HAORUI WANG

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EDUCATION

Georgia Institute of Technology, Atlanta *Aug. 2022 - May 2027 (Expected)*
PhD in Computational Science and Engineering
Advisor: Chao Zhang

Wuhan University, Wuhan *Sept. 2018 - Jun. 2022*
Bachelor of Engineering in Computer Science
GPA 3.84/4 Ranking top 10%

Internship availability: Spring 2026, Summer 2026, Fall 2026

SELECTED PUBLICATIONS

*Equal Contribution

- LLM-Augmented Chemical Synthesis and Design Decision Programs
  Haorui Wang, Jeff Guo, Lingkai Kong, Rampi Ramprasad, Philippe Schwaller, Yuanqi Du, Chao Zhang
  In *ICML 2025*, 2025
- Efficient Evolutionary Search Over Chemical Space with Large Language Models
  Haorui Wang*, Marta Skreta*, Cher-Tian Ser, Wenhao Gao, Lingkai Kong, Felix Strieth-Kalthoff, Chenru Duan, Yuchen Zhuang, Yue Yu, Yanqiao Zhu, Yuanqi Du, Alán Aspuru-Guzik, Kirill Neklyudov, Chao Zhang
  In *ICLR 2025*, 2025
- Aligning Large Language Models with Representation Editing: A Control Perspective
  Lingkai Kong*, **Haorui Wang***, Wenhao Mu*, Yuanqi Du, Yuchen Zhuang, Yifei Zhou, Yue Song, Rongzhi Zhang, Kai Wang, Chao Zhang
  In *NIPS 2024*, 2024
- TPD: Enhancing Student Language Model Reasoning via Principle Discovery and Guidance
  Haorui Wang, Rongzhi Zhang, Yinghao Li, Lingkai Kong, Yuchen Zhuang, Xiusi Chen, Chao Zhang
  In *COLM 2024*, 2024
- Two Birds with One Stone: Enhancing Calibration and Interpretability with Graph Functional Neural Process
  Lingkai Kong, Haotian Sun, Yuchen Zhuang, **Haorui Wang**, Wenhao Mu, Chao Zhang
  In *AISTATS 2024*, 2024
- Assessing Logical Puzzle Solving in Large Language Models: Insights from a Minesweeper Case Study
  Yinghao Li, **Haorui Wang**, Chao Zhang
  In *NAACL 2024*, 2023
- Equivariant and stable positional encoding for more powerful graph neural networks
  Haorui Wang, Haoteng Yin, Muhan Zhang, Pan Li
  In *ICLR 2022*, 2022

INDUSTRY EXPERIENCE

Applied Scientist Intern, Amazon, Palo Alto, CA ***May. 2025 - Dec. 2025***
Advisor: Liqiang Xiao, Rufus Group
Topic: Web-search trajectory synthesis and web-agent training

- Synthesized diverse multi-tool web search trajectories to supervise multi-turn agents.
- Built a multi-turn tool-use training framework based on VeRL; paper in preparation.

Research Intern, NEC Lab America, Princeton, NJ ***May. 2024 - Aug. 2024***
Advisor: LuAn Tang, NEC lab DSSS Team
Topic: Multi-agent system for decision-making

Research Intern, Bytedance AI lab, Shanghai ***May. 2022 - Aug. 2022***
Advisor: Xiaoqin Tan, Bytedance AI lab
Topic: Learning Hierarchical Protein Representations via Graph Neural Networks
Built graph neural networks to learn protein representations from different levels.

- Considered to extract protein representations across various structural levels, including the atom, residue, and surface levels.
- Designed a GNN framework to learn and combine representations from each level to get a protein representation.
- Evaluated the framework on protein-protein interaction task.

RESEARCH EXPERIENCE

Research Assistant, Georgia Institute of Technology, Atlanta, GA ***Jun. 2023 - Now***
Advisor: Chao Zhang, Georgia Institute of Technology
Topic: Building LLM agents for decision-making tasks. 1. Extracting knowledge from LLMs. 2. Self-evolving agents.

- Developed a teacher-student framework enabling advanced language models to mentor weaker agents through principle discovery.
- Developed a representation editing method through a control perspective to align LLMs.
- Combined evolutionary search framework with LLMs for molecular optimization tasks.
- Built LLM-augmented framework for retrosynthesis planning and synthesizable molecule design.

Research Assistant, Georgia Institute of Technology, Atlanta, GA ***Sep. 2022 - May 2023***
Advisor: Chao Zhang, Georgia Institute of Technology
Topic: Generative Active Learning for Decision-focused Learning
Investigated using generative models for data augmentation in the decision-focused learning process.

- Developed a comprehensive framework to generate new data by leveraging model uncertainty in decision-focused learning.
- Tested different uncertainty quantification methods in the framework.
- Evaluated the developed framework in real-world scenarios, such as power scheduling and COVID-19 resource allocation.

Research Assistant, Purdue University, West Lafayette, IN ***Mar. 2021 - Jan. 2022***
Advisor: Pan Li, Purdue University
Topic: Equivariant and Stable Positional Encoding for More Powerful Graph Neural Networks
Studied the failure of GNN on tasks based on sets of nodes in a principled way and proposed a provable solution.

- Considered absolute positions of nodes in the graph as the extra node features.
- Designed a GNN architecture keeping permutation equivariant w.r.t. node features and rotation equivariant w.r.t. positional features.
- Evaluated PEG on traditional link prediction and domain shift link prediction.

SKILLS

Programming languages: Proficient in Python, C#. Familiar with C++, JavaScript, C, MATLAB.
Interests: LLM agents, Large language models for reasoning/decision making, Agents for scientific discovery.

HONORS AND AWARDS

Scholarship
First Class Scholarship(Top 5% in undergraduate) *Sept. 2019*
Second Class Scholarship(Top 10% in undergraduate) *Sept. 2020*