

## EDUCATION

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**Carnegie Mellon University**

*Master of Science in Chemical Engineering*

Pittsburgh, PA

*Dec. 2020*

**University of Tennessee, Knoxville**

*Bachelor of Science in Chemical Engineering*

Knoxville, TN

*May 2019*

## EXPERIENCE

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**U.S. Environmental Protection Agency**

*Data Modeling Specialist (Contractor)*

Durham, NC

*Dec 2021 - Present*

- Transformed a chemical fingerprinting method into a more universal format to allow for expanded applications in toxicology predictions of target chemical substances
- Performed in-depth pairwise comparison analysis across different chemical fingerprint sets to identify differences in information captured across chemical spaces.
- Analyzed the effect of chemical fingerprints on the performance of Generalized Read Across's (GenRA) predictive ability of chemical toxicity properties

**Carnegie Mellon University**

*Graduate Research Assistant*

Pittsburgh, PA

*Aug 2019 - Dec 2020*

- Performed in-depth statistical analysis of composition effects on catalyst surface performance with computational calculations to reduce the required search space for screening by 70%
- Designed a flexible framework with PyTorch for active learning with Deep Learning Neural-Network potentials leading to a reduction of 60% in computational time while maintaining accurate results
- Manipulated large dataframes containing atomic structure information with MongoDB database in Python
- Collaborated in improvement of projects through implementation of continuous integration to improve code structure and reduce errors

**Oak Ridge National Laboratory**

*Research Intern*

Oak Ridge, TN

*June 2019 - Aug 2019*

- 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
- Implemented neural-network assisted molecular dynamics simulations to reduce the error below 10%.
- Ran Python Jupyter notebook experiments for neural network hyper-parameter optimization.

## PROJECTS

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

**Q-Wall Game | Python**

- Developed a Deep Q-Learning agent in TensorFlow capable of accurate navigation inside a game environment

**Twitter Bot Detection | Python**

- Utilized Twitter's API to extract and clean data into a readable format across thousands of individual accounts
- Implemented machine learning algorithms to obtain an overall accuracy of 85% for bot detection and classification.

**Atomic Binding Energy Predictions | Python**

- Performed Feature Engineering on molecular structures to enable predictions for chemical properties
- Constructed and trained a model capable of predicting binding energies with an average error of less than 10%

## SKILLS

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- **Languages:** Python, JavaScript, SQL, CSS/HTML, Shell
- **Frameworks:** PyTorch, TensorFlow, Flask, NodeJS
- **Technologies:** Docker, Kubernetes, MongoDB, Git, CircleCI, VSCode