Limei Wang

Research Scientist, Meta
E-mail: limeiwang.work@gmail.com, Homepage: https://limei0307.github.io/

Education

- **Texas A&M University**, College Station, TX, USA *August 2019 - May 2024*
  Ph.D. in Computer Engineering, Department of Computer Science and Engineering
  Advisor: Prof. Shuiwang Ji
- **University of Science and Technology of China**, Hefei, CHINA *August 2015 - July 2019*
  B.E. in Automation, School of Information Science and Technology
  Advisor: Prof. Jiahu Qin

Experience

- Research Scientist, Meta, Bay Area, CA, USA *February 2024 - present*
- Research Intern, Meta, Bay Area, CA, USA *May 2023 - August 2023*
  Work on scalable machine learning methods for large-scale graphs, design a subgraph sampling method
  Mentor: Dr. Si Zhang, Peers: Hanqing Zeng, Hao Wu, Zhigang Hua, Kaveh Hassani

Research Interests

- Artificial Intelligence, Machine Learning, Deep Learning
- AI for Science, Graph/Geometric ML for Molecules [Related papers: SphereNet, ComENet, ProNet, LEFT-Net, LatentDiff, Geo2Seq, AIRS]
- Large-Scale Graphs, Graph Transformer, Foundation Models [Related papers: GraphFM, S3, GQT]
- Generative Models [Related papers: LatentDiff]
- Large Language Models [Related papers: Geo2Seq]

Publications[Google Scholar]

* indicates equal contribution. † indicates equal senior contribution.

[ICML 2025] **Learning to Generate 3D Molecules via Language Models with Geometry-Aware Tokenization**
Xiner Li*, **Limei Wang***, Youzhi Luo, Carl Edwards, Shurui Gui, Yuchao Lin, Heng Ji, Shuiwang Ji
International Conference on Machine Learning (ICML), 2025

[ICLR 2025] **Learning Graph Quantized Tokenizers**
Limei Wang*, Kaveh Hassani*, Si Zhang, Dongqi Fu, Baichuan Yuan, Weilin Cong, Zhigang Hua, Hao Wu, Ning Yao, Bo Long
International Conference on Learning Representations (ICLR), 2025

[LoG 2023] **A Latent Diffusion Model for Protein Structure Generation**
Cong Fu*, Keqiang Yan*, **Limei Wang**, Wing Yee Au, Michael McThrow, Tao Komikado, Koji Maruhashi, Kanji Uchino, Xiaoning Qian, Shuiwang Ji
Learning on Graphs Conference (LoG), 2023

[NeurIPS 2023] **A New Perspective on Building Efficient and Expressive 3D Equivariant Graph Neural Networks**
Weitao Du*, Yuanqi Du*, **Limei Wang***, Dieqiao Feng, Guifeng Wang, Shuiwang Ji, Carla P Gomes, and Zhi-Ming Ma
Conference on Neural Information Processing Systems (NeurIPS), 2023

[ICLR 2023] **Learning Hierarchical Protein Representations via Complete 3D Graph Networks**
Limei Wang*, Hanran Liu*, Yi Liu*,†, Jerry Kurtin, and Shuiwang Ji†
International Conference on Learning Representations (ICLR), 2023

[NeurIPS 2022] **ComENet: Towards Complete and Efficient Message Passing for 3D Molecular Graphs**
Limei Wang*, Yi Liu*, Yuchao Lin, Haoran Liu, and Shuiwang Ji
Conference on Neural Information Processing Systems (NeurIPS), 2022

[NeurIPS 2022 Track Datasets and Benchmarks] **GOOD: A Graph Out-of-Distribution Benchmark**
Shurui Gui*, Xiner Li*, **Limei Wang**, and Shuiwang Ji
Conference on Neural Information Processing Systems Datasets and Benchmarks Track, 2022

[KDD 2022 Tutorial] **Frontiers of Graph Neural Networks with DIG**
Shuiwang Ji, Meng Liu, Yi Liu, Youzhi Luo, **Limei Wang**, Yaochen Xie, Zhao Xu, Haiyang Yu
ACM SIGKDD Conference on Knowledge Discovery and Data Mining (KDD), 2022

[ICML 2022] **GraphFM: Improving Large-Scale GNN Training via Feature Momentum**
Haiyang Yu*, **Limei Wang***, Bokun Wang*, Meng Liu, Tianbao Yang, and Shuiwang Ji
International Conference on Machine Learning (ICML), 2022

[Bioinformatics 2022] **Advanced Graph and Sequence Neural Networks for Molecular Property Prediction and Drug Discovery**
Zhengyang Wang*, Meng Liu*, Youzhi Luo*, Zhao Xu*, Yaochen Xie*, **Limei Wang***, Lei Cai*, Qi Qi, Zhuoning Yuan, Tianbao Yang, and Shuiwang Ji
Bioinformatics, 2022

[ICLR 2022] **Spherical Message Passing for 3D Molecular Graphs**
Yi Liu*, **Limei Wang***, Meng Liu, Yuchao Lin, Xuan Zhang, Bora Oztekin, and Shuiwang Ji
International Conference on Learning Representations (ICLR), 2022

