

Jiaqing Xie

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RESEARCH INTERESTS

Graph AI for Science, especially chemical science: graph transformers and SE(3)-equivariant graph networks for molecular spectra prediction (IR/Raman/NMR/ECD, forward and inverse), reaction pretraining, molecular property and dynamics prediction; theory and algorithms for graph learning, including positional encodings (Graph-RoPE, Laplacian PE), complexity reduction for GNNs and graph transformers, and parallelizable large-scale training (Graph DeltaNet); reliable molecular generation via graph-guided search (e.g., GNN + MCTS).

EDUCATION

Fudan University w. Shanghai AI Lab

Ph.D., Computer Science

Shanghai, China

Sep. 2026 - Present

- Ph.D. Supervisors: Yuqiang Li, Tianfan Fu, Yuxin Wang, Xipeng Qiu

ETH Zurich

M.Sc., Computer Science

Zurich, Switzerland

2022 - 2025

University of Edinburgh

B.Eng., Electronics and Computer Science

Edinburgh, UK

2019 - 2022

WORK EXPERIENCE

Shanghai Artificial Intelligence Laboratory

Research Assistant

Shanghai, China

Jun. 2025 - Jun. 2026

- Supervisor: Yuqiang Li
- Research in Machine Learning for Spectroscopy Modeling

PUBLICATIONS

Most recent publications. ‡ indicates equal contribution.

Graph Neural Networks

Analytic-Walk Rotary Positional Encodings for Graphs

Jiaqing Xie, Yuxin Wang, Xipeng Qiu
arXiv preprint, 2026.

Equivariant Neural Primal-Dual Assignment for Maximum Common Edge Subgraphs

Jiaqing Xie, Yanchao Li, Zhuo Yang, Yuxin Wang, Tianfan Fu, Yuqiang Li
arXiv preprint, 2026.

Gauge-Invariant Learnable Spectral Positional Encodings for Directed Graphs via Hermitian Block Krylov Subspaces

Jiaqing Xie, Yuxin Wang
Arxiv.

Benchmarking Positional Encodings for GNNs and Graph Transformers

Florian Grotschla[‡], Jiaqing Xie[‡] and Roger Wattenhofer
SIGKDD 2026.

Graph Structure Learning via Lottery Hypothesis at Scale

Yuxin Wang, Xiannian Hu, **Jiaqing Xie**, Zhangyue Yin, Yunhua Zhou, Xipeng Qiu, Xuanjing Huang
ACML 2024.

AI for Physical Science

GSF- χ : Global Stereochemical Fields for Chiral Graph Transformers

Jiaqing Xie, Yuxin Wang, Xipeng Qiu
Under Review, ICLR 2027.

SpectraFlow: Spectroscopy-informed Flow Matching for Bidirectional Infrared–Raman Spectral Translation

Jiaqing Xie, Zhuo Yang, Ben Gao, Shuaike Shen, Tianfan Fu, Yuqiang Li
To be released.

NMRGym: A Comprehensive Benchmark for Nuclear Magnetic Resonance Based Molecular Structure Elucidation

Zheng Fang, Chen Yang, Hai-tao Yu, Haoming Luo, Haitao He, **Jiaqing Xie**, Zhuo Yang, Yuqiang Li, Jun Xia
SIGKDD 2026.

NMRTrans: Structure Elucidation from Experimental NMR Spectra via Set Transformers

Liujia Yang[‡], Zhuo Yang[‡], **Jiaqing Xie**[‡], Yubin Wang[‡], Ben Gao, Tianfan Fu, Xingjian Wei, Jiaxing Sun, Jiang Wu, Conghui He, Yuqiang Li, Qinying Gu
SIGKDD 2026.

SpectrumWorld: Artificial Intelligence Foundation for Spectroscopy

Zhuo Yang[‡], **Jiaqing Xie**[‡], Shuaike Shen, Daolang Wang, Yeyun Chen, Ben Gao, Shuzhou Sun, Biqing Qi, Dongzhan Zhou, Lei Bai, Linjiang Chen, Shufei Zhang, Jun Jiang, Tianfan Fu, and Yuqiang Li
SIGKDD 2026.

PolyReal: A Benchmark for Real-World Polymer Science Workflows

Wanhao Liu[‡], Weida Wang[‡], **Jiaqing Xie**, Suorong Yang, Jue Wang, Benteng Chen, Guangtao Mei, Zonglin Yang, Shufei Zhang, Yuchun Mo, Lang Cheng, Jin Zeng, Houqiang Li, Wanli Ouyang, Yuqiang Li
CVPR 2026 Findings.

