Gang Liu

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Education

University of Notre Dame — Notre Dame, US
Ph.D. student in Computer Science and Engineering, Advisor: Prof. Meng Jiang — 2021–Present

Southwest University — Chongqing, China
B.E. in Software Engineering — 2017–2021

Research and Industrial Experience

MIT-IBM Watson AI Lab, Research Intern — Boston, US
Worked on graph-text multimodal large language models for molecules [C11]. — 05/2024-08/2024

Broad Institute of MIT and Harvard, Research Intern — Boston, US
Worked on multimodal molecular learning with cellular responses [C10]. — 02/2024-05/2024

Amazon, Applied Scientist Intern — Seattle, US
Worked on Transformers with attributes for sequential recommendations [C9]. — 05/2023-08/2023

Awards

- OpenAI Researcher Access Program (Awarded with 10000 USD in API Credits) — 2025–2026
- IBM PhD Fellowship — 2024–2025
- NeurIPS Scholar Award — 2023
- ACM SIGKDD Student Travel Award — 2022
- Notre Dame Graduate School Conference Presentation Grant — 2022
- National Scholarship in China — 2020
- Chongqing Undergraduate Student Innovation Project (with Grants 3000 RMB) — 2019–2020

Publications

Refereed Conference Publications

[C11] **Liu, G.**, Sun M., Matusik W., Jiang M., Chen J. "Multimodal Large Language Models for Inverse Molecular Design with Retrosynthetic Planning". *The Thirteenth International Conference on Learning Representations* (ICLR), 2025.

[C10] **Liu, G.**, Seal S., Arevalo J., Liang Z., Carpenter AE., Jiang M., Singh S. "Learning Molecular Representation in a Cell". *The Thirteenth International Conference on Learning Representations* (ICLR), 2025.

[C9] **Liu, G.**, Yang, F., Yang, J., Garakani, A., Tong, T., Gao, Y, & Jiang, M., "Learning Attribute as Explicit Relation for Sequential Recommendation". *ACM SIGKDD International Conference on Knowledge Discovery and Data Mining* (KDD), 2025. (Research track; Acceptance rate 19% out of 976 submissions)

[C8] Inae E., **Liu G.,** Jiang M. Motif-aware Attribute Masking for Molecular Graph Pre-training. *Learning on Graphs Conference* (LoG), 2024.

[C7] **Liu, G.**, Xu, J., Luo, T., & Jiang, M., "Graph Diffusion Transformers for Multi-Conditional Molecular Generation". *Conference on Neural Information Processing Systems* (NeurIPS), 2024. (**Selected as an oral with a rate of 0.5%=72/15671**)

[C6] Liang Z, **Liu G**, ..., Shi Y., "Graph Learning for Parameter Prediction of Quantum Approximate Optimization Algorithm", The 61st *ACM/IEEE Design Automation Conference* (DAC), 2024.

[C5] Liang Z, Guo K, **Liu G**, ..., Zhang X., "SceMQA: A Scientific College Entrance Level Multimodal Question Answering Benchmark", The 62nd *Annual Meeting of the Association for Computational Linguistics* (ACL), 2024.

[C4] **Liu G**, Inae E, Zhao T, Xu J, Luo T, Jiang M., "Data-Centric Learning from Unlabeled Graphs with Diffusion Model", *Conference on Neural Information Processing Systems* (NeurIPS), 2023. (Acceptance rate 26.1%=3222/12343)

[C3] **Liu, G**., Zhao, T., Inae, E., Luo, T., Jiang, M., "Semi-Supervised Graph Imbalanced Regression", *ACM SIGKDD International Conference on Knowledge Discovery and Data Mining* (KDD), 2023. (Research track; Acceptance rate 22.0% = 313/1416)

[C2] **Liu, G.**, Zhao, T., Xu, J., Luo, T., Jiang, M., "Graph Rationalization with Environment-based Augmentations", *ACM SIGKDD International Conference on Knowledge Discovery and Data Mining* (KDD), 2022. (Research track; Acceptance rate 15.0% = 254/1695)

[C1] Zhao, T., **Liu, G.**, Wang, D., Yu, W., Jiang, M., "Learning from Counterfactual Graph for Link Prediction", *International Conference on Machine Learning* (ICML), 2022. (Acceptance rate 21.9% = 1235/5630)

