Dakota Folmsbee

Computational Chemist | Materials Scientist | Data Scientist

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

Experience

Computational Materials Scientist *April 2024 - July 2025*

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

- 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.

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*

Programming Projects

chemreps *Aug. 2018 - March 2020*

Developer

- https://github.com/chemreps/chemreps
- Directed and developed an open source 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 new graduate students various topics pertaining to computational chemistry

Skills

Chemistry & Materials Science	RDKit, Open Babel, Avogadro, Gaussian, ORCA, xTB, Profex
Programming	Python, Pandas, Scikit-Learn, PyTorch, Tensorflow, Plotly, Dash, Bash, Git, LaTeX, C++, Julia
Computational Biology	Amber, WESTPA, MDAnalysis, PyMOL, VMD, CHARMM-GUI, AlphaFold, GNINA
General	GNU/Linux, VIM, Microsoft Office Suite

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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.

Experience

Computational Materials Scientist *April 2024 - July 2025*

Prometheus Materials, Longmont CO

- Built predictive models using machine learning to estimate material properties from experimental data.
- Created a web-based analytics dashboard with Plotly Dash to enable interactive exploration of concrete mix performance.
- Developed custom data pipelines and centralized databases to streamline R&D and production workflows.
- Designed visualizations and statistical analyses to support experimental interpretation and decision making.

T32 Postdoctoral Scholar *March 2022 - Feb. 2024*

University of Pittsburgh - Koes Group

- Led a team of undergraduates in modeling and analyzing structure-activity relationships in pharmaceutical compounds.
- Developed a computational pipeline for creating, simulating, and analyzing protein-ligand systems in Python.
- Performed virtual screening on large chemical datasets to identify candidate drug molecules.

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

University of Pittsburgh - Hutchison Group

- Engineered molecular feature representations for machine learning models to predict quantum mechanical properties.
- Benchmarked machine learning algorithms against conventional quantum methods.
- Applied optimization algorithms (e.g., genetic algorithms) to materials design problems.
- Created tools for conformer generation based on quantum torsional data.

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*

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.

Skills

Languages	Python, Bash, C++, Julia, LaTeX
Libraries	Scikit-learn, PyTorch, TensorFlow, Pandas, NumPy, Plotly, Dash, Matplotlib
Data	Data cleaning, visualization, feature engineering, model evaluation, deployment
Tools	Tools: Git, Linux, Jupyter, VS Code, Microsoft Office Suite
Science	RDKit, Open Babel, Gaussian, MDAnalysis, AlphaFold