

RESEARCH INTERESTS

Caitlin explores research questions at the intersection of machine learning and computational science. Her Ph.D. research focuses on developing interpretable machine learning pipelines for accurately and efficiently predicting molecular and atomic properties from quantum-mechanical datasets.

RELEVANT RESEARCH PROJECTS

- Designed a physics-informed graph neural network for highly accurate prediction of molecular and atomic properties.
- Developed a scalable adaptive sampling algorithm that leads to greater neural network predictive performance compared to other subset selection algorithms, tested on several Image/NLP datasets and model architectures.
- Designing subset selection metrics to choose informative subsets from chemistry datasets to improve neural network performance and ascertain details about the underlying distribution of the datasets.

PUBLICATIONS

- **Under Review:** Caitlin Whitter, Alex Pothén, and Aurora Clark. PIL-Net: Physics-Informed Graph Convolutional Network for Predicting Atomic Multipoles. *Digital Discovery*, 2025.
- **In Preparation for Submission:** Caitlin Whitter, Young In Kim, and Rajiv Khanna. FARS: A Flatness-aware Adaptive Random Sampling Algorithm for Subset Selection from Heterogeneous Data.