Dakota Folmsbee

Computational Chemist & Materials Scientist

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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

- 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