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

EDUCATION

Carnegie Mellon University — Pittsburgh, PA
PhD in Chemical Engineering — Aug 2022 – Dec 2026 (Expected)
Research Advisors: John R. Kitchin & Andrew J. Gellman
Selected Coursework: Data science & ML – Creating Scientific Software – Deep learning

University of Rochester — Rochester, NY
Bachelor of Science - Chemical Engineering — Aug 2018 - May 2022
Research Advisor: Andrew D. White
Selected Coursework: ML for Molecules and Materials – Organic Chemistry – Thermodynamics

INDUSTRY EXPERIENCE

Entos AI (Iambic Therapeutics) — **San Diego, California (Remote)**
ML Researcher for Drug Discovery — 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 — **Cairo, Egypt**
Chemical Process Engineering Intern — July-August 2019

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

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.

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

PROFESSIONAL ACTIVITIES & LEADERSHIP

Education Chair, Muslim Student Association – Carnegie Mellon University — Jan 2023 – Current

Teaching assistantship

- Data science & ML — Spring 2024
- Introduction of Chemical Engineering lab — Fall 2023
- Chemical Reaction Engineering — Spring 2023
- Mathematical modeling of chemical engineering — Fall 2022

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.

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.

HONORS & AWARDS

- 1st 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.