

Justin B. Gilmer

CONTACT INFORMATION

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EDUCATION

Vanderbilt University, Nashville, TN

M.S., Materials Science

Aug 2016 – Dec 2019 (Expected)

Continued computational chemistry research and became one of the lead developers on a set of open-source Python libraries designed to provide a simulation engine-agnostic platform to initialize chemical systems of interest in a document-able, reproducible fashion (<https://mosdef.org>). Completed course-work in scientific computing, condensed matter physics, and advanced scientific computing.

Clemson University, Clemson, SC

B.S., Materials Science and Chemistry Minor

Aug 2012 – May 2016

Participated in computational chemistry research for 3 semesters, developing helper tools for the lab in Python to detect and enumerate alkane molecules of various lengths from high temperature reactive forcefield molecular dynamics simulations. Completed course-work in multi-variable calculus, differential equations, data structures and algorithms, software development, and physical chemistry.

PROFESSIONAL EXPERIENCE

Vanderbilt University, Nashville, TN

Graduate Research Assistant

Aug 2016 – Present

Conducted various computational studies of organic chemistry-based compounds using molecular modeling as well as open-source Python software development. Notable work includes:

- Designed and implemented an extensible “plug-in” system for our chemical system building library **mBuild** allowing for dynamic discovery of plug-ins through the use of the **setuptools** **entrypoint** functionality.
- Continued development of our lab’s Python libraries by using software development best practices such as unit testing, collaborative code review, continuous integration, object-oriented design patterns, fork and pull request model for code contributions, and input sanitization
- Became one of the lead software developers of the lab’s open-source Python libraries <https://github.com/mosdef-hub>, now involved in a national grant involving 7 other universities.
- Managed and instructed the simulation of over 36 000 chemical systems, performed time-series and statistical analysis of data from these systems to use partly as testing/training data of a random forest regression model from **sklearn**, producing a predictive model linking chemical features to tribological properties.
- Mentored undergraduate and high school students year-round in molecular simulation, data analysis, and scientific software development best practices.

Vanderbilt University, Nashville, TN

Graduate Teaching Assistant

Aug 2016 – Dec 2019

Developed course-work and lecture material for a 3rd year molecular simulation course as well as a 1st year engineering computation course. Created lessons utilizing Jupyter Notebooks, GitHub Classroom, teaching version control and Python to students with little to no experience of programming concepts.

Clemson University, Clemson, SC

Tutor

Aug 2013 – May 2016

Provided academic tutoring to 500 first year science and engineering students as part of the Residents in Science and Engineering (RiSE) Living-Learning Community (LLC) (<https://ln.pm/rise>).

PROGRAMMING EXPERIENCE

Proficient: Python, Bash, Git/Version Control

Comfortable: Unit Testing, Continuous Integration, Statistical Analysis, Time-series Analysis, SciPy, Pandas, scikit-learn, Matplotlib, GNU/Linux, Unix-like operating systems, C, C++, Java, L^AT_EX, Fortran, Gnuplot, Docker, Singularity, Object-oriented Programming