YUYANG WANG

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RESEARCH INTEREST

My research lies at the intersection of machine learning, molecular modeling, and drug discovery. I develop self-supervised learning (SSL) methods with graph neural networks (GNNs) and large language models (LLMs) to learn molecular representations that generalize on large chemical space.

EDUCATION

Carnegie Mellon University — Pittsburgh, PA
Ph.D. in Mechanical Engineering, College of Engineering — *May 2023 (Anticipated)*
› Advisor: Dr. Amir Barati Farimani
› Thesis Proposal: Self-supervised Representation Learning for Molecular Prediction and Analysis

Carnegie Mellon University — Pittsburgh, PA
M.S. in Machine Learning, School of Computer Science — *Dec. 2022 (Anticipated)*

Carnegie Mellon University — Pittsburgh, PA
M.S. in Mechanical Engineering, College of Engineering — *May 2019*

Tongji University — Shanghai, China
B.S. in Engineering Mechanics, School of Aerospace Engineering and Applied Mechanics — *July 2017*

BOOK CHAPTER

[1] Graph Neural Networks for Molecules
A chapter for book "Machine Learning in Molecular Sciences" as one volume in the series "Challenges and Advances in Computational Chemistry and Physics" to be published by Springer Nature.
Yuyang Wang, Zijie Li, Amir Barati Farimani

PUBLICATIONS

*equal contribution

[1] MOFormer: Self-Supervised Transformer model for Metal-Organic Framework Property Prediction
Under review of Journal of the American Chemical Society, 2022
Zhonglin Cao, Rishikesh Magar, ***Yuyang Wang***, Amir Barati Farimani

[2] TransPolymer: a Transformer-based Language Model for Polymer Property Predictions
Under review of npj Computational Materials, 2022
Changwen Xu, ***Yuyang Wang***, Amir Barati Farimani

[3] Predicting CO_2 Absorption in Ionic Liquids with Molecular Descriptors and Explainable Graph Neural Networks
Under review of ACS Sustainable Chemistry & Engineering, 2022
Yue Jian, ***Yuyang Wang***, Amir Barati Farimani

[4] Crystal Twins: Self-supervised Learning for Crystalline Material Property Prediction
npj Computational Materials, 2022
Rishikesh Magar, ***Yuyang Wang***, and Amir Barati Farimani

[5] Improving Molecular Contrastive Learning via Faulty Negative Mitigation and Decomposed Fragment Contrast
Journal of Chemical Information and Modeling, 2022
Yuyang Wang, Rishikesh Magar, Chen Liang, and Amir Barati Farimani

[6] Molecular Contrastive Learning of Representations via Graph Neural Networks
Nature Machine Intelligence, 2022
Yuyang Wang, Jianren Wang, Zhonglin Cao, Amir Barati Farimani

[7] AugLiChem: Data Augmentation Library of Chemical Structures for Machine Learning
Machine Learning: Science and Technology, 2022
Rishikesh Magar*, ***Yuyang Wang****, Cooper Lorsung*, Chen Liang, Hariharan Ramasubramanian, Peiyuan Li, Amir Barati Farimani

[8] Prediction of GPCR activity using Machine Learning
Computational and Structural Biotechnology Journal, 2022
Prakarsh Yadav, Parisa Mollaei, Zhonglin Cao, ***Yuyang Wang***, Amir Barati Farimani

[9] Efficient Water Desalination with Graphene Nanopores Obtained using Artificial Intelligence
npj 2D Materials Applications, 2021
Yuyang Wang*, Zhonglin Cao*, Amir Barati Farimani

[10] Deep Reinforcement Learning for Predicting Kinetic Pathways to Surface Reconstruction in a Ternary Alloy
Machine Learning: Science and Technology, 2021
Junwoong Yoon, Zhonglin Cao, Rajesh K. Raju, ***Yuyang Wang***, Robert Burnley, Andrew J. Gellman, Amir Barati Farimani, Zachary W. Ulissi

[11] Adversarially Robust Imitation Learning
In 5th Annual Conference on Robot Learning (CoRL), 2021
Jianren Wang, Ziwen Zhuang, ***Yuyang Wang***, Hang Zhao

[12] Learning Super-Resolution Electron Density Map of Proteins using 3D U-Net
Machine Learning for Structural Biology Workshop at NeurIPS, 2020
Baishali Mullick, ***Yuyang Wang***, Prakarsh Yadav, Amir Barati Farimani

EXPERIENCE

Momenta.ai Beijing, China
R&D Intern, Momenta Valet Parking Group *May 2018 - Aug 2018*
Implemented and improved deep reinforcement learning to valet car parking in simulation.

TALKS

Molecular Contrastive Learning of Representations via GNNs
Oral presentation, American Chemistry Society Fall 2022, Chicago, IL *Aug. 2022*
Webinar at Nvidia, Virtual *July 2022*
Guest Lecture, 24-789: Deep Learning for Engineers, Virtual *May 2021*

Efficient Graphene Nanopore Designed by AI for Water Desalination
Oral presentation, American Physical Society - DFD Annual Meeting, Virtual *Nov. 2020*

Introduction to Machine Learning and Reinforcement Learning for Precision Engineers
Tutorial, ASPE Spring Meeting (with Dr. Amir Barati Farimani), Virtual *May 2020*

MEDIA COVERAGE

Molecular Contrastive Learning of Representations via GNNs *Spring 2022*
Tech Xplore, *News Azi*, *DrugAI*

Efficient Water Desalination with Graphene Nanopores Obtained using AI *Fall 2021*
CMU College of Engineering, *Phys.org*

HONORS & REWARDS

Milton Shaw Ph.D. Research Award, Carnegie Mellon University *2022-23*
Best Posters Award at MechE Ph.D. Research Symposium, Carnegie Mellon University *2022*
Outstanding Undergraduate Student Scholarship (Top 10%), Tongji University *2014-16*

SKILLS

Programming	Python, C/C++, MATLAB
Packages	PyTorch, PyTorch Geometric, TensorFlow, PySpark, Scikit-learn, RDKit, MDTraj
Languages	English (proficient), Mandarin (native)

SELECTED COURSES

10-701 Introduction to Machine Learning
11-785 Introduction to Deep Learning
10-703 Deep Reinforcement Learning & Control
10-718 Machine Learning in Practice
10-725 Convex Optimization
16-720 Computer Vision
10-605 Machine Learning with Large Dataset
11-777 Multimodal Machine Learning