YUYANG WANG

yuyangw.github.io ◇ Google Scholar ◇ LinkedIn ◇ GitHub

EDUCATION

Carnegie Mellon University — Pittsburgh, PA
Ph.D. in Mechanical Engineering, College of Engineering — *May 2023 (Anticipated)*
› *Thesis*: Self-supervised Representation Learning for Molecular Property Predictions

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

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

Tongji University — Shanghai, China
B.Eng. 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" to be published by Springer Nature
Yuyang Wang, Zijie Li, Amir Barati Farimani

PUBLICATIONS

*equal contribution

[1] Denoise Pre-training on Non-equilibrium Molecules for Accurate and Transferable Neural Potentials
arXiv, 2023
Yuyang Wang, Changwen Xu, Zijie Li, Amir Barati Farimani

[2] Neural Network Predicts Ion Concentration Profiles under Nanoconfinement
arXiv, 2023
Zhonglin Cao, ***Yuyang Wang***, Cooper Lorsung, and Amir Barati Farimani

[3] TransPolymer: a Transformer-based Language Model for Polymer Property Predictions
npj Computational Materials, 2023
Changwen Xu, ***Yuyang Wang***, Amir Barati Farimani

[4] MOFormer: Self-Supervised Transformer model for Metal-Organic Framework Property Prediction
Journal of the American Chemical Society, 2023
Zhonglin Cao, Rishikesh Magar, ***Yuyang Wang***, Amir Barati Farimani

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

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

[7] 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

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

[9] 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

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

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

[12] 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

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

[14] 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 *Summer 2018*
Implemented and improved deep reinforcement learning to valet car parking in simulation.

TALKS

Polymer Property Prediction via Pre-trained Large Language Model
Contributed Oral presentation, American Physical Society (APS) March 2023, Las Vegas, NV *Mar. 2023*

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, Deep Learning for Engineers at CMU, 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*
CMU News, *Tech Xplore*, *News Azi*, *DrugAI*

Efficient Water Desalination with Graphene Nanopores Obtained using AI *Fall 2021*
CMU News, *Phys.org*, *Nanowerk*

DRL for Predicting Kinetic Pathways to Surface Reconstruction in a Ternary Alloy Fall 2021
MarkTechPost

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, PyG, TensorFlow, PySpark, Scikit-learn, RDKit, Biopython, 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