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

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

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, 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

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

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

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

2015 **Walsh Fellow**, Clarkson University