Yusong Wang

130-2295-0985 yusowa0716@gmail.com yusowa0716.github.io

EDUCATION

Xi'an Jiaotong University **Sep. 2017 – Jun. 2021**
Bachelor of Engineering in Automation
- Membership of **Special Class for the Gifted Young (SCGY)** program
- GPA: **90.5 / 100**

Xi'an Jiaotong University & Microsoft Research Asia **Sep. 2021 – Jun. 2026 (Expected)**
Direct Ph.D. in Control Science and Engineering
- Joint training at Institute of Artificial Intelligence and Robotics in Xi'an Jiaotong University (XJTU) & Microsoft Research Asia (MSRA)
- Supervisor:
  - **Dr. Nanning Zheng**, Academician of Chinese Academy of Engineering (XJTU)
  - **Dr. Bin Shao**, Senior Principal Research Manager (MSRA)

SELECTED PUBLICATIONS

Neural P^{3}M: A Long-Range Interaction Modeling Enhancer for Geometric GNNs
Yusong Wang*, Chaoran Cheng*, Shaoning Li*, Yuxuan Ren, Bin Shao, Ge Liu, Pheng-Ann Heng, Nanning Zheng*
(NeurIPS 2024)

Enhancing geometric representations for molecules with equivariant vector-scalar interactive message passing
Yusong Wang*, Tong Wang*, Shaoning Li*, Xinheng He, Mingyu Li, Zun Wang, Nanning Zheng, Bin Shao, Tie-Yan Liu*
*(Nature Communications 2024, **Editor's Highlights in AI and Bio**)*

Geometric Transformer with Interatomic Positional Encoding
Yusong Wang*, Shaoning Li*, Tong Wang, Bin Shao, Nanning Zheng, Tie-Yan Liu*
(NeurIPS 2023)

F^{3}low: Frame-to-Frame Coarse-grained Molecular Dynamics with SE(3) Guided Flow Matching
Shaoning Li, **Yusong Wang***, Mingyu Li*, Jian Zhang, Bin Shao, Nanning Zheng, Jian Tang*
(ICLR 2024 GEM Workshop)

Long-Short-Range Message-Passing: A Physics-Informed Framework to Capture Non-Local Interaction for Scalable Molecular Dynamics Simulation
Yunyang Li, **Yusong Wang***, Lin Huang, Han Yang, Xinran Wei, Jia Zhang, Tong Wang, Zun Wang, Bin Shao, Tie-Yan Liu*
(ICLR 2024)

Improved drug-target interaction prediction with intermolecular graph transformer
Siyuan Liu, **Yusong Wang***, Yifan Deng, Liang He, Bin Shao, Jian Yin, Nanning Zheng, Tie-Yan Liu, Tong Wang*
(Briefings in Bioinformatics 2022)

SELECTED HONORS AND AWARDS

Competitions
- **The** 1^{st} **Prize** in First Global AI Drug Development Competition 2023
- **The** 2^{nd} **Place** in OGB-LSC Graph Regression Track @ NeurIPS 2022 2022
- **The** 3^{rd} **Place** in Open Catalyst Project @ NeurIPS 2022 2022
- **International Excellence Prize** in the 1st IKCEST "the Belt and Road" International Big Data Competition 2019

Honors
- Outstanding Graduates 2021
- Outstanding Student Cadre / Outstanding Student 2017-2020
- Siyuan Scholarship 2017-2020

EXPERIENCE

Microsoft Research AI4Science (Research Intern) **2020 - Present**
Mentor: Bin Shao, Senior Principal Research Manager
- Developed a novel deep learning approach to identify active binding drugs for target proteins.

- Developed an innovative equivariant graph neural network for machine learning force fields.
- Enhanced the Transformer for learning 3D molecular data.
- Designed algorithms to model challenging long-range interactions in large molecules.

Baidu Big Data and Artificial Intelligence Elite Class (Membership) **2018 - 2019**

- Attended courses offered by Baidu.
- Participated in competitions hosted by Baidu.
- Passed the final exam conducted by Baidu.

Technical Competencies

Languages Mandarin Chinese (Native), English

Programming Languages Python, C, C++, MATLAB

Deep Learning Packages PyTorch (PyTorch Geometric), TensorFlow, PaddlePaddle, Jax

Additional Tools Markdown, Latex, Docker, Git ...

SERVICES

Academic Reviewer

- Neural Information Processing Systems (NeurIPS) 2024
- International Conference on Learning Representations (ICLR) 2024, 2025
- International Conference on Artificial Intelligence and Statistics (AISTATS) 2025

Open Source Contributor

- Contributed source code of ViSNet to PyTorh Geometric, which is the most popular graph learning framework. 2023