

# Kareem Abdelmaqsoud

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## INTERESTS

AI for Science, Material Discovery, Deep Learning, Machine Learning, Graph Neural Networks, Knowledge Distillation, Transfer Learning, Density Functional Theory, and Workflow Automation

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## EDUCATION

### Carnegie Mellon University

PhD in Chemical Engineering

Research Advisors: John R. Kitchin & Andrew J. Gellman

Selected Coursework: Data science & ML – Creating Scientific Software – Deep learning

Pittsburgh, PA

Aug 2022 – Dec 2026 (Expected)

### University of Rochester

Bachelor of Science - Chemical Engineering

Research Advisor: Andrew D. White

Selected Coursework: ML for Molecules and Materials – Organic Chemistry – Thermodynamics

Rochester, NY

Aug 2018 - May 2022

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## INDUSTRY EXPERIENCE

### Entos AI (Iambic Therapeutics)

ML Researcher for Drug Discovery

San Diego, California (Remote)

Jan 2022 – July 2022

- Optimizing pretraining and downstream models used for screening by the chemistry and biology teams.
- Implementing new modeling methods from literature and evaluating them on the company internal benchmarks.

### LafargeHolcim

Chemical Process Engineering Intern

- Designed a waste heat recovery system that could reduce the energy need for the plant by 3%.

Cairo, Egypt

July-August 2019

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## CURRENT RESEARCH PROJECTS

### Computational Design of Rare-earth Metal Alloys

Carnegie Mellon University

Aug 2023 – current

- Build a workflow for constructing phase diagrams for rare-earth alloys using Density Functional Theory (DFT), Machine Learning Potentials and CALculation of PHase Diagrams (CALPHAD) models
- Calculate elastic and thermal properties of stable alloy phases to design experiments done by collaborators

### Using Knowledge Distillation to improve the performance of Machine Learning Potentials

Carnegie Mellon University

Aug 2022 – Aug 2023

- Implemented knowledge distillation from a large machine learning model to a smaller model with fewer number of parameters
  - Showed that knowledge distillation improves the accuracy of the small model compared to regular training
  - Currently exploring the effect of choosing different features to distill from on the distillation performance.
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## PUBLICATIONS

### Investigating the error imbalance of large-scale machine learning potentials in catalysis

K Abdelmaqsoud, M Shuaibi, A Kolluru, R Cheula, and J Kitchin

Catalysis Science & Technology, Royal Society of Chemistry

### Structure Sensitive Reaction Kinetics of Chiral Molecules on Intrinsically Chiral Surfaces

K Abdelmaqsoud, M Radetic, C Fernandez-Caban, M Widom, J Kitchin, and A Gellman

The Journal of Physical Chemistry C, American Chemical Society

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## PROFESSIONAL ACTIVITIES & LEADERSHIP

**Education Chair**, Muslim Student Association – Carnegie Mellon University

Jan 2023 – Current

### Teaching assistantship

- Data science & ML
- Introduction of Chemical Engineering lab
- Chemical Reaction Engineering
- Mathematical modeling of chemical engineering

Spring 2024  
Fall 2023  
Spring 2023  
Fall 2022

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## SELECTED ENGINEERING & BUSINESS PROJECTS

### TEDI-London summer school

**Virtual**

Team leader

June-July 2020

- Lead a multinational team designing a mobile application and a device to help people living with dementia.
- The project was ranked the 4th out of 16 teams participating from all over the world.
- Gained the ability to a team of members with different nationalities and different academic backgrounds.

### EZ water Startup

**Rochester, NY**

Team leader & researcher

March 2019- March 2020

- The team built a franchise business model and obtained a license for a novel nanofiber membrane filter. The goal was to provide clean water for people living in Pakistan.
- Was selected to represent the US National Academy of Engineering in the Global Grand Challenge Summit in London, September 2019.
- Raised funds to install 10 water projects that will provide free clean water for over 2,000 people living in the remotest villages in Pakistan over the next 10-15 years.

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## SKILLS

**Programming:** Python

**Frameworks:** Kubernetes, AWS, git

**Deep Learning & Data science:** PyTorch, PyTorch Geometric, Tensorflow, Numpy, Pandas, Scikitlearn

**Packages:** ASE, VASP

**Laboratory skills:**

- Experience with laboratory equipment including Hydrogen fuel cells, heat exchangers and packed-bed reactors.
- Basic and organic chemistry laboratory techniques, including NMR/IR/UV-VIS spectroscopy, gas and thin-layer chromatography, and crystallization.

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## HONORS & AWARDS

- 1<sup>st</sup> Place Award in the Undergraduate Poster Competition at the AIChE conference, Boston, MA.
- Research & Innovation Grant Recipient for my undergraduate research.
- University of Rochester Senior Honoring society
- Tau Beta Pi Engineering Honor Society.
- University of Rochester Dean's List All Semesters.