

Rui Jiao (矫瑞)

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Education

2021.09 – 2026.06

■ **Ph.D. in Computer Science and Technology**

CS Department, Tsinghua University

Advisor: Yang Liu

Research Direction: Molecular Representation Learning and Material Design

2017.09 – 2021.06

■ **B.E. in Computer Science and Technology**

GPA : 3.85/4.0

Senior Thesis: Alternated training with synthetic and authentic data for neural machine translation (A+)

Research Experiences

2025.06 – 2025.09

■ **Research Intern, Microsoft Research Cambridge**

Working on the design of inorganic material generative models.

2024.06 – 2025.06

■ **Research Intern, Alibaba DAMO Lab**

Working on Bayesian Flow Networks (BFN) for the generation of metal-organic frameworks (MOFs).

One first author paper accepted to NeurIPS 2025.

2023.02 – 2024.05

■ **Research Intern, Alibaba Tongyi Lab**

Working on the application of generative models for material design

Proposing a series of works for crystal generation by jointly optimizing lattices and fractional coordinates.

Two first author papers accepted to NeurIPS 2023, ICLR 2024. One paper on lattice permutation invariant and CoM-aware generation accepted to ICML 2024.

Selected Publications

Large Language Models for Science

- DrugTrail: Interpretable Drug Discovery via Structured Reasoning and Druggability-Tailored Preference Optimization
Yurou Liu, Mingyang Li, Xinyuan Zhu, **Rui Jiao**, Yiming Dong, Xinyu Tang, Yang Liu, Jieping Ye, Bing Su, Zheng Wang. ICLR 2026.

Geometric Graph Representation Learning

- An Equivariant Pretrained Transformer for Unified 3D Molecular Representation Learning

Rui Jiao*, Xiangzhe Kong*, Li Zhang*, Ziyang Yu, Fangyuan Ren, Wenjuan Tan, Wenbing Huang, Yang Liu. Nature Communications 2026.

- Learning 3D Anisotropic Noise Distributions Improves Molecular Force Fields
Xixian Liu*, **Rui Jiao***, Zhiyuan Liu, Yurou Liu, Yang Liu, Ziheng Lu, Wenbing Huang, Yang Zhang, Yixin Cao. NeurIPS 2025.
- DenoiseVAE: Learning Molecule-Adaptive Noise Distributions for Denoising-based 3D Molecular Pre-training
Yurou Liu*, Jiahao Chen*, **Rui Jiao***, Jiangmeng Li, Wenbing Huang, Bing Su. ICLR 2025.
- Energy-Motivated Equivariant Pretraining for 3D Molecular Graphs
Rui Jiao, Jiaqi Han, Wenbing Huang, Yu Rong, Yang Liu. AAAI 2023.

Geometric Graph Generation

- Powder Diffraction Crystal Structure Determination using Generative Models
Qi Li*, **Rui Jiao***, Liming Wu, Tiannian Zhu, Wenbing Huang, Shifeng Jin, Yang Liu, Hongming Weng, Xiaolong Chen. Nature Communications 2025.
- Siamese Foundation Models for Crystal Structure Prediction
Liming Wu, Wenbing Huang, **Rui Jiao**, Jianxing Huang, Liwei Liu, Yipeng Zhou, Hao Sun, Yang Liu, Fuchun Sun, Yuxiang Ren, Ji-Rong Wen. Nature Communications 2026.
- Peptide Design through Binding Interface Mimicry with PepMimic
Xiangzhe Kong, **Rui Jiao**, Haowei Lin, Ruihan Guo, Wenbing Huang, Wei-Ying Ma, Zihua Wang, Yang Liu, Jianzhu Ma. Nature Biomedical Engineering 2025.
- MOF-BFN: Metal-Organic Frameworks Structure Prediction via Bayesian Flow Networks
Rui Jiao, Hanlin Wu, Wenbing Huang, Yuxuan Song, Yawen Ouyang, Yu Rong, Tingyang Xu, Pengju Wang, Hao Zhou, Wei-Ying Ma, Jingjing Liu, Yang Liu. NeurIPS 2025.
- UniMoMo: Unified Generative Modeling of 3D Molecules for De Novo Binder Design
Xiangzhe Kong, Zishen Zhang, Ziting Zhang, **Rui Jiao**, Jianzhu Ma, Kai Liu, Wenbing Huang, Yang Liu. ICML 2025.
- 3D Structure Prediction of Atomic Systems with Flow-based Direct Preference Optimization
Rui Jiao, Xiangzhe Kong, Wenbing Huang, Yang Liu. NeurIPS 2024.
- Space Group Constrained Crystal Generation
Rui Jiao, Wenbing Huang, Yu Liu, Deli Zhao, Yang Liu. ICLR 2024.
- Crystal Structure Prediction by Joint Equivariant Diffusion
Rui Jiao, Wenbing Huang, Peijia Lin, Jiaqi Han, Pin Chen, Yutong Lu, Yang Liu. NeurIPS 2023.

Awards

- 2026
 - 📌 Outstanding Graduate (Ph.D.), Tsinghua University
 - 📌 Outstanding Doctoral Dissertation, Tsinghua University
- 2025
 - 📌 Class of 1984 Innovative Future Scholarship, CS Department of Tsinghua University
- 2021
 - 📌 Outstanding Graduate (Bachelor), CS Department of Tsinghua University
 - 📌 Outstanding Graduate (Bachelor), Beijing
- 2017
 - 📌 Outstanding Freshman Award, Tsinghua University

Additional Information

- Teaching Service
 - 📌 (70240033) Principle of Artificial Intelligence
Graduate Level Class, CS Department, Tsinghua University
2023S, 2024S, Instructor: Yang Liu
- Professional Service
 - 📌 Reviewers for ICLR, ICML, NeurIPS, ACL (ARR)
- Skills
 - 📌 Languages: Mandarin (native), English (fluent)
 - Coding: Proficient in Python, C++
 - Deep Learning Framework: PyTorch, PyTorch Geometric
 - Chemistry library: RDKit, Pymatgen, ASE