LUO Yanchen

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Research Interests

My current research interests focus on AI4Science, Agent4Science, and AI4Science Safety. Specifically, I work on foundation and generative models for scientific discovery (e.g., molecules and proteins), scientific agents for autonomous hypothesis generation and experiment planning, and the safety and reliability of scientific AI systems, including robustness, uncertainty estimation, and risk-aware deployment.

Educations & Background

University of Science and Technology of China Sept. 2021 – Mar. 2026
Ph.D. in School of Artificial Intelligence and Data Science,
Advisors: Prof. Xiangnan He and Prof. Xiang Wang.

University of Science and Technology of China Sept. 2017 – Jun. 2021
BSc. in School of the Gifted Young,
Advisor: Prof. Xiangnan He.

Working Experience

Research Assistant Professor,The Hong Kong Polytechnic University May 2026 – Present
Department of Data Science and Artificial Intelligence. Supervisor: Prof. Jian Huang.

Research intern, National University of Singapore Mar. 2025 – May 2025
NExT Research Centre. Supervisor: Prof. Tat-Seng Chua.

Research Intern, Ant Group Oct. 2025 – Feb. 2026
BaiLing Team.

Research Intern, DP Technology May 2025 – Aug. 2025
AI4Science foundation models.

Research Intern, Alibaba Innovative Nov. 2023 – Nov. 2024
Qwen Bailian Team.

Selected Publications

Yanchen Luo, Zhiyuan Liu, Yi Zhao, Sihang Li, Kenji Kawaguchi, Tat-Seng Chua, Xiang Wang. *Towards Unified and Lossless Latent Space for 3D Molecular Latent Diffusion Modeling.* Conference on Neural Information Processing Systems (NeurIPS) 2025

Chang Wu, Zhiyuan Liu, Wen Shu, Liang Wang, **Yanchen Luo**, Wenqiang Lei, Yatao Bian, Junfeng Fang, Xiang Wang. *3D-GSRD: 3D Molecular Graph Auto-Encoder with Selective Remask Decoding.* Conference on Neural Information Processing Systems (NeurIPS) 2025

Zhiyuan Liu* and **Yanchen Luo***, Han Huang, Enzhi Zhang, Sihang Li, Junfeng Fang, Yaorui Shi, Xiang Wang, Kenji Kawaguchi, Tat-Seng Chua. *NExT-Mol: 3D Diffusion Meets 1D Language Modeling for 3D Molecule Generation.* International Conference on Learning Representations (ICLR) 2025

Sihang Li* and **Yanchen Luo***, An Zhang, Xiang Wang, Xiangnan He, Longfei Li, Jun Zhou and Tat-Seng Chua. *Self-attentive Rationalization for Interpretable Graph Contrastive Learning.* ACM Transactions on Knowledge Discovery from Data (TKDD) 2025

Keqin Bao, Jizhi Zhang, Wenjie Wang, Yang Zhang, Zhengyi Yang, **Yanchen Luo**, Fuli Feng, Xiangnan He, Qi Tian. *A Bi-Step Grounding Paradigm for Large Language Models in Recommendation Systems.* ACM Transactions on Recommender Systems (ToRS) 2025

Yanchen Luo, Sihang Li, Zhiyuan Liu, Jiancan Wu, Zhengyi Yang, Xiangnan He, Xiang Wang, Qi Tian. *Text-guided Small Molecule Generation via Diffusion Model.* iScience 2024

Yanchen Luo, Sihang Li, Yongduo Sui, Junkang Wu, Jiancan Wu, Xiang Wang. *Masked Graph Modeling with Multi-View Contrast.* IEEE International Conference on Data Engineering (ICDE) 2024

Sihang Li, Zhiyuan Liu, **Yanchen Luo**, Xiang Wang, Xiangnan He, Kenji Kawaguchi, Tat-Seng Chua, Qi Tian. *Towards 3D Molecule-Text Interpretation in Language Models.* International Conference on Learning Representations (ICLR) 2024

Zhiyuan Liu, Sihang Li, **Yanchen Luo**, Hao Fei, Yixin Cao, Kenji Kawaguchi, Xiang Wang, Tat-Seng Chua. *MolCA: Molecular Graph-Language Modeling with Cross-Modal Projector and Uni-Modal Adapter.* Conference on Empirical Methods in Natural Language Processing (EMNLP) 2023

Underreview Paper

Zhenzhong Wang, Hanghao Li, Shujia Ding, Yongjie Hou, Yipeng Su, **Yanchen Luo**[†], Junfeng Fang. *Bridging the Thermal Gap: Benchmarking Machine Learning Force Fields across Broad Thermal Spectrum.* To be submitted to International Conference on Learning Representations (ICLR) 2026

Yanchen Luo, Zhiyuan Liu, Cheng Yang, Tat-Seng Chua, Xiang Wang. *Unified and Lossless Latent Diffusion Modeling for Structure-Based Drug Design.* To be submitted to Nature Machine Intelligence (NMI)

Zhenzhong Wang[*] and **Yanchen Luo**[*], Yongjie Hou, Shujia Ding, Junfeng Fang, Xiang Wang. *Towards Scalable Machine Learning Interatomic Potentials via Multimodal Blending.* To be submitted to Nature Machine Intelligence (NMI)

Academic Service

Reviewer: NeurIPS2025, ICLR2025, ACL2025, CVPR2024, NeurIPS2024, ICLR2024, *etc.*

Teaching Experience

Data Science Fundamentals	Sept. 2023 – Oct. 2023, Teaching Assistant
Mathematical Logic	Mar. 2020 – Sept. 2020, Teaching Assistant
Analog and Digital Circuits	Sept. 2019 – Jan. 2020, Teaching Assistant

Awards

The 3rd World AI4Science Prize Third Prize 2025
USTC Outstanding Student Scholarship 2017 & 2021 & 2022

[*]Equal contribution
[†]Corresponding author