LIANG WANG

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Education

National University of Singapore   **Singapore**
Visiting Ph.D. Student   *2025 - 2026 (expected)*

- Lab: ZhangLab
- Advisor: Prof. Yang Zhang   Mentor: Dr. Zhiyuan Liu
- Research Interests: AI for Science, Diffusion Models, LLM Reasoning

Institution of Automation, Chinese Academy of Sciences   **Beijing, China**
Ph.D. in Pattern Recognition and Intelligent Systems (selected for the PhD honors program)   *2021 - 2026 (expected)*

- Lab: State Key Laboratory of Multimodal Artificial Intelligence Systems (MAIS)
- Advisor: Prof. Liang Wang   Co-advisors: Prof. Shu Wu and Prof. Qiang Liu
- Honors and Awards: National Scholarship for PhD Students

Tongji University   **Shanghai, China**
B.Eng. in Software Engineering   *2017 - 2021*

- GPA: 4.86/5.00 (Ranking 3/214, Top 1.4%)
- Honors and Awards: National Scholarship for Undergraduate Students, Outstanding Graduate of Shanghai

Selected Publications (* denotes co-first authorship)

1. **MolSpectra: Pre-training 3D Molecular Representation with Multi-modal Energy Spectra**
   - Liang Wang, Shaozhen Liu, Yu Rong, Deli Zhao, Qiang Liu, Shu Wu, Liang Wang
   - *ICLR 2025*

2. **Pin-Tuning: Parameter-Efficient In-Context Tuning for Few-Shot Molecular Property Prediction**
   - Liang Wang, Qiang Liu, Shaozhen Liu, Xin Sun, Shu Wu, Liang Wang
   - *NeurIPS 2024*

3. **Rethinking Graph Masked Autoencoders through Alignment and Uniformity**
   - Liang Wang*, Xiang Tao*, Qiang Liu, Shu Wu, Liang Wang
   - *AAAI 2024*

4. **Bi-Level Graph Structure Learning for Next POI Recommendation**
   - Liang Wang, Shu Wu, Qiang Liu, Yanqiao Zhu, Xiang Tao, Mengdi Zhang, Liang Wang
   - *IEEE Transactions on Knowledge and Data Engineering 2024*

5. **CAMLO: Cross-Attentive Multi-View Network for Long-Term Origin-Destination Flow Prediction**
   - Liang Wang, Hao Fu, Shu Wu, Qiang Liu, Xuelei Tan, Fangsheng Huang, Mengdi Zhang, Wei Wu
   - *SDM 2024*

6. **DIVE: Subgraph Disagreement for Graph Out-of-Distribution Generalization**
   - Xin Sun, Liang Wang, Qiang Liu, Shu Wu, Zilei Wang, Liang Wang
   - *KDD 2024*

7. **GSLB: The Graph Structure Learning Benchmark**
   - Zhixun Li, Liang Wang, Xin Sun, Yifan Luo, Yanqiao Zhu, Dingshuo Chen, Yingtao Luo, Xiangxin Zhou, Qiang Liu, Shu Wu, Liang Wang, Jeffrey Xu Yu
   - *NeurIPS 2023*

8. **Semantic Evolvement Enhanced Graph Autoencoder for Rumor Detection**
   - Xiang Tao, Liang Wang, Qiang Liu, Shu Wu, Liang Wang
   - *WWW 2024*

9. **S²DN: Learning to Denoise Unconvincing Knowledge for Inductive Knowledge Graph Completion**
   - Tengfei Ma, Yujie Chen, Liang Wang, Xuan Lin, Bosheng Song, Xiangxiang Zeng
   - *AAAI 2025*

10. **EnzyControl: Adding Functional and Substrate-Specific Control for Enzyme Backbone Generation**
    - Chao Song, Zhiyuan Liu, Han Huang, <u>Liang Wang</u>, Qiong Wang, Jianyu Shi, Hui Yu, Yihang Zhou, Yang Zhang
    - *NeurIPS 2025*

11. **3D-GSRD: 3D Molecular Graph Auto-Encoder with Selective Re-mask Decoding**
    - Chang Wu, Zhiyuan Liu, Wen Shu, <u>Liang Wang</u>, Yanchen Luo, Wenqiang Lei, Yatao Bian, Junfeng Fang, Xiang Wang
    - *NeurIPS 2025*

12. **Chain-of-History Reasoning for Temporal Knowledge Graph Forecasting**
    - Yuwei Xia, Ding Wang, Qiang Liu, <u>Liang Wang</u>, Shu Wu, Xiaoyu Zhang
    - *ACL 2024*

