

Dakota Folmsbee

CHEMISTRY GRADUATE STUDENT · UNIVERSITY OF PITTSBURGH

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Education

University of Pittsburgh

PH.D. STUDENT IN PHYSICAL CHEMISTRY

Aug. 2016 - PRESENT

Pittsburgh, PA

Clarkson University

B.S. IN CHEMISTRY

Aug. 2012 - May 2016

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

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

Jan. 2017 - PRESENT

General Chemistry Teaching Assistant/Fellow

UNIVERSITY OF PITTSBURGH

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

Aug. 2016 - Dec. 2017

Undergraduate Researcher

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

Aug. 2013 - May 2016

General Chemistry Teaching Assistant/Mentor

CLARKSON UNIVERSITY

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

Aug. 2013 - May. 2016

Publications

2021

Folmsbee, D., Koes, D., Hutchison, G. Evaluation of Thermochemical Machine Learning for Potential Energy Curves and Geometry Optimization. *J. Phys. Chem. A*. 2021. <https://doi.org/10.1021/acs.jpca.0c10147>

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

POSTER PRESENTATION

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

Online

October 2020

ACS National Meeting & Expo, Online

POSTER PRESENTATION

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

Online

March 2020

Covestro Lecture Series, University of Pittsburgh

POSTER PRESENTATION

Assessing Conformer Energies: Machine Learning vs Conventional Quantum Chemistry

Pittsburgh, PA

Jan. 2020

Frederick Kaufman Memorial Lecture Series, University of Pittsburgh

POSTER PRESENTATION

Assessing Conformer Energies: Machine Learning vs Conventional Quantum Chemistry

Pittsburgh, PA

Oct. 2019

Science 2019, University of Pittsburgh

POSTER PRESENTATION

Assessing Conformer Energies: Machine Learning vs Conventional Quantum Chemistry

Pittsburgh, PA

Oct. 2019

Advancing Research through Computing 2019, University of Pittsburgh

POSTER PRESENTATION

Rapid Predictive Methods to Aid in Screening of Organic Dielectric Materials

Pittsburgh, PA

Mar. 2019

Science 2018, University of Pittsburgh

POSTER PRESENTATION

Rapid Predictive Methods to Aid in Screening of Organic Dielectric Materials

Pittsburgh, PA

Oct. 2018

Frederick Kaufman Memorial Lecture Series, University of Pittsburgh

POSTER PRESENTATION

Rapid Predictive Methods to Aid in Screening of Organic Dielectric Materials

Pittsburgh, PA

Oct. 2018

Covestro Lecture Series, University of Pittsburgh

POSTER PRESENTATION

Rapid Predictive Methods to Aid in Screening of Organic Dielectric Materials

Pittsburgh, PA

Sept. 2018

Simulators Meeting 2018, Carnegie-Mellon University

ORAL PRESENTATION

Machine Learning to Aid in Screening for Organic Dielectric Materials

Pittsburgh, PA

May 2018

Covestro Lecture Series, University of Pittsburgh

POSTER PRESENTATION

Genetic Algorithms & Machine Learning for Rapid Materials Screening

Pittsburgh, PA

Oct. 2017

Frederick Kaufman Memorial Lecture Series, University of Pittsburgh

POSTER PRESENTATION

Genetic Algorithms & Machine Learning for Rapid Materials Screening

Pittsburgh, PA

Oct. 2017

Programming Projects

chemreps

DEVELOPER

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

Aug. 2018 - PRESENT

QM/MM Study Group

INSTRUCTOR & ORGANIZER

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

July 2018 - Dec. 2018

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