

OpenPathSampling



<http://openpathsampling.org>

Twitter: @pathsampling

Development at: <http://github.com/openpathsampling/>

A Python library for path sampling simulations

- ✓ **Easy to use:** Beginners can quickly learn to use it
- ✓ **Easy to extend:** Advanced users can use it to develop new methods
- ✓ **Independent of dynamics engine:** Useful in many fields and to the broadest audience

Core Python library, plus separate command line interface

OpenPathSampling is modular

Big package: 250+ Python files with 43000+ lines of code; 400+ classes.
But you can make a contribution in one part without needing to understand others.

