
Molecules Experiments Documentation

Release 0.0.1

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1.1 Stable release

To install molexperiments, run this command in your terminal:

```
pip install molexperiments
```

This is the preferred method to install molexperiments, 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.

1.2 From sources

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

You can either clone the public repository:

```
git clone git://github.com/yngtodd/molexperiments
```

Or download the [tarball](#):

```
curl -OL https://github.com/yngtodd/molexperiments/tarball/master
```

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

```
python setup.py install
```


CHAPTER 2

Usage

To use Molecules Experiments in a project:

```
import molexperiments
```


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

3.1 Types of Contributions

3.1.1 Report Bugs

Report bugs at <https://github.com/yngtodd/molexperiments/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.

3.1.2 Fix Bugs

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

3.1.3 Implement Features

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

3.1.4 Write Documentation

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

3.1.5 Submit Feedback

The best way to send feedback is to file an issue at <https://github.com/yngtodd/molexperiments/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 :)

3.2 Get Started!

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

1. [Fork](#) the *molexperiments* repo on GitHub.
2. Clone your fork locally:

```
git clone git@github.com:your_name_here/molexperiments.git
```

3. Create a branch for local development:

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

Now you can make your changes locally.

4. When you're done making changes, check that your changes pass style and unit tests, including testing other Python versions with tox:

```
tox
```

To get tox, just pip install it.

5. 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
```

6. Submit a pull request through the GitHub website.

3.3 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 ≥ 3.6 and for PyPy. Check <https://travis-ci.org/yngtodd/molexperiments> under pull requests for active pull requests or run the `tox` command and make sure that the tests pass for all supported Python versions.

3.4 Tips

To run a subset of tests:

```
py.test test/test_molexperiments.py
```


4.1 Development Lead

- Todd Young GitHub: [yngtodd](#)

4.2 Contributors

None yet. Why not be the first?

5.1 0.0.1 (2018-11-30)

- First release on PyPI.

CHAPTER 6

Feedback

If you have any suggestions or questions about **Molecules Experiments** feel free to email me at youngmt1@ornl.gov.

If you encounter any errors or problems with **Molecules Experiments**, please let me know! Open an Issue at the GitHub <http://github.com/yngtodd/molexperiments> main repository.