Refereed Journal Publications

[J9] Xu, J., Suleiman, A., **Liu, G.**, Zhang, R., Jiang, M., Guo, R., Luo, T. "Transcend the Boundaries: Machine Learning for Designing Polymeric Membrane Materials for Gas Separation", *Chemical Physics Reviews*, 2024. (IF=6.6)

[J8] Jin, B.*, **Liu, G.***, Han, C.*, Jiang, M., Ji, H., & Han, J., "Large Language Models on Graphs: A Comprehensive Survey". *IEEE Transactions on Knowledge and Data Engineering*. 2024. (IF=8.9)

[J7] Xu, J.*, Suleiman, A.*, **Liu, G.***, Perez, M., Zhang, R., Jiang, M., Guo, R., & Luo, T., "Superior Polymeric Gas Separation Membrane Designed by Explainable Graph Machine Learning", *Cell Reports Physical Science*, 2024. (IF=7.9)

[J6] **Liu G.**, Inae E., Luo T., Jiang M., "Rationalizing Graph Neural Networks with Data Augmentation", *ACM Transactions on Knowledge Discovery from Data*, 2024. (IF=4.4)

[J5] Zhao, T., Jin, W., Liu, Y., Wang, Y., **Liu, G.**, Günnemann, S., Shah, N., Jiang, M., "Graph Data Augmentation for Graph Machine Learning: A Survey", *IEEE Data Engineering Bulletin*, 2023.

[J4] **Liu, G.**, Deng, Y., & Cheong, K. H., "Network Immunization Strategy by Eliminating Fringe Nodes: A Percolation Perspective", *IEEE Transactions on Systems, Man, and Cybernetics: Systems*, 2023. (IF=11.471)

[J3] **Liu, G.**, Xiao, F., Lin, C.-T., & Cao, Z., "A Fuzzy Interval Time-Series Energy and Financial Forecasting Model Using Network-Based Multiple Time-Frequency Spaces and the Induced-Ordered Weighted Averaging Aggregation Operation", *IEEE Transactions on Fuzzy Systems*, 2020. (IF=12.029)

[J2] **Liu, G.**, & Xiao, F., "A Data-Driven Dynamic Data Fusion Method Based on Visibility Graph and Evidence Theory", *IEEE Access*, 2019. (IF=3.367)

[J1] **Liu, G.**, & Xiao, F., "Time Series Data Fusion Based on Evidence Theory and OWA Operator", *Sensors*, 2019. (IF=3.576)

Refereed Conference Tutorial

[T1] Tong Zhao, Kaize Ding, Wei Jin, **Gang Liu**, Meng Jiang, and Neil Shah., "Augmentation Methods for Graph Learning", *SIAM International Conference on Data Mining* (SDM). 2023.

Teaching and Mentorship Experience

- **Teaching Assistant** at University of Notre Dame
  - Theory of Computing (CSE 30151) — Spring 2022
  - Database Systems Concepts (CSE 30331) — Fall 2021
- **Mentorship Experience:**
  - Eric Inae, Ph.D. Student at the University of Notre Dame — 08/2022-Present
  - Ms. Yihan Zhu, Ph.D. Student at the University of Notre Dame — 08/2024-Present
  - Jackson Ballow, Undergraduate at the University of Notre Dame. — 01/2022-05/2023
  - Ryan Pairitz, Undergraduate at the University of Notre Dame. — 01/2022-05/2022

Professional Services and Activities

- **Conference Reviewer:**
  - Neural Information Processing Systems (NeurIPS)
    2024, 2023, 2022
  - ACM SIGKDD Conference on Knowledge Discovery and Data Mining (KDD)
    2025 Aug/Feb, 2024, 2023
  - International Conference on Learning Representations (ICLR)
    2025, 2024
  - International Conference on Machine Learning (ICML)
    2024, 2023, 2022
  - ACM International Conference on Web Search and Data Mining (WebConf)
    2024
  - AAAI Conference on Artificial Intelligence (AAAI)
    2025, 2024, 2023
  - SIAM International Conference on Data Mining (SDM)
    2024
- **Journal Reviewer:**

  - IEEE Transactions on Knowledge and Data Engineering (TKDE)
  - Information Sciences (INS)
  - IEEE Transactions on Cybernetics (TCYB)
  - Digital Signal Processing

- **Volunteer** at ACM KDD 2022.
- **Organizer** of Learning on Graphs (LoG) MidNorth Local Meetup 2023.