Dakota Folmsbee

Computational Chemist & Materials Scientist

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Education

University of Pittsburgh *Aug. 2016 - Feb. 2022*

Ph.D. 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
Computational Biology	Amber, WESTPA, MDAnalysis, PyMOL, VMD, CHARMM-GUI, AlphaFold, GNINA
Programming	Python, Scikit-Learn, Tensorflow, Keras, PyTorch, Bash, Git, LaTeX, C++, Julia
General	GNU/Linux, VIM, Microsoft Office Suite

Professional Experience

Computational Materials Scientist *April 2024 - Present*

Prometheus Materials, Longmont CO

- Applied machine learning tools to existing data to predict the strength of concrete mixes.
- Created analysis and visualization tools for FTIR and Raman spectroscopy.
- Constructed a new database and tools for production and R&D.

T32 Postdoctoral Scholar *March 2022 - Feb. 2024*

University of Pittsburgh - Koes Group

- Analyzed the effect of allosteric modulation of ion channels for pain relief.
- Led a team of undergraduate researchers in uncovering the structural basis of drug potency and efficacy.
- Developed a computational pipeline for creating, simulating, and analyzing ion channels in a membrane bilayer.
- Performed pharmacophore searches to effectively screen known compounds for additional hits, resulting in the identification of promising candidates for further investigation.

Computational/Physical Chemistry Graduate Student Researcher *Jan. 2017 - Feb. 2022*

University of Pittsburgh - Hutchison Group

- Assisted in developing a genetic algorithm for screening dielectric materials.
- Engineered machine learning representations for rapid property prediction of molecules.
- Benchmarked state of the art machine learning methods against conventional quantum methods.
- Devised a novel approach to generate conformers based on quantum torsional information as an alternative to crystal structure data-based methods.

General Chemistry Teaching Assistant/Fellow *Aug. 2016 - Dec. 2017*

University of Pittsburgh

- Taught recitation and laboratory sections for multiple general chemistry courses.
- Mentored and supervised new graduate and undergraduate teaching assistants in their teaching duties.

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

- Taught recitation and laboratory sections for multiple general chemistry courses.

Publications

2023
Folmsbee, D., Koes, D., Hutchison, G. Systematic Comparison of Experimental Crystallographic Geometries and Gas-Phase Computed Conformers for Torsion Preferences. *J. Chem. Inf. Model.* 2023. https://doi.org/10.1021/acs.jcim.3c01278

2022
Hiener, D., Folmsbee, D., Langkamp, L., Hutchison, G. Evaluating Fast Methods for Static Polarizabilities on Extended Conjugated Oligomers *Phys. Chem. Chem. Phys.* 2022. https://doi.org/10.1039/D2CP02375J

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

Anesthesiology Research Rounds Seminar, University of Pittsburgh *Pittsburgh, PA*
Oral Presentation *Feb. 2024*
Computational Illumination of Allosteric Modulation of Glycine Receptors

Postdoctoral Data & Dine Symposium, University of Pittsburgh *Pittsburgh, PA*
Poster Presentation *May 2023*
Evaluating Positive-Allosteric-Modulator-Induced Conformational Changes of α3 Glycine Receptor

Safar Symposium, University of Pittsburgh *Pittsburgh, PA*
Poster Presentation *May 2023*
Evaluating Positive-Allosteric-Modulator-Induced Conformational Changes of α3 Glycine Receptor

ACS Spring 2023 National Meeting & Expo *Indianapolis, IN*
Oral Presentation *March 2023*
Assessing Torsional Preferences for Conformer Sampling: Experimental Crystallographic Geometries versus Gas-Phase Computed Conformers

ACS Spring 2023 National Meeting & Expo *Indianapolis, IN*
Poster Presentation *March 2023*
Evaluating Positive-Allosteric-Modulator-Induced Conformational Changes of Glycine Receptors

Biophysical Society Meeting *San Diego, CA*
Poster Presentation *February 2023*
Evaluating Positive-Allosteric-Modulator-Induced Conformational Changes of Glycine Receptors

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

2016 **Magna Cum Laude**, Clarkson University

2015 **Walsh Fellow**, Clarkson University