Dakota Folmsbee

Computational Chemist | Materials Scientist | Data Scientist

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Summary

Ph.D.-trained scientist with over 7 years of experience applying machine learning and data analysis techniques to complex scientific problems. Skilled in developing predictive models, interactive dashboards, and data pipelines. Proven ability to translate technical insight into actionable solutions across chemistry, materials science, and biotechnology.

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

Professional Experience

Computational Materials Scientist *April 2024 - Present*

Prometheus Materials, Longmont CO

- Applied machine learning models to both concrete and biomineralization datasets to predict material properties and extract key performance indicators.
- Developed a machine learning interface using Dash to predict concrete mix performance, enabling interactive exploration of mix designs and outcomes.
- Created data visualization and analysis tools to interpret characterization results from biomineralization experiments.
- Built and maintained a centralized database and custom analysis pipelines to support R&D and production efficiency.

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 3 Glycine Receptor

Safar Symposium, University of Pittsburgh *Pittsburgh, PA*

Poster Presentation *May 2023*

Evaluating Positive-Allosteric-Modulator-Induced Conformational Changes of 3 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

Projects

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: Dash, Plotly, Scikit-learn, Pandas

chemreps *Aug. 2018 - March 2020*

Developer

- Created an open-source Python package for generating molecular representations for ML models in chemistry.
- https://github.com/chemreps/chemreps

QM/MM Study Group *July 2018 - Dec. 2018*

Instructor & Organizer

- https://github.com/shivupa/QMMM_study_group
- Designed and delivered a curriculum introducing computational chemistry and Python to graduate students.

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