaded from the [Github repo](#).

You can either clone the public repository:

```
$ git clone git://github.com/paulsaxe/molssystem
```

Or download the [tarball](#):

```
$ curl -OL https://github.com/paulsaxe/molssystem/tarball/master
```

Once you have a copy of the source, you can install it with:

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



## USAGE

To use MolSystem in a project:

```
import molsystem
```



## CONTRIBUTING

Contributions are welcome, and they are greatly appreciated! Every little bit helps, and credit will always be given. You can contribute in many ways:

### 4.1 Types of Contributions

#### 4.1.1 Report Bugs

Report bugs at <https://github.com/molssi-seamm/molssystem/issues>.

If you are reporting a bug, please include:

- Your operating system name and version.
- Any details about your local setup that might be helpful in troubleshooting.
- Detailed steps to reproduce the bug.

#### 4.1.2 Fix Bugs

Look through the GitHub issues for bugs. Anything tagged with “bug” and “help wanted” is open to whoever wants to implement it.

#### 4.1.3 Implement Features

Look through the GitHub issues for features. Anything tagged with “enhancement” and “help wanted” is open to whoever wants to implement it.

#### 4.1.4 Write Documentation

Molssystem could always use more documentation, whether as part of the official Molssystem docs, in docstrings, or even on the web in blog posts, articles, and such.

### 4.1.5 Submit Feedback

The best way to send feedback is to file an issue at <https://github.com/molssi-seamm/molsystem/issues>.

If you are proposing a feature:

- Explain in detail how it would work.
- Keep the scope as narrow as possible, to make it easier to implement.
- Remember that this is a volunteer-driven project, and that contributions are welcome :)

## 4.2 Get Started!

Ready to contribute? Here's how to set up *molsystem* for local development.

1. Fork the *molsystem* repo on GitHub.
2. Clone your fork locally:

```
$ git clone git@github.com:your_name_here/molsystem.git
```

3. Install your local copy into a virtualenv. Assuming you have virtualenvwrapper installed, this is how you set up your fork for local development:

```
$ mkvirtualenv molsystem
$ cd molsystem/
$ python setup.py develop
```

4. Create a branch for local development:

```
$ git checkout -b name-of-your-bugfix-or-feature
```

Now you can make your changes locally.

5. When you're done making changes, check that your changes pass flake8 and the tests, including testing other Python versions with tox:

```
$ flake8 molsystem tests
$ python setup.py test or py.test
$ tox
```

To get flake8 and tox, just pip install them into your virtualenv.

6. Commit your changes and push your branch to GitHub:

```
$ git add .
$ git commit -m "Your detailed description of your changes."
$ git push origin name-of-your-bugfix-or-feature
```

7. Submit a pull request through the GitHub website.

## 4.3 Pull Request Guidelines

Before you submit a pull request, check that it meets these guidelines:

1. The pull request should include tests.
2. If the pull request adds functionality, the docs should be updated. Put your new functionality into a function with a docstring, and add the feature to the list in README.rst.
3. The pull request should work for Python 3.5, 3.6, and 3.7, and for PyPy. Check [https://travis-ci.org/molssi-seamm/molsystem/pull\\_requests](https://travis-ci.org/molssi-seamm/molsystem/pull_requests) and make sure that the tests pass for all supported Python versions.

## 4.4 Tips

To run a subset of tests:

```
$ py.test tests.test_molsystem
```





CREDITS

## 5.1 Development Lead

- Paul Saxe <[psaxe@vt.edu](mailto:psaxe@vt.edu)>

## 5.2 Contributors

None yet. Why not be the first?



## HISTORY

### 6.1 0.1.0 (2019-05-05)

- First release on PyPI.



## INDICES AND TABLES

- `genindex`
- `modindex`
- `search`