

OpenPathSampling



<http://openpathsampling.org>

Twitter: @pathsampling

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

A Python library for path sampling simulations

New features!

- Gromacs integration
- PLUMED integration
- Reactive Flux (Bennett-Chandler)
- Faster datafile format
- Spring Shooting*
- Hooks for simulation customization*

* will be in next release (1.5)

***Now with a command
line interface!***

Coming soon:

- Parallel RETIS
- Simulation setup wizard

Acknowledgments

DNA



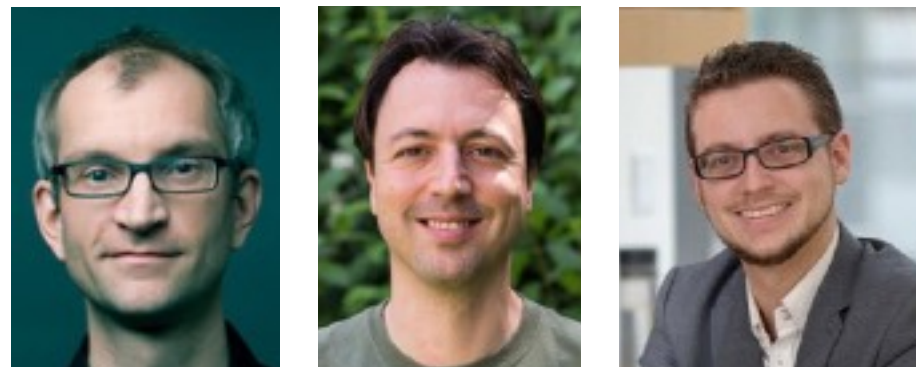
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OpenPathSampling



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