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 statistical 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%
- Created a feature engineering pipeline that processed and transformed raw data into feature vectors improving model performance.
- Designed a flexible framework for active learning with Deep Learning Neural-Network potentials leading to a reduction of 55% 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%
- Manipulated large dataframes containing atomic structure information with MongoDB database in Python (PyMongo)

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
- Organized experimental datasets through Excel spreadsheets for data analysis and visualization.
- 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 10%.
- Ran Python Jupyter notebook experiments for neural network hyperparameter optimization.

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 less than 10%
- Analyzed and visualized data trends in active site binding energies through Python.

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

- Performed Exploratory Data Analysis and interpreted previous results from previous scientific publications focused on methods for bot detection.
- Utilized Twitter's API to extract and clean data into a readable format across thousands of individual accounts
- Investigated feature importance and implemented machine learning algorithms to obtain an overall accuracy of 85% for bot detection and classification.

SKILLS

Software: Excel, GitHub, Linux, Tableau, MongoDB, Docker, AWS, CI/CD, Kubeflow
Programming: Python, PyTorch, Flask, OpenCV, JavaScript, Bash, SQL, Matlab