

YUYANG WANG

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EDUCATION

- Carnegie Mellon University**, Pittsburgh, PA, USA *Aug. 2019 - Present*
Ph.D. in Mechanical Engineering, Department of Mechanical Engineering, College of Engineering
- Carnegie Mellon University**, Pittsburgh, PA, USA *Aug. 2021 - Present*
M.S. in Machine Learning, Machine Learning Department, School of Computer Science
- Carnegie Mellon University**, Pittsburgh, PA, USA *Aug. 2017 - May 2019*
M.S. in Mechanical Engineering, Department of Mechanical Engineering, College of Engineering
- Tongji University**, Shanghai, China *Sept. 2013 - June 2017*
B.Eng. in Engineering Mechanics, School of Aerospace Engineering and Applied Mechanics

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, and Amir Barati Farimani. "MolCLR: Molecular contrastive learning of representations via graph neural networks." arXiv preprint arXiv:2102.10056 (2021).
- Yuyang Wang***, Zhonglin Cao*, and Amir Barati Farimani. "Efficient water desalination with graphene nanopores obtained using artificial intelligence." npj 2D Materials and Applications 5, no. 1 (2021): 1-9.
- Jianren Wang*, Ziwen Zhuang*, **Yuyang Wang**, and Hang Zhao. "Adversarially Robust Imitation Learning." In 5th Annual Conference on Robot Learning (2021).
- Junwoong Yoon*, Zhonglin Cao*, Rajesh K. Raju*, **Yuyang Wang**, Robert Burnley, Andrew J. Gellman, Amir Barati Farimani, and 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.
- Mullick, Baishali, **Yuyang Wang**, Prakarsh Yadav, and 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, and Amir Barati Farimani. "Bio-informed Protein Sequence Generation for Multi-class Virus Mutation Prediction." bioRxiv (2020).

TEACHING

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

SKILLS

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