

GRADUATE STUDENT RESEARCHER

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Dedicated researcher pivoting from chemical engineering to computer science

Education

Carnegie Mellon University

Pittsburgh, PA

M.S. IN CHEMICAL ENGINEERING, GPA: 3.91

Sep. 2019 - Dec. 2020

• Competed in several hackathons including the Covestro Hackathon, Hack the Northeast, and the Pitt Challenge.

West Virginia University

Morgantown, WV

B.S. IN CHEMICAL ENGINEERING, CUM LAUDE

Sep. 2016 - Aug. 2019

• Graduated with Presidential Honors from the WVU Honors college.

Publications

Demystifying the Chemical Ordering of Multimetallic Nanoparticles $[\mathscr{O}]$

Sep. 2022

ACCOUNTS OF CHEMICAL RESEARCH (UNDER REVIEW)

- Developed a novel method for calculating the cohesive energy of a bimetallic nanoparticle that overcomes major weaknesses in previous models. On the systems we investigated, our method led to a 71% reduction in the RMSE compared to the original.
- Generalized this method to be applicable to any number of metals (multimetallic nanoparticles). GitHub <u>link</u>

Size-dependent shape distributions of platinum nanoparticles [\mathscr{E}]

Aug. 2022

VANOSCALE ADVANCES

- · Used Boltzmann statistics to support experimental findings on nanoparticle shape and size distributions.
- · Selected for the 2022 Popular Advances collection which includes articles which have been very well received by the community.

Resolving Electrocatalytic Imprecision in Atomically Precise Metal Nanoclusters $[\mathscr{O}]$

Nov 2021

CURRENT OPINIONS IN CHEMICAL ENGINEERING

- Electrocatalysis applications of ligand-protected nanoclusters.
- Prospective section on current and possible future applications of machine learning in the field.

Research Experience

Computer-Aided Nano and Energy Lab (CANELa)

University of Pittsburgh

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June 2021 - PRESENT

- · Developed a novel method for calculating cohesive energies of metal nanoparticles that led to a 71% improvement to the previous model.
- Applied quantum/statistical mechanics through Density Functional Theory, Boltzmann statistics, and mixed integer optimization using the genetic algorithm to better understand structure property relationships of metal nanoparticles.
- Organized and presented in several machine learning and software development meetings within the CANELa research group. Notable presentations include: version control using git/GitHub, an introduction to PyTorch and logistic regression, and developing custom Python packages.
- Mentored members of the group (grad and undergrad) about public [𝓔] and private code I have developed, ML fundamentals, building models
 with PyTorch, and evaluating ML results.

The Kitchin GroupCarnegie Mellon University

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Dec 2019 - Dec 2020

- Recreated image analysis tools in Python (originally in Mathematica) to be interactive, fast, and intuitive.
- · Trained and deployed a convolutional neural network classifier to extract valuable information from experimental image data.
- Developed a Python package, nb_search [𝚱], to efficiently sort through, locate and open Jupyter Notebook files.
- Regressed parameters and used them to cluster different bimetallic catalysts.

Control, Optimization and Design for Energy and Sustainability (CODES)

West Virginia University

Undergraduate Researcher

Apr. 2017 - Aug. 2019

· Modeled, optimized, and economically evaluated a chemical process in MATLAB — Funded by the National Science Foundation.

Volunteering and Outreach

Fundraising, Organized a profit sharing event with Chipotle to raise funds for people suffering from the flooding in Pakistan

Leadership

Outreach, Organized outreach events with local public schools to help encourage students to consider STEM STEM Education, Volunteered at the Carnegie Science Center, where I conducted science experiments with

Leadership

and answered questions from elementary students

Volunteering

Work Experience __

KEF RoboticsPittsburgh, PA

COMPUTER VISION ENGINEER Jan. 2023 - Start of Ph.D.

· Responsibilities will include: conducting literature reviews on computer vision topics and developing software for tethered drone autonomy.

