Dakota Folmsbee

Computational Chemist | Materials Scientist | Data Scientist

(+1) 802-683-4502 | dfolmsbee@gmail.com | dlf57.github.io | dlf57 | dakota-folmsbee-b610645a

Summary

Ph.D.-trained scientist with over 7 years of experience applying computational chemistry, machine learning, and data science to complex molecular and materials problems. Skilled in developing predictive models, analyzing simulation and chemical data, and applying cheminformatics tools. Proficient in Python, DFT, molecular dynamics, and modern ML methods. Strong collaborator and communicator with a track record of translating scientific insights into practical solutions.

Professional Experience

Computational Materials Scientist

April 2024 - Current

Prometheus Materials, Longmont CO

- Developed machine learning models to predict material properties for concrete and biomineralization systems.
- Applied modeling and optimization methods to advance discovery of sustainable material compositions.
- Developed interactive ML dashboards for performance prediction and design optimization.
- Built and maintained data pipelines and centralized databases for R&D data.
- Collaborated cross-functionally to translate data insights into actionable materials solutions.

T32 Postdoctoral Scholar – Computational Drug Discovery

March 2022 - Feb. 2024

University of Pittsburgh - Koes Group

- Built computational pipelines for molecular dynamics simulations of ion channels in membranes.
- Implemented enhanced sampling approaches to produce protein structures for binding interaction studies.
- Applied cheminformatics to analyze structure-function relationships affecting drug efficacy.
- Utilized pharmacophore searches and data analysis techniques to identify and prioritize promising drug-like compounds.
- Directed undergraduate research teams conducting computational modeling studies.

Graduate Researcher – Computational Chemistry & ML

Jan. 2017 - Feb. 2022

University of Pittsburgh - Hutchison Group

- Conducted first-principles (DFT) calculations to predict optical, electronic, and dielectric properties of organic materials.
- Benchmarked ML models against ab initio methods for property prediction, enabling speed-ups in screening workflows.
- Designed novel molecular representation methods (chemreps) to improve ML accuracy for quantum chemical properties.
- Developed and applied genetic algorithms for material property optimization and dielectric material discovery.
- Implemented distance geometry method using quantum torsion as an alternative to crystal-structure-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 - Medicinal Chemistry

Aug. 2014 - May 2016

Clarkson University - Melman Group

- Synthesized carriers for cancer detecting molecules and chemotherapy drugs
- Analyzed compounds using techniques such as NMR, TOF-MS, and HPLC

General Chemistry Teaching Assistant/Mentor

Aug. 2013 - May. 2016

Clarkson University

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

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

Certifications

IBM Deep Learning with PyTorch, Keras and Tensorflow

Credential ID SJZLWDAK8H6T

Google Data Analytics

Credential ID WOADFVJ190RU

Projects

diamondfp
Aug 2025 - Present

Developer

- Developed a Python library for generating statistical fingerprints of baseball players to enable similarity searches and ML.
- Technologies: Python, NumPy, Pandas, Polars, Scikit-Learn, Matplotlib, Git, Pytest
- https://github.com/dlf57/diamondfp

Concrete Mix Optimization Dashboard
April 2024 - July 2025

Developer, Prometheus Materials

- Developed and deployed a web dashboard for exploring ML-driven predictions of concrete mix properties.
- Technologies: Python, Scikit-learn, Pandas, Plotly Dash

chemreps
Aug. 2018 - March 2020

Developer

- Created an open-source Python package for generating molecular representations for ML models in chemistry.
- Technologies: Python, NumPy, cclib, qcelemental, Git, Pytest
- https://github.com/chemreps/chemreps

QM/MM Study Group
July 2018 - Dec. 2018

Instructor & Organizer

- Designed and led a course teaching computational chemistry and Python fundamentals to graduate students.
- Technologies: Python, PySCF, Psi4NumPy, Git
- https://github.com/shivupa/QMMM_study_group

MolecularLearning
Sept. 2017 - Aug. 2018

Developer

- Implementation of PhD work for creating custom molecular representations for ML.
- Technologies: Python, Open Babel, Scikit-Learn, Git, Pytest
- https://github.com/dlf57/MolecularLearning

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

Skills

Programming Languages	Python, R, SQL, Bash, C++, Julia, LaTeX
Computational Chemistry	RDKit, Open Babel, Avogadro, Gaussian, ORCA, PySCF, xTB
Computational Biology	Amber, GROMACS, MDAnalysis, PyMOL, VMD, CHARMM-GUI, AlphaFold, GNINA
Python Libraries	Scikit-learn, PyTorch, Keras, TensorFlow, Pandas, NumPy, Plotly, Dash, Matplotlib
Data Science	Data cleaning, visualization, feature engineering, model evaluation & deployment
General	Git, GNU/Linux, SLURM, HPC environments, VIM, Jupyter, Microsoft Office Suite

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