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 2021 - Sep. 2021
Research Intern, Artificial Intelligence
With Larry Zitnick

- Worked on physically inspired graph neural networks to model quantum-mechanical atomistic simulations.
- Co-Organized the Open Catalyst Challenge, hosted at NeurIPS 2021.

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 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 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

[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
ACS Catalysis, 2021.

[4] **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.

[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 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