

# Justin Gilmer

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## CONTACT INFORMATION

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GitHub: <https://github.com/justinGilmer>

## EDUCATION

**Vanderbilt University**, Nashville, TN

*M.S., Materials Science*

**Aug 2016 – Present**

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 multivariable 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 3<sup>rd</sup> year molecular simulation course as well as a 1<sup>st</sup> 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<sup>A</sup>T<sub>E</sub>X, FORTRAN, Gnuplot, Docker, Singularity, Object-oriented Programming