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 2019 - present
Ph.D. in Mechanical Engineering, College of Engineering
Advisor: Prof. Amir Barati Farimani

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, Mechanical & AI Lab

- Developed molecular contrastive learning frameworks with graph neural networks (GNNs).
- Modeled protein-ligand complexes via GNNs to predict the binding affinities for drug screening.
- Developed GNNs on MD simulation data of biomolecules for structural and dynamics analysis.

Momenta Beijing, China May 2018 - Aug. 2018
R&D Intern, Momenta Valet Parking Group

- Implemented DRL to park the simulated car to the target parking spot given locomotion positions.
- Accelerated the DRL training by deploying asynchronous distributed training on TensorFlow.

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

Publications

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

[2] **Improving Molecular Contrastive Learning via Faulty Negative Mitigation and Decomposed Fragment Contrast**
arXiv preprint arXiv:2202.09346 (2022)
Yuyang Wang, Rishikesh Magar, Chen Liang, and Amir Barati Farimani

[3] **AugLiChem: Data Augmentation Library of Chemical Structures for Machine Learning**
arXiv preprint arXiv:2111.15112 (2021)
Rishikesh Magar*, ***Yuyang Wang****, Cooper Lorsung*, Chen Liang, Hariharan Ramasubramanian, Peiyuan Li, Amir Barati Farimani

[4] **Efficient Water Desalination with Graphene Nanopores Obtained using Artificial Intelligence**
npj 2D Materials Applications 5, no. 1 (2021): 1-9
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 2, no. 4 (2021): 045018
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

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

Talks

Contrastive Learning and its Application on Molecules May 2021
Guest Lecture, 24-789 Deep Learning for Engineers, Virtual

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

Introduction to ML and RL for Precision Engineers May 2020
Tutorial, ASPE Spring Meeting (with Prof. Amir Barati Farimani), Virtual

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 News, *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 & 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	10-708 Probabilistic Graphic Model
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)