[JMLR 2021] **DIG: A Turnkey Library for Diving into Graph Deep Learning Research**
Meng Liu*, Youzhi Luo*, **Limei Wang***, Yaochen Xie*, Hao Yuan*, Shurui Gui*, Haiyang Yu*, Zhao Xu, Jingtun Zhang, Yi Liu, Keqiang Yan, Haoran Liu, Cong Fu, Bora Oztekin, Xuan Zhang, and Shuiwang Ji
Journal of Machine Learning Research (JMLR), 2021

[NeurIPS-W 2021] **Fast Quantum Property Prediction via Deeper 2D and 3D Graph Networks**
Meng Liu*, Cong Fu*, Xuan Zhang, **Limei Wang**, Yaochen Xie, Hao Yuan, Youzhi Luo, Zhao Xu, Shenglong Xu, and Shuiwang Ji
AI for Science Workshop at NeurIPS, 2021

[Chemistry-Methods 2021] **Development of Xanthene-Based Fluorescent Dyes: Machine Learning-Assisted Prediction vs. TD-DFT Prediction and Experimental Validation**
Yingying Wang*, Lei Cai*, Wei Chen, Difei Wang, Shi Xu, **Limei Wang**, Martin A. Kononov, Shuiwang Ji, and Ming Xian
Chemistry-Methods, 2021

Preprints

* indicates equal contribution.

How to Make LLMs Strong Node Classifiers?
Zhe Xu, Kaveh Hassani, Si Zhang, Hanqing Zeng, Michihiro Yasunaga, **Limei Wang**, Dongqi Fu, Ning Yao, Bo Long, Hanghang Tong

Artificial Intelligence for Science in Quantum, Atomistic, and Continuum Systems
Xuan Zhang*, **Limei Wang***, Jacob Helwig*, Youzhi Luo*, Cong Fu*, Yaochen Xie*, Meng Liu, Yuchao Lin, Zhao Xu, Keqiang Yan, Keir Adams, Maurice Weiler, Xiner Li, Tianfan Fu, Yucheng Wang, Haiyang Yu, YuQing Xie, Xiang Fu, Alex Strasser, Shenglong Xu, Yi Liu, Yuanqi Du, Alexandra Saxton, Hongyi Ling, Hannah Lawrence, Hannes Stärk, Shurui Gui, Carl Edwards, Nicholas Gao, Adriana Ladera, Tailin Wu, Elyssa F. Hofgard, Aria Mansouri Tehrani, Rui Wang, Ameya Daigavane, Montgomery Bohde, Jerry Kurtin, Qian Huang, Tuong Phung, Minkai Xu, Chaitanya K. Joshi, Simon V. Mathis, Kamyar Azizzadenesheli, Ada Fang, Alán Aspuru-Guzik, Erik Bekkers, Michael Bronstein, Marinka Zitnik, Anima Anandkumar, Stefano Ermon, Pietro Liò, Rose Yu, Stephan Günnemann, Jure Leskovec, Heng Ji, Jimeng Sun, Regina Barzilay, Tommi Jaakkola, Connor W. Coley, Xiaoning Qian, Xiaofeng Qian, Tess Smidt, Shuiwang Ji

Staleness-based Subgraph Sampling for Large-Scale GNNs Training
Limei Wang, Si Zhang, Hanqing Zeng, Hao Wu, Zhigang Hua, Kaveh Hassani, Andrey Malevich, Bo Long, Shuiwang Ji

Professional Services

Program Committee Member & Reviewer

- International Conference on Machine Learning (**ICML**) *2022, 2023, 2024*
- Conference on Neural Information Processing Systems (**NeurIPS**) *2022, 2023*
- NeurIPS Datasets and Benchmarks Track *2022, 2023*
- AI4Science Workshop @ NeurIPS *2022, 2023*
- International Conference on Learning Representations (**ICLR**) *2023, 2024*
- Learning on Graphs Conference (**LoG**) *2022, 2023*
- ACM SIGKDD International Conference on Knowledge Discovery and Data Mining (**KDD**) *2022*

Talks, Lecture, & Tutorials

Invited Talks

- Geometric Deep Learning for 3D Molecules *Lawrence Livermore National Laboratory, 2024*
- Improving Large-Scale GNN Training via Feature Momentum *Meta, 2023*
- Learning Hierarchical Protein Representations via 3D Graph Networks *Fujitsu Research of America, 2022*

Tutorial

- PyTorch Tutorial *CSCE 421, Texas A&M University, 2023*
- Frontiers of Graph Neural Networks with DIG Texas A&M Institute of Data Science, 2023; KDD, 2022

Scholarships, Awards, & Honors

- **EECS Rising Star, Georgia Tech** *2023*
- **NeurIPS Travel Award** *2022, 2023*
- **Travel Grant, CSE@TAMU** *2021, 2022, 2023*
- **Third place on the Open Catalyst Challenge** *2021*
- **Runner-Up Award of KDD Cup on Open Graph Benchmark Large-Scale Challenge (OGB-LSC)** *2021*
- **1st Place, MIT AI Cures Challenge for COVID-19 Drug Discovery** 2020
- **Outstanding Graduates, USTC** *2019*

News Coverage

- Ph.D. Student Attends Workshop for Rising Stars *TAMU News 2024*
- Ji and his team earn top showing at premier data mining competition *TAMU News 2021*
- Computer scientists using artificial intelligence to fight secondary effects of COVID-19 *TAMU News 2020*