Dakota Folmsbee

Computational Chemist | Data Scientist | Materials Scientist

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Summary

Ph.D.-trained data and computational scientist with 7+ years of experience applying machine learning, statistical analysis, and scientific computing to accelerate discovery in chemistry, materials science, and biotechnology. Proven track record building predictive models, deploying interactive analytics tools, and automating R&D workflows. Skilled in translating complex technical data into actionable insights and scalable software tools.

Experience

Computational Materials Scientist *April 2024 - Current*

Prometheus Materials, Longmont CO

- Built supervised ML models to predict concrete mix properties from experimental parameters, improving formulation efficiency.
- Developed and deployed a web-based analytics dashboard (Plotly Dash) for real-time materials performance exploration.
- Developed custom data pipelines and centralized databases to streamline R&D and production workflows.
- Delivered statistical reports and visualizations to guide production and experimental decision-making.

T32 Postdoctoral Scholar – Computational Drug Discovery *March 2022 - Feb. 2024*

University of Pittsburgh - Koes Group

- Led a team of undergraduates in modeling protein–ligand interactions and analyzing SAR data for novel pharmaceuticals.
- Developed a computational pipeline for creating, simulating, and analyzing protein-ligand systems in Python.
- Performed virtual screens on 100k+ compound libraries to identify candidate drug molecules.

Graduate Researcher – Computational Chemistry & ML *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 a conformer generation tool leveraging quantum torsion scans as an alternative to crystal-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*

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: 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.
- 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.
- https://github.com/shivupa/QMMM_study_group

Skills

Languages	Python, SQL, R, Bash, C++, Julia, LaTeX
Libraries	Scikit-learn, PyTorch, TensorFlow, Pandas, NumPy, SciPy, Plotly, Dash, Matplotlib
Data	Data cleaning, visualization, feature engineering, ML modeling, pipeline deployment
Tools	Git, Linux, Jupyter, SLURM, HPC environments, VIM, Microsoft Office Suite
Science	RDKit, Open Babel, Gaussian, ORCA, xTB, MDAnalysis, AlphaFold, AMBER, GROMACS