AithELITEPittsburgh, PA

DATA SCIENTIST/SOFTWARE ENGINEER

- Dec. 2020 May. 2021
- · Developed web scraping scripts using Beautifulsoup and Selenium to automate data retrieval and updating.
- Developed and automated the feature engineering with Numpy and Pandas.
- · Applied machine learning algorithms using Numpy and SkLearn to generate intelligent predictions and insights from the data.
- Built and maintained relational (MySQL) and graph (Neo4J) databases, hosted on AWS.
- Built the frontend and backend of the AithELITE EliteAl website with Django, hosted on AWS.

Projects

SkinsAl $[\mathscr{S}]$ Pitt Challenge Hackathon

COMPUTER VISION, DEEP LEARNING

- Developed a free-access, diagnosis tool for classifying moles as benign or malignant.
- Classification model was a small convolutional neural network built with PyTorch and website was built with Django web-framework and deployed with Heroku.

Question Answering Model [\mathscr{O}]

CMU Course

NATURAL LANGUAGE PROCESSING

Developed models using SpaCy that can generate questions from a provided text and also find answers to questions about a given text.

Disparity Map Generation [\mathscr{D}]

CMU Course

COMPUTER VISION, DEEP LEARNING

- Modified the PSMnet architecture for disparity map generation to be used for 3D object detection.
- Implemented asymmetric convolutions and redesigned the SPP module of the PSMNet using residual blocks.
- Modifications led to a 53.65% reduction in parameters and a higher 3-pixel accuracy on I.R. images.

Speech to Text Transcription [\mathscr{O}]

CMU Course

DEEP LEARNING

Implemented a combination of recurrent neural networks (more specifically BLSTMs) and dense networks for speech to text transcription.

American Sign Language (ASL) Active Learning $[\mathscr{O}]$

Personal Project

COMPUTER VISION, DEEP LEARNING

• Developed a GUI that uses machine learning techniques such as a vanilla convolutional neural network classifier and YOLOv3 object detection to tell a user if they have correctly signed a letter in American sign language.

Honors & Awards & Activities

University of Pittsburgh

2022	2nd Flace, The Fitt Chatteringe, built Skinshi which was awarded 2nd place over all (\$2,000 cash phize) out of	Pittsburgh, PA
2022	24 teams from Pittsburgh universities, including CMU	rittsburgii, rA
2022	GSA President , Elected President of the Chemical Engineering Graduate Student Association	Pittsburgh, PA

2nd Place. The Pitt Challenge, built Skins Al which was awarded 2nd place everall (\$2,000 cash prize) out of

CARNEGIE MELLON UNIVERSITY

2020	3rd Place , Chemical Engineering Masters Student Association Research Forum, Poster Competition	Pittsburgh, PA
2020	Category Winner, The Pitt Challenge, "Largest Impact on Healthcare Workers" Category	Pittsburgh, PA

WEST VIRGINIA UNIVERSITY

2019	1st Place, AVEVA's National Simulation Competition (Advanced Category)	Morgantown, WV
2019	Vice President, American Institute of Chemical Engineers (WVU Chapter)	Morgantown, WV
2018	2nd Place , Computing and Process Control Division at the National 2018 AIChE Poster Presentations	Morgantown, WV
2018	Member, Omega Chi Epsilon Chemical Engineering Honor Society	Morgantown, WV

Relevant Courses

2021	Natural Language Processing, Carnegie Mellon University (cross-registration), Graduate	Pittsburgh, PA
2020	Introduction to Deep Learning, Carnegie Mellon University, Graduate	Pittsburgh, PA
2020	Introduction to Machine Learning, Carnegie Mellon University, Graduate	Pittsburgh, PA
2019	Linear Optimization (supply chain focused), Carnegie Mellon University, Graduate	Pittsburgh, PA
2017	Numerical Methods and Optimization, West Virginia University, Undergraduate	Morgantown, WV

DECEMBER 2, 2022 DENNIS J. LOEVLIE · CURRICULUM VITAE