

YUSONG WANG

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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

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)

F³low: 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

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|--|------|
| – The 1st Prize in First Global AI Drug Development Competition | 2023 |
| – The 2nd Place in OGB-LSC Graph Regression Track @ NeurIPS 2022 | 2022 |
| – The 3rd 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

Open Source Contributor

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