Yuyang Wang

CONTACT INFORMATION	Carnegie Mellon University 5000 Forbes Avenue Pittsburgh, PA 15213, USA	Email: yuyangw@cmu.edu Website: yuyangw.github.io Google Scholar

EDUCATION

Carnegie Mellon University 2019 - present
Ph.D. in Mechanical Engineering, College of Engineering
Advisor: Prof. Amir Barati Farimani
Thesis Proposal: Self-supervised Representation Learning for Molecular Prediction and Analysis

Carnegie Mellon University 2021 - present
M.S. in Machine Learning, School of Computer Science

Carnegie Mellon University 2017 - 2019
M.S. in Mechanical Engineering, College of Engineering

Tongji University 2013 - 2017
B.Eng. in Engineering Mechanics, School of Aerospace Engineering and Applied Mechanics

EMPLOYMENT

Carnegie Mellon University Pittsburgh, PA, USA 2019 - present
Graduate Research Assistant

Momenta Beijing, China Summer 2018
R&D Intern, Momenta Valet Parking Group

HONORS AND AWARDS

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, Tongji University 2014-16

PEER-REVIEWED PUBLICATIONS

*equal contribution

[1] 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

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

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

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

[5] 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

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

[7] 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

PRE-PRINTS

[1] Crystal Twins: Self-supervised Learning for Crystalline Material Property Prediction
arXiv preprint, 2022
Rishikesh Magar, **Yuyang Wang**, and Amir Barati Farimani

[2] AugLiChem: Data Augmentation Library of Chemical Structures for Machine Learning
arXiv preprint, 2021
Rishikesh Magar*, **Yuyang Wang***, Cooper Lorsung*, Chen Liang, Hariharan Ramasubramanian, Peiyuan Li, Amir Barati Farimani

[3] Bio-informed Protein Sequence Generation for Multi-class Virus Mutation Prediction
bioRxiv preprint, 2020
Yuyang Wang, Prakarsh Yadav, Rishikesh Magar, Amir Barati Farimani

TALKS

Molecular Contrastive Learning of Representations via GNNs
Guest Lecture, 24-789 Deep Learning for Engineers, Carnegie Mellon University   May 2021

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

Introduction to Machine Learning and Reinforcement Learning for Precision Engineers
Tutorial, ASPE Spring Meeting (with Prof. 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

Deep Reinforcement Learning for Predicting Kinetic Pathways to Surface Reconstruction in a Ternary Alloy   Fall 2021
MarkTechPost

TEACHING

24-789: Deep Learning for Engineers   Spring 2020 & Spring 2021
Teaching Assistant, Carnegie Mellon University

24-677: Linear Control Systems   Fall 2018
Teaching Assistant, Carnegie Mellon University

SELECTED COURSES

10-701 Introduction to Machine Learning	10-725 Convex Optimization
11-785 Introduction to Deep Learning	16-720 Computer Vision
10-703 Deep Reinforcement Learning & Control	10-605 Machine Learning with Large Dataset
10-718 Machine Learning in Practice	24-783 Advanced Engineering Computation

SKILLS

Programming: Python, C/C++, MATLAB, Java, PyTorch, TensorFlow, PySpark, Scikit-learn
Languages: English (proficient), Chinese (native)