

# Adeesh KOLLURU

## PhD Student at Carnegie Mellon University

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🌐 Personal Website



**Interests :** Graph Neural Networks, Computational Catalysis

## 🎓 EDUCATION

2020-2025   *PhD in Chemical Engineering, Carnegie Mellon University*; Advisor : Zachary Ulissi  
2016-2020   *B. Tech in Chemical Engineering, Indian Institute of Technology Delhi*

## 💻 PROJECTS

### ROTATION INVARIANT GRAPH NEURAL NETWORK USING SPIN CONVOLUTION

*Carnegie Mellon University and Facebook AI Research*

- Worked on developing a novel Graph Neural Network that predicts energies and forces of molecules and catalyst systems.
- This model captures 3D complex angular features in a novel way and is rotationally invariant.
- Results are demonstrated on OC20, QM9, MD17 Datasets.

Graph Neural Networks

### ACCELERATING GEOMETRY OPTIMIZATION WITH GRAPH NEURAL NETWORKS

*Carnegie Mellon University and Facebook AI Research*

- Developed a baseline for direct prediction of optimized geometry with Graph Neural Networks
- Analyzed and showed relative importance of various important metrics across conventional and recent methods

Geometric Optimization

Graph Neural Networks

Catalysts

### TRANSFER LEARNING FOR CATALYTIC/MOLECULAR PREDICTIONS USING OC20

*Carnegie Mellon University*

- Conducted fine tuning experiments with pre-trained models on OC20 dataset to get close to 15% improvement in performance on other small scale catalyst as well as molecular databases.

Transfer Learning

Graph Neural Networks

Catalysts

Small Molecules

### DELTA LEARNING FOR LARGE SCALE CATALYST DATASET

DEC '20 - FEB '21

*Carnegie Mellon University*

- Calculated and compared results for delta learning methods with multiple tight binding potentials (xTB, DFTB) for OC20 dataset. Explored various referencing schemes for energy targets.

Machine Learning potentials

Delta Learning

Graph Neural Networks

### MACHINE LEARNING BASED CONTROL OF AERATION RATE FOR MAMMALIAN CELLS IN A BIOREACTOR

AUGUST 2019 - MAY 2020

*B.Tech Thesis, Indian Institute of Technology Delhi | Advisor : Prof. Anurag Rathore*

- Developed a machine learning based control model to optimize aeration rate for mammalian cell in a stirred tank reactor.
- It predicts Viable Cell Concentration (VCC) through a random forest model and the mass transfer coefficient from theoretical approach and combined them to determine the optimal aeration rate.

Machine Learning

Process Control

Reactor Modeling

## 🎓 FELLOWSHIPS, AWARDS & RECOGNITION

2020	Merit Award : For being in the Top 7% of Chemical Engineering batch of IIT Delhi
2018	Distinctive performance in Overall Activities from Chemical Engineering Society, IIT Delhi
2018	Colors Award : For being a promising sportsperson of IIT Delhi
2016	KVPY fellowship : Awarded by Govt. of India for being in the Top 1% in math and science across the country
2016	National Science Talent Search Exam (NSTSE) : Awarded Gold Medal, Tablet for securing All India Rank 1

## SKILLS

**Languages :** Python (PyTorch, PyTorch Geometric, DGL, TensorFlow, Keras), C++    **Software :** Ansys, Fluent, Matlab, Gromacs

## RELEVANT COURSEWORK

**ChemE :** Advanced Process Control, Molecular Modeling and Simulations, Advanced Chemical Engineering Thermodynamics

**CS & Math :** Linear Algebra, Probability & Statistics, Machine Learning, Advanced Machine Learning, Historical Advances in Machine Learning, Crafting Software

**Economics :** Microeconomics & Game Theory, Macroeconomics and Economic Policies

## PUBLICATIONS

### > Rotation Invariant Graph Neural Network using Spin Convolution

M.Shuaibi, A. Kolluru, A. Das, A. Grover, A. Sriram, Z. Ulissi, C.L. Zitnick

[Arxiv Link](#)

## PROFESSIONAL ACTIVITIES

### > Summer Schools Participation

London Geometry and Machine Learning Summer School 2021 [LOGML]

Machine Learning Summer School 2021 Taipei [MLSS]

### > Teaching Assistant

Advanced Chemical Engineering Thermodynamics - *Fall 2021*

Mathematical Methods of Chemical Engineering - *Spring 2021*

### > Challenge Organization

Open Catalyst Challenge - NeurIPS 2021 Competition Track [link]

### > Tutorial Organization

Open Catalyst Project - Climate Change with ML workshop, NeurIPS 2021

## EXTRACURRICULAR ACTIVITIES

### Leadership

- Served as Sports Secretary of the Board for Sports Activities, IIT Delhi
- Captained the Aquatics and Water polo team in Intra-College competitions
- Conducted various National debating tournaments as Representative of Debating Club, IIT Delhi

### Sports

- Represented IIT Delhi in Waterpolo and won Silver medal in 4x100 Medley Relay Aavhan Sports Meet 2018, IIT Bombay
- Won Best Waterpolo Player award twice consecutively in Intra-College competitions of IIT Delhi

### Cultural

- Breaking Adjudicator, Intra-IIT Parliamentary Debate'18    • Breaking Speaker, Intra-IIT Parliamentary Debate'19

### Voluntary work

- Mentored a group of students as a part of Student Mentorship Program
- Volunteered for Humanity Foundation that works for the welfare of visually impaired students