

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 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 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 <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>[3] The Open Catalyst 2020 (OC20) Dataset and Community Challenges L. Chanussot*, A. Das*, S. Goyal*, T. Lavril*, M. Shuaibi*, M. Riviere, J. Heras-Domingo, W. Hu, A. Palizhati, A. Sriram, J. Yoon, D. Parikh, C. L. Zitnick, Z. Ulissi <i>in prep to American Chemical Society Catalysis, 2020.</i></p> <p>[2] An Introduction to Electrocatalyst Design using Machine Learning for Renewable Energy Storage C. L. Zitnick, L. Chanussot, A. Das, S. Goya, J. Heras-Domingo, C. Ho, W. Hu, T. Lavril, A. Palizhati, M. Rivière, M. Shuaibi, A. Sriram, K. Tran, B. Wood, J. Yoon, D. Parikh, Z. Ulissi <i>arXiv preprint, 2020.</i></p> <p>[0] Enabling robust offline active learning for machine learning potentials using simple physics-based priors M. Shuaibi, S. Sivakumar, R. Q. Chen, Z. W. Ulissi <i>arXiv preprint arXiv:2008.10773; under review Machine Learning Science & Technology, 2020.</i></p>	

Projects	Open Catalyst Project [opencatalystproject.org] <i>Facebook AI Research and Carnegie Mellon University</i> 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 <i>Carnegie Mellon University</i> 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 <i>Carnegie Mellon University</i> Aug. 2018 - Present Main developer of <i>AMPTorch</i> , 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 <i>Carnegie Mellon University</i> 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 <i>Illinois Institute of Technology</i> 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