

Education

Ph.D. candidate **Carnegie Mellon University** **Expected Fall 2024**

- Department of Chemical Engineering, emphasis in Machine Learning.
- Advised by John Kitchin and Zachary Ulissi.

Bachelor of Science **Iowa State University** **Graduated December 2019**

- Major in Chemical Engineering, *summa cum laude*.
- Minor in Computer Science.

Research Experience

Ph.D. Researcher **Carnegie Mellon University** **November 2020 - Present**

- Studying uncertainty quantification, active learning, and transfer learning methods for machine learning graph potentials in computational catalysis.
- Develop property prediction techniques for graph neural networks, such as Gibbs free energy prediction.
- Collaborate with researchers at Meta AI on the Open Catalyst Project to improve methods for dataset generation and uncertainty quantification of graph neural networks.
- Principal developer of the *Finetuna* Python package, implementing active learning methods for accelerating atomistic simulations. github.com/ulissigroup/finetuna
- Responsible for maintenance and troubleshooting of the Ulissi Group Kubernetes compute cluster.

Undergraduate Researcher **Iowa State University** **September 2016 - May 2019**

- Designed and built high-throughput fluorimeters for carbon nanotube biosensors in enzyme assays.
- Automated data collection instruments throughout the lab by programming custom controllers.
- Coauthored two published papers regarding carbon nanotubes for enzyme characterization.

Professional Experience

Research Scientist Intern **Meta AI** **May 2023 - October 2023**

- Benchmarked uncertainty prediction methods for use in the Open Catalyst Demo. open-catalyst.metademolab.com
- Implemented transformer sequence models, mean variance estimation models, latent distance methods, and ensemble methods for estimating neural network uncertainty.
- Developed novel improvements to uncertainty methods for graph neural network potentials.
- Manuscript documenting these results presented at the NeurIPS 2023 AI4Science workshop.

Process Development Intern **Genentech** **May 2019 - August 2019**

- Evaluated a process camera for automating single-use bioreactors in a pilot plant environment.
- Designed experiments to demonstrate camera compatibility with the cell culture process.
- Implemented computer vision code to analyze images from the camera and control the cell culture process in real time.

Process Development Co-op **Hutchinson Technology** **January 2018 - August 2018**

- Led the scale-up of a low-cost oxidation process used to replace a more expensive plating process.
- Investigated the effectiveness of various etchants on a new alloy and developed a novel etching process.

Leadership Experience

Teaching Assistant Carnegie Mellon University August 2020 - December 2021

- TA for Thermodynamics, Process Control, and Mathematical Modeling in Chemical Engineering
- Prepared homework problems and led weekly help sessions for undergraduate students.

Process Team Leader NASA X-Hab Challenge August 2018 - May 2019

- Led a team of undergraduate engineers in an interdisciplinary effort to design a working prototype carbon scrubber for the Artemis missions.
- Collaborated with researchers at the Ames National Laboratory to model and test a CO₂ adsorbing bed incorporating novel metal organic frameworks.

Nationals Team Leader ISU Chem-E-Car June 2017 - November 2018

- Led a team of engineers in building a chemistry-driven car for a precision-distance competition.

Publications and Presentations

Publications

- *Improved Uncertainty Estimation of Graph Neural Network Potentials Using Engineered Latent Space Distances.* **J. Musielewicz**, J. Lan, M. Uyttendaele, J. Kitchin; ArXiv, Jul. 2024.
- *Generalization of Graph-Based Active Learning Relaxation Strategies Across Materials.* **J. Musielewicz**, X. Wang, R. Tran, S. Ethirajan, X. Fu, H. Mera, J. Kitchin, R. Kurchin, and Z. Ulissi; Machine Learning: Science & Technology, Apr. 2024.
- *Robust and scalable uncertainty estimation with conformal prediction for machine-learned interatomic potentials.* Y. Hu, **J. Musielewicz**, and Z. Ulissi, and A. Medford; Machine Learning: Science & Technology, Dec. 2022.
- *Finetuna: Fine-tuning accelerated molecular simulations.* **J. Musielewicz**, X. Wang, T. Tian, and Z. Ulissi; Machine Learning: Science & Technology, Sep. 2022.
- *Substrate-Wrapped, Single-Walled Carbon Nanotube Probes for Hydrolytic Enzyme Characterization.* N. Kallmyer, **J. Musielewicz**, J. Sutter, and N. Reuel; Analytical Chemistry, Mar. 2018.

Presentations

- *Predictive Uncertainty Quantification for Graph Neural Network Driven Relaxed Energy Calculations.* **J. Musielewicz**, J. Lan, and M. Uyttendaele; Poster presented at NeurIPS 2023 AI for Science Workshop; Dec. 2023.
- *Accelerating Geometric Optimizations by Finetuning Open Catalyst Project Models with Active Learning.* **J. Musielewicz**, Z. Ulissi; Talk presented at 27th North American Catalysis Society Meeting; May 2022.
- *Accelerating on-the-Fly Active Learning of Catalyst Simulations Using Large Scale Pretrained Models.* **J. Musielewicz**, Z. Ulissi; Poster presented at AIChE annual meeting; Nov. 2021.

Skills

- Python and its scientific computing stack (NumPy, SciPy, Pandas, etc.).
- Machine learning libraries, particularly PyTorch and Scikit-learn.
- Atomistic simulations, particularly using codes such as VASP and ASE.
- Version control systems such as Git, for collaboration and with continuous integration tools for developing packages.
- Distributed and cloud computing tools, particularly Kubernetes and AWS.
- Setting up and replicating scientific Python environments in Linux using tools like Conda and Docker.
- Object-oriented programming in languages such as Python and Java.