# Dakota Folmsbee

Chemistry Graduate Student · University of Pittsburgh
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## Education

**University of Pittsburgh** — *Aug. 2016 - PRESENT*
Ph.D. Student in Phyiscal Chemistry — *Pittsburgh, PA*

**Clarkson University** — *Aug. 2012 - May 2016*
B.S. in Chemistry — *Potsdam, NY*

## Skills

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|---|---|
| Chemistry | NMR, HPLC, Mass Spectrometry, FTIR, UV/Vis |
| Programming | Python, Scikit-Learn, Tensorflow, Keras, PyTorch, Bash, LaTeX, C++, Julia |
| General | GNU/Linux, VIM, Microsoft Office Suite |

## Professional Experience

**Computational/Physical Chemistry Graduate Student** — *Jan. 2017 - PRESENT*
University of Pittsburgh

- Instituted fast property prediction models to aid a genetic algorithm in rapid material screening
- Developed a molecular machine learning representation for chemical property predictions
- Bench marked state of the art machine learning methods for thermochemical applications

**General Chemistry Teaching Assistant/Fellow** — *Aug. 2016 - Dec. 2017*
University of Pittsburgh

- Recitation & Lab Honors General Chemistry
- Recitation & Lab General Chemistry
- Lab General Chemistry for Engineers

**Undergraduate Researcher** — *Aug. 2013 - May 2016*
Clarkson University

- Synthesized carriers for cancer detecting molecules and chemotherapy drugs
- Analyzed compounds using techniques such as NMR, TOF-MS, and HPLC
- Researched procedures and applications for Gold nanoparticles and nanorods
- Synthesized Gold nanorods and analyzed with thermogravimetric analysis

**General Chemistry Teaching Assistant/Mentor** — *Aug. 2013 - May. 2016*
Clarkson University

- Recitation & Lab General Chemistry for Engineers
- Recitation & Lab General Chemistry for Chemistry and Chemical Engineering

## Publications

**2020**
Folmsbee, D., Koes, D., Hutchison, G. Evaluation of Thermochemical Machine Learning for Potential Energy Curves and Geometry Optimization. *ChemRxiv preprint* 2020. https://doi.org/10.26434/chemrxiv.13029437.v1

**2020**
Folmsbee, D., Hutchison, G. Assessing conformer energies using electronic structure and machine learning methods. *Int J Quantum Chem.* 2020. https://doi.org/10.1002/qua.26381

**2019**
D. Folmsbee, S. Upadhyay, A. Dumi, D. Hiener, & D. Mulvey. *chemreps/chemreps: Molecular Machine Learning Representations (Version 0.1.1).* 2019.Zenodo. http://doi.org/10.5281/zenodo.3333856

# Presentation

**PQI Quantum 2020, Online** *Online*

Poster Presentation *October 2020*

Evaluation of Thermochemical Machine Learning Methods
https://www.pqi.org/content/quantum2020-poster-gallery

**ACS National Meeting & Expo, Online** *Online*

Poster Presentation *March 2020*

Assessing Conformer Energies: Machine Learning vs Conventional Quantum Chemistry
https://doi.org/10.1021/scimeetings.0c00132

**Covestro Lecture Series, University of Pittsburgh** *Pittsburgh, PA*

Poster Presentation *Jan. 2020*

Assessing Conformer Energies: Machine Learning vs Conventional Quantum Chemistry

**Frederick Kaufman Memorial Lecture Series, University of Pittsburgh** *Pittsburgh, PA*

Poster Presentation *Oct. 2019*

Assessing Conformer Energies: Machine Learning vs Conventional Quantum Chemistry

**Science 2019, University of Pittsburgh** *Pittsburgh, PA*

Poster Presentation *Oct. 2019*

Assessing Conformer Energies: Machine Learning vs Conventional Quantum Chemistry

**Advancing Research through Computing 2019, University of Pittsburgh** *Pittsburgh, PA*

Poster Presentation *Mar. 2019*

Rapid Predictive Methods to Aid in Screening of Organic Dielectric Materials

**Science 2018, University of Pittsburgh** *Pittsburgh, PA*

Poster Presentation *Oct. 2018*

Rapid Predictive Methods to Aid in Screening of Organic Dielectric Materials

**Frederick Kaufman Memorial Lecture Series, University of Pittsburgh** *Pittsburgh, PA*

Poster Presentation *Oct. 2018*

Rapid Predictive Methods to Aid in Screening of Organic Dielectric Materials

**Covestro Lecture Series, University of Pittsburgh** *Pittsburgh, PA*

Poster Presentation *Sept. 2018*

Rapid Predictive Methods to Aid in Screening of Organic Dielectric Materials

**Simulators Meeting 2018, Carnegie-Mellon University** *Pittsburgh, PA*

Oral Presentation *May 2018*

Machine Learning to Aid in Screening for Organic Dielectric Materials

**Covestro Lecture Series, University of Pittsburgh** *Pittsburgh, PA*

Poster Presentation *Oct. 2017*

Genetic Algorithms & Machine Learning for Rapid Materials Screening

**Frederick Kaufman Memorial Lecture Series, University of Pittsburgh** *Pittsburgh, PA*

Poster Presentation *Oct. 2017*

Genetic Algorithms & Machine Learning for Rapid Materials Screening

# Programming Projects

**chemreps** *Aug. 2018 - PRESENT*

Developer

- https://github.com/chemreps/chemreps
- Developed a molecular representation library for machine learning in chemistry.

**QM/MM Study Group** *July 2018 - Dec. 2018*

Instructor & Organizer

- https://github.com/shivupa/QMMM_study_group
- Organized and taught various lessons surrounding computational chemistry.

## Honors & Awards

2020 **PQI Quantum2020 Remote Poster Session Poster Award**, PQI

2017 **Safford Teaching Award**, University of Pittsburgh

2017 **First Year Graduate Teaching Assistant Mentor**, University of Pittsburgh

2015 **Walsh Fellow**, Clarkson University