

# JOSEPH MUSIELEWICZ

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## Education

### **Carnegie Mellon University Ph.D. in Chemical Engineering**

- Advised by John Kitchin and Zachary Ulissi.
- Emphasis in Machine Learning.

**Pittsburgh, PA  
January 2025**

### **Iowa State University Bachelor of Science in Chemical Engineering**

- Graduated *summa cum laude*.
- Minor in Computer Science.

**Ames, IA  
December 2019**

## Ph.D. Research Experience

### **Carnegie Mellon University Ph.D. Researcher**

**Pittsburgh, PA  
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.
- Implement transition state finding methods which converge 3 times more often than previous state of the art.
- 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 on Github, implementing active learning methods for accelerating atomistic simulations by 90%.
- Responsible for maintenance and troubleshooting of the Ulissi Group Kubernetes compute cluster.

## Professional Experience

### **Meta AI Research Scientist Intern**

**San Francisco, CA  
May 2023 - October 2023**

- Benchmarked uncertainty prediction methods for use in the Open Catalyst Demo.
- 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 resulting in a 50% improvement in uncertainty calibration on the relaxed structure to relaxed energy task.
- Presented a manuscript documenting these results at the NeurIPS 2023 AI4Science workshop.

### **Genentech Process Development Intern**

**South San Francisco, CA  
May 2019 - August 2019**

- Evaluated a process camera for automating single-use bioreactors in a pilot plant environment.
- Designed experiments to demonstrate compatibility with the cell culture process within light exposure tolerance.
- Implemented computer vision code to analyze images from the camera and control the cell culture process in real time, saving an estimated 10 operator hours per week.

### **Hutchinson Technology Process Development Co-op**

**Hutchinson, MN  
January 2018 - August 2018**

- Led the scale-up of a low-cost oxidation process used to replace a 10 times more expensive plating process.
- Investigated the effectiveness of etchants on a new alloy and developed a novel etching process.

## Skills

### **Programming Languages and Libraries**

- Python and its scientific computing stack, including NumPy, SciPy, Pandas, etc.
- Machine learning libraries, particularly PyTorch and Scikit-learn.
- Atomistic simulations, particularly using codes such as VASP and ASE.
- Object-oriented programming in languages such as Python and Java.

### **Computing Tools**

- Version control systems such as Git, and its use for collaboration
- Continuous integration tools for developing packages, including Github Actions and CircleCI.
- Distributed and cloud computing tools, including Kubernetes, Slurm, and AWS.
- Setting up and replicating scientific Python environments using tools like Conda and Docker.

## Publications and Presentations

### Publications

- *Accessing Numerical Energy Hessians with Graph Neural Network Potentials and Their Application in Heterogeneous Catalysis*. **J. Musielewicz**, B. Wander, R. Cheula, J. Kitchin; ArXiv, Oct. 2024.
- *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.

## Leadership Experience

**Carnegie Mellon University**  
**Undergraduate Research Mentor**

**Pittsburgh, PA**  
**May 2022 - August 2022**

- Mentored an undergraduate student in conducting computational chemistry research in the Ulissi group.

**Carnegie Mellon University**  
**Teaching Assistant**

**Pittsburgh, PA**  
**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.

**NASA X-Hab Challenge**  
**Process Team Leader**

**Ames, IA**  
**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, which passed NASA evaluation.
- Collaborated with researchers at the Ames National Laboratory to model and test a CO<sub>2</sub> adsorbing bed incorporating novel metal organic frameworks.

**ISU Chem-E-Car**  
**Nationals Team Leader**

**Ames, IA**  
**June 2017 - November 2018**

- Led a team of engineers in building a chemistry-driven car for a precision-distance competition.
- Set a record for Iowa State Chem-E-Car performance at the national competition.

## Undergraduate Research Experience

**Iowa State University**  
**Undergraduate Researcher**

**Ames, IA**  
**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.