JOSEPH MUSIELEWICZ

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Education

Carnegie Mellon University **Pittsburgh, PA**
Ph.D. in Chemical Engineering **February 2025**
- Advised by John Kitchin and Zachary Ulissi.
- Emphasis in Machine Learning.

Iowa State University **Ames, IA**
Bachelor of Science in Chemical Engineering **December 2019**
- Graduated *summa cum laude*.
- Minor in Computer Science.

Professional Experience

Entalpic AI **Paris, France**
Machine Learning Scientist for Chemistry **March 2025 - Present**
- Leading the development of the active learning workflow for accelerating the discovery of novel materials, including building the initial codebase from scratch.
- Building production scale pipelines on AWS for ML inference, training, and quantum chemistry calculations.
- Orchestrating the flow of millions of datapoints to continuously train new generative and predictive models.
- Guiding junior researchers in scientific investigations into improvements of our models and algorithms.

Meta AI **San Francisco, CA**
Research Scientist Intern **May 2023 - October 2023**
- Benchmarked uncertainty prediction methods for use in the Open Catalyst Demo.
- Implemented transformer sequence models, mean-variance estimation, 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 **South San Francisco, CA**
Process Development Intern **May 2019 - August 2019**
- Evaluated a process camera for automating single-use bioreactors in a pilot plant environment.
- Implemented a computer vision tool to analyze images of the cell culture and control the process in real time, saving an estimated 10 operator hours per week.

Ph.D. Research Experience

Carnegie Mellon University **Pittsburgh, PA**
Ph.D. Researcher **November 2020 – February 2025**
- Investigated active learning, transfer learning, and uncertainty quantification methods for graph neural network models in computational catalysis.
- Collaborated with researchers at Meta AI on the Open Catalyst Project to improve training methods 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% over competing algorithms.
- Implemented transition state finding methods which converge 3 times more often than previous state of the art.
- Developed hessian estimations and other property prediction techniques for machine learned force fields.
- Responsible for maintenance and troubleshooting of the Ulissi Group Kubernetes compute cluster.

Skills

Programming Languages and Libraries
- Machine learning libraries, particularly PyTorch and Scikit-learn.
- Python and its scientific computing and data science stack, including NumPy, SciPy, Pandas, etc.
- Atomistic simulation libraries, particularly using codes such as VASP, ASE, and Pymatgen.

Computing Tools
- Git for version control and collaboration, and Github Actions for continuous integration testing.
- Distributed HPC and cloud computing, using tools such as AWS, GCP, Kubernetes, and Slurm.
- Orchestration tools such as Apache Airflow and Jobflow interfacing with MongoDB and SQLite.

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; The Journal of Physical Chemistry C, Feb. 2025.
- *Improved Uncertainty Estimation of Graph Neural Network Potentials Using Engineered Latent Space Distances.* **J. Musielewicz**, J. Lan, M. Uyttendaele J. Kitchin; The Journal of Physical Chemistry C, Nov. 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

- *Improving Uncertainty Estimation Based on Latent Space Distance for Graph Neural Network Potentials.* **J. Musielewicz**, John Kitchin; Talk presented at AIChE annual meeting; Oct. 2024.
- *Predictive Uncertainty Quantification for Graph Neural Network Driven Relaxed Energy Calculations.* **J. Musielewicz**, J. Lan, and M. Uyttendaele; Poster presented at NeurIPS 2023 AI4Science Workshop; Dec. 2023.
- *Finetuna: Fine-Tuning accelerated molecular simulations.* **J. Musielewicz**, X. Wang, T. Tian, and Z. Ulissi; Talk presented at AIChE annual meeting; Nov. 2022.
- *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 — **Pittsburgh, PA**
Undergraduate Research Mentor — **May 2022 - August 2022**

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

Carnegie Mellon University — **Pittsburgh, PA**
Teaching Assistant — **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 — **Ames, IA**
Process Team Leader — **August 2018 - May 2019**

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

ISU Chem-E-Car — **Ames, IA**
Nationals Team Leader — **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 — **Ames, IA**
Undergraduate Researcher — **September 2016 - May 2019**

- Automated data collection by 3D printing robots and programming custom controllers.
- Designed and built high-throughput fluorometers for carbon nanotube biosensors in enzyme assays.
- Coauthored two published papers regarding carbon nanotubes for enzyme characterization.