

JIAQI HAN

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[Github](#) | [Webpage](#) | [Google Scholar](#)

EDUCATION

Tsinghua University

B. Eng in Computer Science

Beijing, China

Sep. 2017 – July 2021

- Selected awards: First Place in Open Catalyst 2022 Competition, Outstanding Graduate of Beijing, Academic Excellence Award 2018 & 2019
- Research interests: Graph neural networks - theories and applications; AI4Science – molecular and protein modeling, 3D geometric models, physics-inspired model designs.

Stanford University

PhD in Computer Science

Stanford, CA, USA

Sep. 2023 – Present

PUBLICATIONS

1. Rui Jiao, Wenbing Huang, Peijia Lin, **Jiaqi Han**, Pin Chen, Yutong Lu, Yang Liu. “[Crystal Structure Prediction by Joint Equivariant Diffusion](#)”. *Advances in Neural Information Processing Systems (NeurIPS 2023)*
2. **Jiaqi Han**, Wenbing Huang, Yu Rong, Tingyang Xu, Fuchun Sun, and Junzhou Huang. “[Structure-Aware DropEdge Towards Deep Graph Convolutional Networks](#)”. *IEEE Transactions on Neural Networks and Learning Systems (TNNLS)*, 2023
3. Runfa Chen*, **Jiaqi Han***, Fuchun Sun, Wenbing Huang. “[Subequivariant Graph Reinforcement Learning in 3D Environments](#)”. *International Conference on Machine Learning (ICML 2023)*, **Oral Presentation (155/6538, ~2.3%)**
4. Rui Jiao, **Jiaqi Han**, Wenbing Huang, Yu Rong, and Yang Liu. “[Energy-Motivated Equivariant Pretraining for 3D Molecular Graphs](#)”. *AAAI Conference on Artificial Intelligence (AAAI 2023)*
5. **Jiaqi Han**, Wenbing Huang, Hengbo Ma, Jiachen Li, Joshua B. Tenenbaum, and Chuang Gan. “[Learning Physical Dynamics with Subequivariant Graph Neural Networks](#)”. *Advances in Neural Information Processing Systems (NeurIPS 2022)*
6. **Jiaqi Han**, Wenbing Huang, Tingyang Xu, and Yu Rong. “[Equivariant Graph Hierarchy-Based Neural Networks](#)”. *Advances in Neural Information Processing Systems (NeurIPS 2022)*
7. Wenbing Huang*, **Jiaqi Han***, Yu Rong, Tingyang Xu, Fuchun Sun, and Junzhou Huang. “[Equivariant Graph Mechanics Networks with Constraints](#)”. *International Conference on Learning Representations (ICLR 2022)*
8. **Jiaqi Han**, Yu Rong, Tingyang Xu, and Wenbing Huang. “[Geometrically Equivariant Graph Neural Networks: A Survey](#)”. *arXiv preprint 2202.07230*.
9. Zhihan Li, Youjian Zhao, **Jiaqi Han**, Ya Su, Rui Jiao, Xidao Wen, and Dan Pei. “[Multivariate Time Series Anomaly Detection using Hierarchical Inter-Metric and Temporal Embedding](#)”. *The 27th ACM SIGKDD Conference on Knowledge Discovery and Data Mining (KDD 2021)*

* denotes equal contribution. Publications are listed in chronological order.

RESEARCH EXPERIENCE

Tencent AI Lab, Machine Learning Center

Research Intern to Dr. Yu Rong, Prof. [Junzhou Huang](#), and Prof. [Wenbing Huang](#)

Shenzhen, China

Feb. 2020 – May 2023

[Geometric Graph Neural Networks for Science](#)

- Investigated injecting equivariance (symmetry constraint) in modeling constrained physical and biochemical systems like molecules, as well as for larger and hierarchical systems like proteins.
- The designed models improved the molecular dynamics simulation precision by up to 26% and protein dynamics simulation by 20%, verifying the efficacy of the proposed equivariant GNN in modeling complex systems of different scales.
- Two first author papers accepted to ICLR 2022 and NeurIPS 2022. One paper on building deep graph convolutional networks accepted to IEEE TNNLS journal.
- Selected into Tencent Rhino Bird Elite Program 2020.

MIT, CSAIL

Research Assistant to Dr. [Chuang Gan](#) and Prof. [Joshua B. Tenenbaum](#)

Cambridge, United States

Mar. 2022 – June 2022

[Modeling Physical interactions with Proper Symmetry as Prior](#)

- Designed a particle-based GNN that considers physical symmetry of the system with external forces.
- Demonstrated model is 3x more data-efficient and generalizable on physical scene simulation tasks.
- First author paper accepted to NeurIPS 2022.

Tsinghua University, Institute of AI Industry Research (AIR)

Beijing, China

Research Assistant to Prof. [Wenbing Huang](#)

Sep. 2021 – Feb. 2022

Geometrically Equivariant Graph Neural Networks: Survey and Applications

- Surveyed recent advances in geometrically equivariant GNNs; First author paper available on arXiv.
- Proposed a novel 3D pretraining framework for molecular graphs, equipped with an energy-based representation model. The pretraining framework is also theoretically guaranteed to meet the symmetry constraint by leveraging the Riemann-Gaussian distribution.
- Paper on 3D molecular pretraining accepted to AAAI 2023, on crystal generation accepted to NeurIPS 2023.

University of Chicago, Department of Computer Science

Chicago, United States

Research Assistant to Prof. [Yuxin Chen](#)

July 2020 – Sep. 2020

Multi-fidelity Bayesian Optimization for Physical PDE Solvers

- Studied multi-fidelity Bayesian Optimization in combinatorial setting to bring down the simulation cost of finding proper parameter configuration of physical simulations.
- Implemented a toolkit that achieved the goal by cutting down the cost by half over existing approaches.

Tsinghua University, Netman Lab

Beijing, China

Research Assistant to Prof. [Dan Pei](#)

June 2019 – Jan. 2020

Anomaly Detection on Multivariate Time Series

- Developed a novel framework for anomaly detection and interpretation of multivariate time series data. The method takes a two-view modeling approach with both inter-metric and temporal embeddings. The framework has been deployed in a network company and received positive feedbacks.
- Paper accepted to KDD 2021.

AWARDS AND HONORS

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| • NeurIPS'22 Open Catalyst Challenge 2022 , received first place and invited to give speech | 2022 |
| • Outstanding Graduate of Tsinghua University | 2021 |
| • Outstanding Graduate of Beijing | 2021 |
| • Academic Excellence Award, Tsinghua University | 2019 |
| • Academic Excellence Award, Tsinghua University | 2018 |
| • Outstanding Freshman Award, Tsinghua University | 2017 |

ADDITIONAL INFORMATION

Professional Service

- Serve as reviewer for ICML 2022-2023, KDD 2022, NeurIPS 2022-2023, ICLR 2023-2024

Other Interests

- Piano: Proficient with amateur level-10 national certificate.

Computer and Language Skills

- Coding language: Proficient in Python, C++, Java.
- Deep learning framework: PyTorch, PyG (PyTorch Geometric).
- Biochemistry library: RDKit, MDAnalysis, PyMol
- Languages: Chinese (native), English (proficient)