Yuyang Wang

CONTACT INFORMATION

Carnegie Mellon University
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Pittsburgh, PA 15213, USA

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Google Scholar

EDUCATION

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

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

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

Tongji University Shanghai, China 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.AI 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 (Top 10%), Tongji University 2014-16

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" (Series Editor: Dr. Jerzy Leszczynski) to be published by Springer Nature.
Yuyang Wang, Zijie Li, Amir Barati Farimani

PUBLICATIONS

*equal contribution

[1] **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

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

[4] **Crystal Twins: Self-supervised Learning for Crystalline Material Property Prediction**

npj Computational Materials (accepted in principle), 2022
Rishikesh Magar, ***Yuyang Wang***, and Amir Barati Farimani

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

[6] **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

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

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

[9] **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

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

[11] **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

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

On-going Projects

[1] **Equivariant Self-supervised Representation Learning for Molecules in 3D**
Learning by predicting force fields of perturbed molecular conformations with equivariant GNNs.

[2] **Fragment-based Ligand Generation via Diffusion Model**
Generating ligands from fragment hits in binding pockets via diffusion generative model.

Talks

Molecular Contrastive Learning of Representations via GNNs
Oral presentation, American Chemistry Society Fall 2022, Chicago — 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

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
Head 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	11-777 Multimodal Machine Learning
24-783 Advanced Engineering Computation	24-703 Numerical Methods in Engineering

Skills

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