

## Caleb Gallops

[cegallo2@gmail.com](mailto:cegallo2@gmail.com)

2082 Courtland Place, Memphis, TN 38104

(860) 712-0063

### TECHNICAL SKILLS

**Modeling Software:** AMBER, VASP, CPMD, Psi4, Gaussian, MOE, ChemDraw  
**General Software:** Jupyter Notebook, Mathematica, MATLAB, Microsoft Office, Google Suite  
**Languages:** Python, C/C++, Java, SQL  
**Tools:** Psi4, RDKit, Git/Github, Numpy, Pandas, Matplotlib, Plotly, Scipy, Scikit-Learn, XGBoost, Tensorflow, Keras, BigQuery, MAMP  
**Operating Systems:** Macintosh, Windows, Linux

### PROFESSIONAL SKILLS

**Molecular Dynamics (MD) Simulations:** MM, QM/MM, Car-Parrinello, Born-Oppenheimer and Coarse-grained methods  
**Other Chemical Modeling:** conformational searching, geometry optimization, single-point energy, nudged elastic band method for reaction path prediction  
**Data Analysis:** data visualization, quantitative analysis, optimization, statistics, predictive modeling, unsupervised and supervised machine learning, neural networks  
**Communication:** presentations, project development, scientific writing  
**Personal:** detail-oriented, desire to learn, teaching/tutoring experience

### EDUCATION

**Currently pursuing PhD: Expected May 2021**

**Master of Science in Physical Chemistry: Graduated May 2018**

- University of Memphis, Memphis, TN 38104
- GPA: 3.83

**Bachelor of Science in Chemistry: Graduated May 2015**

- Minor in Physics
- Loyola University New Orleans, New Orleans, Louisiana 70118
- Major GPA: 3.467, Minor GPA: 3.321

**LaunchCode LC101 Course: Expected July 2019**

- Learning Python, SQL and Java for backend/frontend software development

### PROJECTS

**Computational Studies of Nanomaterials in Biomedicine:**

<https://pubs.acs.org/doi/10.1021/acsomega.9b00066>

- Performed molecular dynamics simulations of polycationic transfection vectors in non-viral gene delivery
- Evaluated structural changes of polyethyleneimine (PEI) in response to changes in pH and ionic strength.

**Chem\_Strip - Molecular Dynamics Analysis:**

[https://github.com/cegallo2/Chem\\_Strip-1](https://github.com/cegallo2/Chem_Strip-1)

- Wrote program in C++ to reduce size of molecular data files
- Removes unwanted molecules and atoms to shrink files

**2018 Kaggle Survey:**

<https://www.kaggle.com/cegallo2/professional-development-in-2018-kaggle-survey>

- Analyzed the responses to the 2018 Kaggle survey, in which Kaggle users provided information on their professional and technical backgrounds.
- Investigated the correlation between respondents' education and yearly income by creating graphs using Pandas and Plotly libraries in Python.

### WORK EXPERIENCE

**Teaching/Research Assistant:** Fall 2016-Present

Department of Chemistry, University of Memphis, Memphis, TN, 38152,

- Teaching General Chemistry laboratory courses during Academic Year
- Research Assistant in Laboratory of Dr. Yongmei Wang during Summer Sessions

**Software Tutor:** April 2015

Department of Chemistry, Loyola University New Orleans, New Orleans, LA 70118,

- Taught visualization of atomic orbitals for undergraduate Physical Chemistry course using Mathematica