Matthew Adams
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EDUCATION

Carnegie Mellon University Pittsburgh, PA
Master of Science in Chemical Engineering **Dec 2020**

University of Tennessee, Knoxville Knoxville, TN
Bachelor of Science in Chemical Engineering **May 2019**

RESEARCH EXPERIENCE

Carnegie Mellon University **Nov 2019 – Dec 2020**
Graduate Research Assistant (Advisor: Dr. Zachary Ulissi)

- Performed in-depth analysis of composition effects on catalyst surface performance with DFT (Density-Functional Theory) calculations to reduce the required search space for computational catalyst screening by 70%
- Designed a flexible framework for active learning with machine learning potentials leading to a reduction of 50% in the number of required DFT calculations while maintaining accurate results
- Collaborated in improvement of projects through implementation of continuous integration to improve code structure and reduce errors by 80%

University of Tennessee, Knoxville **May 2017 – May 2019**
Undergraduate Research Assistant (Advisor: Dr. Siris O. Laursen)

- Performed analysis of DFT calculations on atomic systems to gain additional insight into the relationship between surface Nickel concentration and Hydrogen selectivity
- Presented findings at multiple conferences and received both an Award of Merit and Bronze Award
- Trained undergraduate students in gas flow reactor operations and catalyst performance analysis resulting in increased group research productivity

INTERNSHIP EXPERIENCE

Oak Ridge National Laboratory **June 2019 – Aug 2019**
Science Undergraduate Laboratory Internship (Advisor: Dr. Stephan Irle)

- Constructed a unique framework through combining density functional tight binding with metadynamics which accelerated scanning of the free energy profile of a system by a factor of 1000
- Collected and analyzed data of particle size and temperature effects to further improve the understanding of nanoparticle formation in material development
- Implemented neural-network assisted molecular dynamics simulations to reduce the error against DFT below 1.0 kcal/mol

ACADEMIC PROJECTS

For additional projects and source code, visit https://mattaadams.github.io/

Using Machine-Learning to Predict Adsorbate Binding Energies of Active Sites **Spring 2020**
Data Science in Chemical Engineering – Carnegie Mellon University

- Developed a program capable of automatically generating atomistic structures using user-specified elements reducing required manual entry time by 90%
- Constructed and trained a model capable of predicting binding energies with an average error of 0.05 eV

Using Machine-Learning Methods to Identify Twitter Bots **Fall 2019**
Artificial Intelligence and Machine Learning for Engineers – Carnegie Mellon University

- Utilized Twitter's API to collect and cleanse data into a readable format across thousands of individual accounts
- Investigated feature importance and implemented algorithms to obtain an overall accuracy of 85% for bot detection

SKILLS

Software: Excel, Git, Ubuntu, Tableau, MongoDB, Docker, AWS, CI/CD, MATLAB
Programming: Python, PyTorch, OpenCV, Bash, SQL