Dakota Folmsbee

Computational Chemist | Materials Scientist | Data Scientist

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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 chem-informatics 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 Physical 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