Website: jmusiel.github.io

JOSEPH MUSIELEWICZ

Email: jmus [AT] cmu.edu

Education

Ph.D. candidate **Carnegie Mellon University** **Expected May 2025**

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

Bachelor of Science **Iowa State University** **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 graph models in computational catalysis.
- Principal developer of the *Finetuna* Python package, implementing active learning methods for accelerating atomistic simulations. *github.com/ulissigroup/finetuna*
- Develop and test novel transfer learning techniques for graph neural networks applied to molecular simulation in very low data regimes.
- Collaborate with researchers at Meta AI on the Open Catalyst Project to improve methods for dataset generation and uncertainty quantification of machine learning potentials.
- 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 fluorometers 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 graph neural network potentials.
- Developed novel improvements to uncertainty methods for graph neural network potentials.
- Manuscript documenting these results accepted to 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 an inexpensive oxidation process used to replace a costly plating process in manufacturing.
- 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 designing and building a chemically powered car for a precision-distance competition.

Publications and Presentations

Publications

- *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; ArXiv, Nov. 2023.
- *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.