

Patrick B. Louden

PhD, Computational Chemistry

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Summary

Computational chemist with **10 years' experience in software development, predictive modeling, and data analytics**. Senior graduate developer of OpenMD, an open source molecular simulation software package. High level of proficiency at advanced mathematics and statistics, with excellent interpersonal, oral, and written communication skills. Passionate about designing, developing, and collaborating on software used to generate actionable insights.

Programming and Development Skills

Languages C++, Python, Fortran95, SQL, R, shell scripting
Tools Git, UNIX environments, numpy, scipy, matplotlib, Mathematica, MS Office

Experience

- 2012 - **Graduate Research Assistant – University of Notre Dame**
Present
- Developed analysis software to extract key features from large data sets.
 - Automated mathematical fitting procedures for obtaining parameters for predictive models.
 - Took vaguely described research problems with unclear solutions from concept development through to publication.
 - Derived a predictive model for molecular friction at solid/liquid interfaces.
 - Developed software to generate solids for molecular simulation, rapidly increasing ability to screen chemical composition as well as surface features in studies of friction.
 - Derived new mathematical expressions for solid/liquid friction independent of boundary conditions.
 - Developed software to perform two-dimensional Fourier Transforms on surfaces from atomistic simulations.
- 2012 - **Graduate Teaching Assistant – University of Notre Dame**
Present
- Independently led classes in general chemistry I & II, including office hours and review sessions.
 - Strove to consistently improve my teaching performance by completing 18 workshops covering teaching skills and utilizing technology in the classroom.
- 2009 - 2012 **Undergraduate Research Assistant – Grand Valley State University**
- Developed software for atomistic simulations of cloud formation.
 - Designed, characterized, and published a new atomistic model for water.

Education

- 2018 **PhD Chemistry**, *University of Notre Dame*, Notre Dame IN, USA
2012 **Bachelor of Science Chemistry**, *Grand Valley State University*, Allendale MI, USA