

Haorui Li

CONTACT INFORMATION

Dept. of Computer Sci. & Eng.
The Chinese University of Hong Kong,
Shatin, New Territories, Hong Kong

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RESEARCH TOPICS

Deep Learning; Generative Models; AI for Science;

EXPERIENCES

The Chinese University of Hong Kong

Ph.D. Student in Computer Science
Advisor: Prof. Shengchao Liu

Aug. 2025 – Present

Huazhong University of Science and Technology

B.E. in Computer Science, GPA: 91.0/100
B.S. in Chemistry, GPA: 91.2/100, Ranking: 1st

Sep. 2021 – June 2025

California Institute of Technology

Undergraduate Researcher, CMS Department
Advisors: Dr. Shengchao Liu & Prof. Anima Anandkumar

July 2024 – Dec. 2024

National University of Singapore

Intern, School of Computing
Advisor: Dr. Hsiang Hui Lek

July 2023 – Aug. 2023

PUBLICATIONS

Haorui Li, Weitao Du, Yuqiang Li, Hongyu Guo, Shengchao Liu. InertialAR: Autoregressive 3D Molecule Generation with Inertial Frames. Preprint (under review).

Haorui Li, Weitao Du, Hongyu Guo, Shengchao Liu. InertialTransformer: Early Explorations and Insights into Transformer-based Geometric Representation. *LLM for Scientific Discovery Workshop, 2nd Conference on Language Modeling (COLM 2025)*

Haorui Li*, Shengchao Liu*, Hongyu Guo, Anima Anandkumar. Geometry-text Multimodal Foundation Model for Reactivity-oriented Molecule Editing. *AI for New Drug Modalities Workshop, 38th Conference on Neural Information Processing Systems (NeurIPS 2024)*

HONORS & AWARDS

National Scholarship $\times 3$ in 2022, 2023, 2024

(highest scholarship for undergraduate awarded by the Chinese government, $< 0.1\%$)

Merit Student Scholarship $\times 2$ in 2022, 2023

(given to students that excel in academics, athletics, arts of special interest, $< 1\%$)

Outstanding Undergraduates in Term of Academic Performance

(greatest honor for undergraduate in HUST, $< 0.1\%$)

Outstanding Graduate