

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) <i>Research Intern, Artificial Intelligence</i> <i>With Larry Zitnick</i>	May 2021 - Present
	<ul style="list-style-type: none">• Working on physically inspired graph neural networks to model quantum-mechanical atomistic simulations.• Organizing the Open Catalyst Challenge, hosted at NeurIPS 2021.	
	Facebook AI Research, Menlo Park (virtual) <i>Research Intern, Artificial Intelligence</i> <i>With Larry Zitnick and Devi Parikh</i>	May 2020 - Sep. 2020
	<ul style="list-style-type: none">• 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 <i>Environmental Engineer</i>	Jan. 2017 - Aug. 2018
	<ul style="list-style-type: none">• Inspected industrial facilities to review records, conduct plant walkthroughs, 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 <i>Ph.D. in Chemical Engineering</i> Research Areas: Catalysis, Computational Chemistry, Deep Learning, Graph Neural Networks, Active Learning	2018 - 2022
	Illinois Institute of Technology <i>M.A.S in Chemical Engineering</i> <i>B.Sc in Chemical Engineering</i>	2013 - 2017
Publications	<p>* Co-First authors</p> <p>[5] 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 <i>ACS Catalysis</i>, 2021.</p> <p>[4] Rotation Invariant Graph Neural Networks using Spin Convolutions M. Shuaibi, A. Kolluru, A. Das, A. Grover, A. Sriram, Z. Ulissi, C. L. Zitnick <i>arXiv 2106.09575</i>, 2021.</p>	

- [3] **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.
- [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. Current efforts include new model development, pipelines for high-throughput catalyst screening, and organizing community challenges.

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]

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