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	RDKit, Open Babel, Avogadro, Gaussian, ORCA, xTB
Programming	Python, Scikit-Learn, Tensorflow, Keras, PyTorch, Bash, Git, LaTeX, C++, Julia
General	GNU/Linux, VIM, Microsoft Office Suite

Professional Experience

Computational/Physical Chemistry Graduate Student Researcher *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

2021
Matlock, M., Hoffman, M., Dang, N., Folmsbee, D., Langkamp, L., Hutchison, G., Kumar, N., Sarullo, K., Swamidass, S. J. Deep Learning Coordinate-Free Quantum Chemistry. *J. Phys. Chem. A.* 2021. https://doi.org/10.1021/acs.jpca.1c04462

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 *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