JOSEPH MUSIELEWICZ

Personal Website: https://jmusiel.github.io/ | Github: https://github.com/jmusiel

Education

Carnegie Mellon University **Expected May 2025**

Ph.D. candidate in Chemical Engineering

Iowa State University **December 2019**

Bachelor of Science in Chemical Engineering, *summa cum laude*

Minor in Computer Science

Presentations and Publications

Publications

- **J. Musielewicz**, X. Wang, T. Tian, and Z. Ulissi, "Finetuna: Fine-tuning accelerated molecular simulations" Machine Learning: Science and Technology, Sep. 2022.
- Y. Hu, **J. Musielewicz**, and Z. Ulissi, and A. Medford, "Robust and scalable uncertainty estimation with conformal prediction for machine-learned interatomic potentials" ArXiv, Aug. 2022.
- N. Kallmyer, T. Huynh, J. Graves, **J. Musielewicz**, D. Tamiev, and N. F. Reuel "Influence of sonication conditions and wrapping type on yield and fluorescent quality of noncovalently functionalized single-walled carbon nanotubes" Carbon, vol.139, pp. 609-613, Nov. 2018.
- N. Kallmyer, **J. Musielewicz**, J. Sutter, and N. Reuel "Substrate-Wrapped, Single-Walled Carbon Nanotube Probes for Hydrolytic Enzyme Characterization" Analytical Chemistry, vol. 90 (8), pp. 5209-5216, Mar. 2018.

Presentations

- **J. Musielewicz**, Z. Ulissi. "Accelerating Geometric Optimizations by Finetuning Open Catalyst Project Models with Active Learning." Talk presented at 27th North American Catalysis Society Meeting; May 2022; New York City, NY.
- **J. Musielewicz**, Z. Ulissi. "Accelerating on-the-Fly Active Learning of Catalyst Simulations Using Large Scale Pretrained Models." Poster presented at AIChE annual meeting; November 2021; Boston, MA.

Research Experience

PhD Researcher in Computational Catalysis November 2020 - Present

Ulissi Group, CMU Chemical Engineering *Pittsburgh, PA*

- Principal developer and maintainer of the *Finetuna* Python package, implementing active machine learning methods for accelerating atomistic simulations. G*ithub repository: https://github.com/ulissigroup/finetuna*
- Develop and test novel implementations of machine learning potentials for molecular simulations, especially transfer learning techniques for graph neural networks in very low data regimes.
- Collaborate with other researchers in the Open Catalyst Project at Facebook AI Research to improve methods for dataset generation and uncertainty quantification of machine learning potentials.
- Responsible for maintenance and troubleshooting of the Kubernetes-enabled Ulissi Group computer cluster.
- Implement unit tests and a continuous integration pipeline for the *Finetuna* Python package.

Undergraduate Researcher September 2016 - May 2019

Reuel Group, ISU Chemical Engineering *Ames, IA*

- Built and programmed high-throughput instruments to measure carbon nanotube biosensors in biochemical assays.
- Wrote Python scripts for data collection and analysis used on Raspberry Pis throughout the lab.
- Coauthored two published papers regarding carbon nanotube biosensors.

Professional Experience

Process Development Engineering Intern May 2019 - August 2019

Genentech *South San Francisco, CA*

- Evaluated automation applications of a process camera for single-use bioreactors in a pilot plant environment.
- Designed experiments to prove camera compatibility with the cell culture process and allowed it to be implemented.
- Implemented computer vision methods to analyze images from the camera in real time to control the process.

Process Development Engineering Co-op January 2018 - August 2018

Hutchinson Technology *Hutchinson, MN*

- 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.
- Identified consistency problems and coordinated with engineers to improve maintenance of etchant composition.

Leadership Experience

Teaching Assistant August 2020 - December 2021

Thermodynamics, Process Control, Mathematical Modeling in Chemical Engineering *Pittsburgh, PA*

- Prepared homework problems and led weekly help sessions for undergraduate students.

Deep Space Carbon Scrubber Process Team Leader August 2018 - May 2019

NASA X-Hab 2019 Academic Innovation Challenge *Ames, IA*

- Led a team in an interdisciplinary effort to design a working prototype 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 June 2017 - November 2018

ISU Chem-E-Car *Ames, IA*

- Led a team of engineers in designing and building a chemically powered car for a precision-distance competition.

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.