

Muhammed Shuaibi

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Interests Computational catalysis, climate change, graph neural networks, deep learning, active learning.

Experience **Facebook AI Research, Menlo Park (virtual)** May 2020 - Sep. 2020

Research Intern, Artificial Intelligence

With Larry Zitnick and Devi Parikh

- Worked on the Open Catalyst Dataset (OC20) - the largest catalyst dataset to enable broader machine learning applications to quantum chemistry and catalysis.
- Core developer in the OC20 repo, containing baseline models and trainers for the community to work from.
- Worked on graph neural networks to model quantum-mechanical atomistic simulations.

U.S. Environmental Protection Agency, Chicago

Jan. 2017 - Aug. 2018

Environmental Engineer

- Inspected industrial facilities to review records, conduct plant walk-throughs, analyze pollution control measures, and discuss process designs for emission points.
- Utilized 3D CAD and CFD software to model and simulate facility ventilation studies, determining capture efficiency and particulate matter emissions

Education **Carnegie Mellon University** 2018 - 2022

Ph.D. in Chemical Engineering

Research Areas: Catalysis, Computational Chemistry, Deep Learning, Graph Neural Networks, Active Learning

Illinois Institute of Technology

2013 - 2017

M.A.S in Chemical Engineering

B.Sc in Chemical Engineering

Publications * Co-First authors

[4] **ForceNet: A Graph Neural Network for Large-Scale Quantum Calculations**

W. Hu, M. Shuaibi, A. Das, S. Goyal, A. Sriram, J. Leskovec, D. Parikh, C. L. Zitnick
arXiv 2103.01436, 2021.

[3] **The Open Catalyst 2020 (OC20) Dataset and Community Challenges**

L. Chanussot*, A. Das*, S. Goyal*, T. Lavril*, M. Shuaibi*, M. Riviere, K. Tran,
J. Heras-Domingo, C. Ho, W. Hu, A. Palizhati, A. Sriram, B. Wood, J. Yoon, D. Parikh,
C. L. Zitnick, Z. Ulissi
arXiv 2010.09990, 2020.

[2] **An Introduction to Electrocatalyst Design using Machine Learning for Renewable Energy Storage**

C. L. Zitnick, L. Chanussot, A. Das, S. Goyal, J. Heras-Domingo, C. Ho, W. Hu, T. Lavril,
A. Palizhati, M. Riviere, M. Shuaibi, A. Sriram, K. Tran, B. Wood, J. Yoon, D. Parikh, Z. Ulissi
arXiv 2010.09435, 2020.

[1] **Enabling robust offline active learning for machine learning potentials using simple physics-based priors**

M. Shuaibi, S. Sivakumar, R. Q. Chen, Z. W. Ulissi

Machine Learning: Science and Technology, 2020.

Projects

Open Catalyst Project [opencatalystproject.org]

Facebook AI Research and Carnegie Mellon University

Nov. 2019 - Present

The development of renewable energy technologies has been limited by the availability of efficient and economical catalysts. To address this, I work closely with collaborators at Facebook AI to explore broader catalysis and machine learning applications. We developed the Open Catalyst Dataset (OC20) to enable the development of accurate machine learning models for large-scale atomistic simulations and catalyst screening. I am a core developer of the corresponding repository, which includes baseline models, data loaders, evaluators and tools necessary to run ML-based atomistic simulations. Additionally, we will host various challenges to encourage participation from the ML/catalysis communities. Future efforts will focus on new model development and, if successful, large-scale catalyst screening.

Code: [github.com/Open-Catalyst-Project/ocp]

Active Learning Atomistic Simulations

Carnegie Mellon University

Aug. 2019 - Present

Developing active learning frameworks to improve the quality of a machine learning model over the course of a dynamic molecular simulation, minimizing the number of highly expensive quantum mechanical calculations necessary.

AMPtorch: Atomistic Machine-learning Package - PyTorch

Carnegie Mellon University

Aug. 2018 - Present

Main developer of *AMPtorch*, an open-source software package that aims to provide researchers with the tools to carry out machine-learning applications to molecular systems.

Code: [github.com/ulissigroup/amptorch]

Physics-coupled Machine Learning Models

Carnegie Mellon University

Aug. 2019 - May. 2020

Developed a hybrid physics-based and machine-learning model to enable for more accurate predictions of molecular simulations, improving the predictive ability of machine-learning frameworks.

Hydroponics Technology Solutions to Enable Improved Nutrition

Illinois Institute of Technology

Jan. 2016 - Sep. 2016

Contributed to the design and development of a pilot scale, three-phase reactor to accelerate the growth of microgreens. Design and constructed an apparatus to promote uniform air distribution. Awarded for technological and social innovation among hundreds of other projects.

Skills

Software: Python, PyTorch, Git, CI/CD, Linux, High Performance Computing, MATLAB,

Modeling: Aspen HYSYS/Plus, CFD, CAD

Languages: English and Arabic

Awards &
Recognition

Camras Scholar, Illinois Institute of Technology (top 1% awarded)

2013-17

Faculty Choice Award: Academic Excellence, Illinois Institute of Technology

2013-17

Dean's List, Illinois Institute of Technology

2013-17