Selected Preprint Papers (* denotes co-first authorship)

1. **DiffSpectra: Molecular Structure Elucidation from Spectra using Diffusion Models**
   - <u>Liang Wang</u>, Yu Rong, Tingyang Xu, Zhenyi Zhong, Zhiyuan Liu, Pengju Wang, Deli Zhao, Qiang Liu, Shu Wu, Liang Wang, Yang Zhang
   - *arXiv preprint 2025*

2. **Diffusion Models for Molecules: A Survey of Methods and Tasks**
   - <u>Liang Wang</u>, Chao Song, Zhiyuan Liu, Yu Rong, Qiang Liu, Shu Wu, Liang Wang
   - *arXiv preprint 2025*

3. **Materials Generation in the Era of Artificial Intelligence: A Comprehensive Survey**
   - Zhixun Li*, Bin Cao*, Rui Jiao*, <u>Liang Wang</u>*, Ding Wang, Yang Liu, Dingshuo Chen, Jia Li, Qiang Liu, Yu Rong, Liang Wang, Tong-yi Zhang, Jeffrey Xu Yu
   - *arXiv preprint 2025*

Selected Projects

PyGCL: A PyTorch Library for Graph Contrastive Learning　　　　https://github.com/PyGCL/PyGCL
- ☆ Github Star: 960
- An easy-to-use library for graph contrastive learning with PyTorch. It implements a wide variety of contrastive objectives, data augmentations, contrasting modes and other utilities useful for implementing and evaluating contrastive learning on graphs.

GSLB: A Benchmark of Graph Structure Learning　　　　https://github.com/GSL-Benchmark/GSLB
- ☆ Github Star: 123
- An open-source library built for easy implementation and evaluation of graph structure learning model family. It offers a versatile control of graph dataset laoding, structure learners, structure processors, and a bunch of reproduced models.

ScienceOne (S1) - Scientific Foundation Model　　　　https://www.scienceone.cn
- Strategic Priority Research Program of the Chinese Academy of Sciences
- A scientific foundation model designed for comprehensive understanding of scientific data. It is designed with a heterogeneous mixture-of-experts architecture and is trained on curated scientific knowledge and data, enabling in-depth comprehension of complex scientific modalities, including waves, spectra, and fields.

Internship

DP Technology　　　　**Beijing, China**
Research Intern　　　　*Apr. 2025 - Now*
- Conducting research on large language models for reasoning and planning complex scientific problems using reinforcement learning.

Language And Science AI Lab, Alibaba DAMO Academy　　　　**Hangzhou, China**
Research Intern　　　　*Aug. 2024 - Mar. 2025*
- Advised by Dr. <u>Yu Rong</u> and Dr. <u>Tingyang Xu</u>.
- Conducted research on AI for chemistry and life science. The research work has been published in ICLR 2025.

NLP Center, Meituan Inc.　　　　**Beijing, China**
Research Intern　　　　*Sept. 2021 - Oct. 2022*
- Conducted research on graph self-supervised learning and graph-based spatial-temporal data mining. The research works have been published in IEEE TKDE and SDM 2024.

Advertising Department, ByteDance Inc.　　　　**Shanghai, China**
Machine Learning Engineer Intern　　　　*Jul. 2020 - Dec. 2020*
- Supported the improvement of advertising machine learning models, and the development of the advertising system.

Talks

Molecular Representation and Structure-Activity Relationship, at Bytedance Seed, 2025, <u>Slides</u>
Molecular Spectroscopy, at Alibaba DAMO Academy, 2024, <u>Slides</u>
Molecular Representation Learning and Property Prediction, at DP Technology, 2024, <u>Slides</u>
Denoising-based 3D Molecular Pre-training, 2024, <u>Slides</u>
Generative Graph Self-Supervised Learning, 2023, <u>Slides</u>
Graph Transformers, 2022, <u>Slides</u>
Graph Self-Supervised Learning and Pre-Training, 2021, <u>Slides</u>

Academic Services

Conference Reviewers : NeurIPS (2024 2025), ICLR (2025, 2026), ICML (2025), KDD (2024 2025, 2026), AAAI (2026), AISTATS (2025, 2026)

Journal Reviewers : IEEE TKDE, IEEE TCBB

Technical Skills

Programming Languages: Python, C++, Java, Go, C#, Matlab
Machine Learning Frameworks: PyTorch, PyTorch Geometric (PyG), Deep Graph Library (DGL), Hugging Face Transformers, Hugging Face Diffusers
Others: LaTeX, Git