Adeesh Kolluru

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Interests. *AI for Science and Climate Change, Deep Learning, Graph Neural Networks, Multi-task Learning, Transfer Learning, Diffusion Models, LLMs, Molecular and Material Discovery, Density Functional Theory.*

Education

Carnegie Mellon University — Pittsburgh, PA
Ph.D. in Chemical Engineering — *Aug 2020 – December 2024 (Expected)*
Thesis: Deep Learning Frameworks for Atomic Simulation — *Advisors: John Kitchin, Zachary Ulissi*

Indian Institute of Technology (IIT) Delhi — Delhi, India
B.Tech in Chemical Engineering — *August 2016 – July 2020*
Thesis: Machine Learning for Bioprocess Control — *Advisor: Anurag Rathore*

Industry Experience

Machine Learning Research Intern — Boston, MA
Samsung Semiconductors — *May 2024 – August 2024*

- Working with *Eric Wang* in Advanced Materials Lab on discovering next-gen batteries and semiconductors.
- Combining LLMs and Diffusion models to significantly expand the known materials space.

Machine Learning Research Intern — London, UK (Remote)
Orbital Materials — *May 2023 – August 2023*

- Worked with the founding team; *Mark Neumann (Head of ML), Jonathan Godwin (CEO, Co-founder)*
- Worked on developing generative foundation model for material design in the application of porous materials.

Research Intern (AI) — Menlo Park, CA
Meta — *May 2022 – August 2022*

- Worked with *Brandon Wood, Larry Zitnick* from Open Catalyst Project team at FAIR, Meta AI.
- Worked on developing a foundation model that works across molecules, materials, and proteins; Paper, Web, Code
- Created graph neural network benchmark for Open Catalyst 2022 Dataset; Paper, Code
- Contributed to developing novel Graph Neural Network for atomic interaction; Paper, Code

Skills

Programming: Python, MATLAB, SQL; **Frameworks:** Kubernetes, AWS, GCP, Azure
Deep Learning: PyTorch, PyTorch Geometric, DGL, Jax, Tensorflow, Keras
Packages: ASE, VASP, Gromacs, Ansys, Fluent

Publications

*Google Scholar; 9 publications; Citations: 250+; h-index: 6; i10-index: 5, * represents equal contribution*

AdsorbDiff: Adsorbate Placement via Conditional Denoising Diffusion
***A Kolluru**, J Kitchin*
ICML 2024, ICML AI4Science Spotlight

From Molecules to Materials: Pre-training Large Generalizable Models for Atomic Property Prediction
*N Shoghi, **A Kolluru**, J Kitchin, ZW Ulissi, CL Zitnick, BM Wood*
ICLR 2024

Spherical Channels for Modeling Atomic Interactions
*CL Zitnick, A Das, **A Kolluru**, J Lan, M Shuaibi, A Sriram, ZW Ulissi, B Wood*
NeurIPS 2022

Transfer Learning using Attentions across Atomic Systems with Graph Neural Networks (TAAG)
***A Kolluru**, N Shoghi, M Shuaibi, S Goyal, A. Das, L. Zitnick, ZW Ulissi*
JCP 2022

Open Challenges in Developing Generalizable Large Scale Machine Learning Models for Catalyst Discovery
A Kolluru, M Shuaibi*, A Palizhati, N Shoghi, A Das, BM Wood, L Zitnick, JR Kitchin, ZW Ulissi*
ACS Catalysis 2022

The Open Catalyst 2022 (OC22) Dataset and Challenges for Oxide Electrocatalysis
R Tran, J Lan*, M Shuaibi*, BM Wood*, S Goyal*, A Das, J Heras-Domingo,* ***A Kolluru****, A Rizvi, N Shoghi, et al*
ACS Catalysis 2023

Materials cartography: A forward-looking perspective on materials representation and devising better maps
SB Torrisi, MZ Bazant, AE Cohen, MG Cho, JS Hummelshøj, L Hung, G Kamat, A Khajeh, ***A Kolluru****, X Lei, et al*
APL Machine Learning 2023

