Muhammed Shuaibi

1 Bayard Rd
Pittsburgh, PA 15213

e-mail: mshuaibi@andrew.cmu.edu
website: mshuaibii.github.io

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, Artifical 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. Envriomental 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

[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
in prep to American Chemical Society Catalysis, 2020.

[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
arXiv preprint, 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
arXiv preprint arXiv:2008.10773; under review Machine Learning Science & 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 Perofrmance 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