Justin Gilmer

CONTACT INFORMATION

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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.
- Maintained lab computational equipment, including a 14 node computing cluster.
- Ensured cluster uptime by performing maintenance

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. Also performed teaching-assistant duties for a 3rd year mechanical engineering lab, as well as an additional 1st year engineering course.

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://1n.pm/rise`). Led general chemistry study sessions for exam preparation. Mentored minority students through a program offered by the RiSE LLC.

PROGRAMMING SKILLS

Proficient: Python, Bash, Git/Version Control

SciPy, Pandas, scikit-learn, Matplotlib, GNU/Linux, Unix-like operating systems, C, C++, Java, LaTeX, FORTRAN, Gnuplot, Docker, Singularity, Object-oriented Programming