YUYANG WANG

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EDUCATION

Carnegie Mellon University — Pittsburgh, PA, USA
Ph.D. in Mechanical Engineering, College of Engineering — *2019 - Present*
M.S. in Machine Learning, School of Computer Science — *2021 - Present*
M.S. in Mechanical Engineering, College of Engineering — *2017 - 2019*

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

EXPERIENCE

Mechanical and AI Lab, Carnegie Mellon University — Pittsburgh, PA, USA
Ph.D. Research Assistance, advised by Prof. Amir Barati Farimani — *Aug. 2019 - Present*

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

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

- Implemented Deep Reinforcement Learning (DRL) algorithms to control the simulated car parking autonomously in the target parking space with Cartesian coordinate and posture of the car as inputs.
- Accelerated the DRL training by deploying asynchronous-updated distributed training on TensorFlow.

PUBLICATIONS

Yuyang Wang, Jianren Wang, Zhonglin Cao, Amir Barati Farimani. "MolCLR: Molecular Contrastive Learning of Representations via Graph Neural Networks." arXiv preprint arXiv:2102.10056 (2021).

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

Yuyang Wang*, Zhonglin Cao*, Amir Barati Farimani. "Efficient Water Desalination with Graphene Nanopores Obtained using Artificial Intelligence." npj 2D Materials Applications 5, no. 1 (2021): 1-9.

Junwoong Yoon*, Zhonglin Cao*, Rajesh K. Raju*, **Yuyang Wang**, Robert Burnley, Andrew J. Gellman, Amir Barati Farimani†, Zachary W. Ulissi†. "Deep Reinforcement Learning for Predicting Kinetic Pathways to Surface Reconstruction in a Ternary Alloy." Machine Learning: Science and Technology 2, no. 4 (2021): 045018.

Jianren Wang*, Ziwen Zhuang*, **Yuyang Wang**, Hang Zhao. "Adversarially Robust Imitation Learning." In 5th Annual Conference on Robot Learning (2021).

Mullick, Baishali, **Yuyang Wang**, Prakarsh Yadav, Amir Barati Farimani. "Learning Super-Resolution Electron Density Map of Proteins using 3D U-Net." ML4SB Workshop at NeurIPS (2020).

Yuyang Wang, Prakarsh Yadav, Rishikesh Magar, Amir Barati Farimani. "Bio-informed Protein Sequence Generation for Multi-class Virus Mutation Prediction." bioRxiv (2020).

INVITED TALKS & POSTERS

Contrastive Learning and Implementation on Molecules — Virtual
Guest Lecture, 24-789 Deep Learning for Engineers — *May 2021*

Efficient Graphene Nanopore Designed by Artificial Intelligence for Water Desalination — Virtual
American Physical Society - Division of Fluid Dynamics Annual Meeting (APS-DFD) — *Nov. 2020*

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

TEACHING

24-789: Deep Learning for Engineers — Pittsburgh, PA, USA
Head Teaching Assistant, Carnegie Mellon University — *Spring 2020 & Spring 2021*

24-677: Linear Control Systems — Pittsburgh, PA, USA
Teaching Assistant, Carnegie Mellon University — *Fall 2018*

SELECTED COURSES

10-701 Introduction to Machine Learning
11-785 Introduction to Deep Learning
16-720 Computer Vision
10-718 Machine Learning in Practice
10-725 Convex Optimization
10-703 Deep Reinforcement Learning & Control
10-708 Probabilistic Graphic Model
24-783 Advanced Engineering Computation

HONORS & REWARDS

1st Prize, Tongji University undergraduate outstanding student scholarship (TOP 10%). *2014 & 2016*
2nd Prize, Tongji University undergraduate outstanding student scholarship (TOP 20%). *2015*

SKILLS

Programming Python, C/C++, MATLAB, Java, PyTorch, TensorFlow
Languages English (proficient), Mandarin (native)