

# YUYANG WANG

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## EDUCATION

### Carnegie Mellon University

Ph.D. in Mechanical Engineering, College of Engineering

M.S. in Machine Learning, School of Computer Science

M.S. in Mechanical Engineering, College of Engineering

Pittsburgh, PA, USA

2019 - Present

2021 - Present

2017 - 2019

### Tongji University

B.Eng. in Engineering Mechanics, School of Aerospace Engineering and Applied Mechanics

Shanghai, China

2013 - 2017

## EXPERIENCE

### Mechanical and AI Lab, Carnegie Mellon University

Ph.D. Research Assistance, advised by Prof. Amir Barati Farimani

Pittsburgh, PA, USA

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

R&D Intern, Momenta Valet Parking Group

Beijing, China

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<sup>†</sup>, Zachary W. Ulissi<sup>†</sup>. “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

Guest Lecture, 24-789 Deep Learning for Engineers

Virtual

May 2021

### Efficient Graphene Nanopore Designed by Artificial Intelligence for Water Desalination

American Physical Society - Division of Fluid Dynamics Annual Meeting (APS-DFD)

Virtual

Nov. 2020

### Introduction to Machine Learning and Reinforcement Learning for Precision Engineers

Tutorial, Precision Engineers at ASPE Spring Meeting (with Prof. Amir Barati Farimani)

Virtual

May 2020

## TEACHING

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**24-789: Deep Learning for Engineers**  
*Head Teaching Assistant, Carnegie Mellon University*

Pittsburgh, PA, USA  
*Spring 2020 & Spring 2021*

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

Pittsburgh, PA, USA  
*Fall 2018*

## SELECTIVE COURSES

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10-701 Introduction to Machine Learning  
11-785 Introduction to Deep Learning  
10-720 Computer Vision

10-725 Convex Optimization  
10-703 Deep Reinforcement Learning & Control  
10-708 Probabilistic Graphic Model

## HONORS & REWARDS

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1st Prize, Tongji University undergraduate outstanding student scholarship (TOP 10%).	<i>Sept. 2016</i>
2nd Prize, Tongji University undergraduate outstanding student scholarship (TOP 20%).	<i>Sept. 2015</i>
1st Prize, Tongji University undergraduate outstanding student scholarship (TOP 10%).	<i>Sept. 2014</i>

## SKILLS

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