The Open Catalyst Challenge 2021: Competition Report
A Das, M Shuaibi, A Palizhati, S Goyal, A Grover, ***A Kolluru****, J Lan, A Rizvi, A Sriram, B Wood, et al*
NeurIPS 2021 Competitions and Demonstrations Track

Rotation Invariant Graph Neural Network using Spin Convolution
M Shuaibi, ***A Kolluru****, A Das, A Grover, A Sriram, Z Ulissi, CL Zitnick*
arXiv preprint arXiv:2106.09575

Fellowships, Awards & Recognitions

R.R Rothfus Graduate Fellowship from CMU

Phillips and Huang Family Fellowship in Energy from CMU College of Engineering

Merit Award for being in the **Top 7%** of Chemical Engineering batch of IIT Delhi

Distinctive Performance in Overall Activities from Chemical Engineering Society, IIT Delhi

Colors Award for being a promising sportsperson of IIT Delhi

KVPY Fellowship: Awarded by Govt. of India for being in the **Top 1%** in math and science across the country

National Science Talent Search Exam (NSTSE): Awarded gold medal, tablet for securing **All India Rank 1**

Projects

Generative AI for simulations

- Developed a diffusion model for rigid 3D simulation of molecules conditioned on energies to find global optima during adsorbate placement on a surface. Paper, Code

Foundation model development, multi-task learning and transfer learning

- Developed a novel transfer learning framework using attention framework across different layers of the model that gives improved results on out-of-domain molecular datasets. Paper, Code
- Worked on developing a foundation model using supervised multi-task pretraining and demonstrated state-of-the-art results on datasets across molecules, materials, and proteins Paper, Web, Code

Developing novel graph neural network architectures for representing atoms

- A novel approach to achieving rotation invariance in a graph neural network by incorporating a per-edge local coordinate frame and a novel spin convolution to effectively model angular information between sets of neighboring atoms in the network's edge messages. Paper, Code
- A graph neural network architecture, for modeling atomic energies and forces, leveraging atom embeddings represented by spherical functions (spherical channels) using spherical harmonics, and incorporating rotation of embeddings based on 3D edge orientation to enhance information utilization while preserving rotational equivariance of messages. Paper, Code
- Both models were state-of-the-art methods for predicting atomic energies and forces on large scale OC20 dataset.

Large scale dataset development and benchmarking

- Contributed to developing the Open Catalyst 2022 (OC22) dataset, consisting of 62,331 Density Functional Theory (DFT) relaxations (9M single point calculations) across a range of oxide materials, coverages, and adsorbates.
- We tested baseline performance of several graph neural networks; and provided predefined dataset splits to establish clear benchmarks for future efforts. Paper, Code

Professional Activities

Reviewing
NeurIPS 2022-24; Learning on Graphs 2022-24; ICML'24 AI4Science, ML4LMS

Talks
Transfer Learning with Large Scale GNNs across Molecular Datasets - AIChE 2021, TRI Workshop 2022
Open Challenges in developing generalizable ML models for material discovery - AIChE 2022

Teaching assistantship
Mathematical Methods of Chemical Engineering - Spring 2021, Spring 2022
Advanced Chemical Engineering Thermodynamics - Fall 2021

Organization
Learning on Graph Conference (LoG) 2024
Open Catalyst Challenge - NeurIPS 2021-23

Tutorials
Open Catalyst Project Tutorial - Climate Change with AI workshop - NeurIPS 2021-22

Extra-curricular Activities

- Served as Sports Secretary of the Board for Sports Activities, IIT Delhi
- Captained the Aquatics and Water polo team in Intra-College competitions of IIT Delhi
- Conducted various National debating tournaments as Representative of Debating Club, IIT Delhi
- Volunteered for Humanity Foundation that works for the welfare of visually impaired students