Muhammed Shuaibi

San Francisco, CA

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Interests

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

Position

Fundamental AI Research (FAIR), Meta AI 2022 - Present
Research Engineer
Open Catalyst Project

Experience

Facebook AI Research, Menlo Park (virtual) Summer 2021
Research Intern, Artificial Intelligence
With Larry Zitnick

- Worked on physically inspired graph neural networks to model quantum-mechanical atomistic simulations.

Facebook AI Research, Menlo Park (virtual) Summer 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.

U.S. Environmental Protection Agency, Chicago Jan. 2017 - Aug. 2018
Environmental Engineer

Education

Carnegie Mellon University 2018 - 2022
Ph.D. in Chemical Engineering; Zachary Ulissi
Thesis: Generalizable Machine Learning Models for Electrocatalyst Discovery
Research Areas: Catalysis, Computational Chemistry, 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

[11] **AdsorbML: Accelerating Adsorption Energy Calculations with Machine Learning**
J. Lan*, A. Palizhati*, M. Shuaibi*, B. M. Wood*, B. Wander, A. Das, M. Uyttendaele, C. L. Zitnick, Z. W. Ulissi
arXiv 2211.16486, 2022.

[10] **Spherical Channels for Modeling Atomic Interactions**
C. L. Zitnick, A. Das, A. Kolluru, J. Lan, M. Shuaibi, A. Sriram, Z. Ulissi, B. Wood
arXiv 2206.14331, 2022.

[9] **The open catalyst 2022 (OC22) dataset and challenges for oxide electrocatalysis**
R. Tran*, J. Lan*, M. Shuaibi*, S. Goyal*, B. M. Wood*, A. Das, J. Heras-Domingo, A. Kolluru, A. Rizvi, N. Shoghi, *et al.*
ACS Catalysis, 2022.

[8] **Open Challenges in Developing Generalizable Large-Scale Machine-Learning Models for Catalyst Discovery**
A. Kolluru, M. Shuaibi, A. Palizhati, N. Shoghi, A. Das, B. Wood, C. L. Zitnick, J. R. Kitchin, Z. W. Ulissi
ACS Catalysis, 2022.

[7] **Transfer learning using attentions across atomic systems with graph neural networks (TAAG)**
A. Kolluru, N. Shoghi, M. Shuaibi, S. Goyal, A. Das, C. L. Zitnick, Z. Ulissi
The Journal of Chemical Physics, 2022.

[6] **GemNet-OC: developing graph neural networks for large and diverse molecular simulation datasets**
J. Gasteiger, M. Shuaibi, A. Sriram, S. Günnemann, Z. Ulissi, C. L. Zitnick, A. Das
Transactions on Machine Learning Research, 2022.

[5] **Rotation Invariant Graph Neural Networks using Spin Convolutions**
M. Shuaibi, A. Kolluru, A. Das, A. Grover, A. Sriram, Z. Ulissi, C. L. Zitnick
arXiv 2106.09575, 2021.

[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
ACS Catalysis, 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 - Aug. 2022
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 - Aug. 2022
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 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