

Jiaqing Xie

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RESEARCH INTERESTS

Flow Matching and Diffusion Models; Graph Neural Networks and Graph Transformers; applications of machine learning in physical science, including spectroscopy, molecular dynamics, and protein sequence learning.

EDUCATION

Fudan University

Ph.D., Computer Science

- Incoming / Ph.D. candidate in Computer Science.

Shanghai, China
Sep. 2026 - Present

ETH Zurich

M.Sc., Computer Science

Zurich, Switzerland
2022 - 2025

University of Edinburgh

B.Eng., Electronics and Computer Science

Edinburgh, UK
2019 - 2022

PUBLICATIONS

Most recent publications. ‡ indicates equal contribution.

Graph Neural Networks

Scaling Learnable Laplacian Positional Encodings with Random-Probe Krylov Methods

Jiaqing Xie

To be released.

Benchmarking Positional Encodings for GNNs and Graph Transformers

Florian Grotschla[‡], **Jiaqing Xie**[‡] and Roger Wattenhofer

SIGKDD 2026.

AI for Physical Science

Antibody Design via On-Policy Self-Distillation

Zhuo Yang, Jiaying He, **Jiaqing Xie** et al.

To be released.

SpectraFlow: Physics-guided Flow Matching for IR-Raman Spectral Interconversion

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

Liuja Yang[‡], Zhuo Yang[‡], **Jiaqing Xie**[‡], Yubin Wang[‡], Ben Gao, Tianfan Fu, Xingjian Wei, Jiaying 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

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

GeoBA: Geometry-Biased Attention for Molecular Property Prediction

Jiaqing Xie, Ziheng Chi, Zhuo Yang
Under Review, arXiv.

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: A Human-Calibrated Multimodal Reasoning Benchmark Across 19 Materials Science Subfields

Wanhao Liu[‡], **Jiaqing Xie**[‡], Qian Tan, Weida Wang, Jue Wang, Ran Sun, Zhuo Yang, Lei Bai, Tianfan Fu, Lu Chen, Xin Chen, Yuqiang Li

Under Review, arXiv.

SpecMol: A Unified Framework for Spectroscopy-Grounded Molecular Modeling and Evaluation

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

Under Review, arXiv.

ACADEMIC
SERVICES

Reviewer: ACL, CVPR, EMNLP, ICONIP, NeurIPS

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 55'30". Weiqi / Go: Chinese Weiqi Association amateur 1 dan. Codeforces: 1200.