DeepProtein: Deep Learning Library and Benchmark for Protein Sequence Learning

Jiaqing Xie, Yuqiang Li and Tianfan Fu
Bioinformatics 2025.

Large Language Models

R2-Seg: Training-Free OOD Medical Tumor Segmentation via Anatomical Reasoning and Statistical Rejection

Shuaike Shen[‡], Ke Liu[‡], **Jiaqing Xie**, Shangde Gao, Chunhua Shen, Ge Liu, Mireia Crispin-Ortuzar, Shangqi Gao
CVPR 2026 (Best Paper Candidate).

QCBench: Evaluating Large Language Models on Domain-Specific Quantitative Chemistry

Jiaqing Xie[‡], Weida Wang[‡], Ben Gao[‡], Zhuo Yang, Haiyuan Wan, Shufei Zhang, Tianfan Fu, and Yuqiang Li
JCIM 2025.

Deep Research Arena: The First Exam of LLMs' Research Abilities via Seminar-Grounded Tasks

Haiyuan Wan, Chen Yang, Junchi Yu, Meiqi Tu, Jiaxuan Lu, Di Yu, Jianbao Cao, Ben Gao, **Jiaqing Xie**, Aoran Wang, Wenlong Zhang, Philip Torr, Dongzhan Zhou
AAAI 2026.

Technical Reports

Disagree to Accelerate: Closing the Loop on Diffusion Feature Forecasts

Yanchao Li, **Jiaqing Xie**, Ben Gao, Wanhao Liu, Yanbo Wang, T. Y. Tsui, Jinfei Liu, Yuqiang Li, Tianfan Fu
arXiv preprint, 2026.

Reachability Is Not Realization: Tracing the Sources of LLM Benchmark Gains

Yanchao Li, Wanhao Liu, **Jiaqing Xie**, Ben Gao, Yanbo Wang, Tianfan Fu, Yuqiang Li
arXiv preprint, 2026.

MolAct: An Agentic RL Framework for Molecular Editing and Property Optimization

Zhuo Yang[‡], Yeyun Chen[‡], **Jiaqing Xie**, Ben Gao, Shuaike Shen, Wanhao Liu, Liujia Yang, Beilun Wang, Tianfan Fu, Yuqiang Li
Under Review, arXiv.

When to Use SAEs for LLM Steering: A Comparative Study with Mean Activation Differences

Jiaqing Xie

Under Review, arXiv.

Under Review

SkillsInjector: Dynamic Skill Context Construction for LLM Agents

Yanchao Li, Wanhao Liu, Ben Gao, **Jiaqing Xie**, Zhehong Ai, Na Zou, Yuqiang Li, Tianfan Fu
Under Review, arXiv.

OmniMatBench: An Expert-Curated Benchmark for Materials Science Reasoning and Execution

Wanhao Liu[‡], **Jiaqing Xie**[‡], Qian Tan, Weida Wang, Jue Wang, Ran Sun, Zhuo Yang, Wanli Ouyang, Lei Bai, Tianfan Fu, Lu Chen, Xin Chen, Yuqiang Li
Under Review, ACL ARR (COLING 2027).

SpecMol: A Spectroscopy-Grounded Foundation Model for Multi-Task Molecular Learning

Shuaike Shen[‡], **Jiaqing Xie**[‡], Zhuo Yang, Antong Zhang, Shuzhou Sun, Ben Gao, Tianfan Fu, Biqing Qi, Yuqiang Li
Under Review, arXiv.

CONTESTS

Tongji University Skills Contest with TT Design College, Third Prize RMB 3000	2026
Chinese Chemistry Olympiad (CCHO) Shanghai Second Prize	2016

ACADEMIC SERVICES

Reviewer: ICLR, ACL ARR, JCIM	2026
Reviewer: ACL, CVPR, EMNLP, ICONIP, NeurIPS, JCIM	2025
Reviewer: ACML, NeurIPS	2024

**SELECTED
LINKS**

[Google Scholar](#) [X / Twitter](#) [LinkedIn](#) [GitHub](#)

**PERSONAL
INFO**

Running PB: 50 m 6.5 s; 1000 m 3'22"; 5000 m 27'30"; 10000 m 51'00". Weiqi / Go: Chinese
Weiqi Association amateur 1 dan. Codeforces: 1200.