

# Yinan Huang

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## Education

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- Georgia Institute of Technology, USA**, Ph.D. in Machine Learning Sept 2023 – 2027 (Expected)
- Advisor: Pan Li
- Duke University, USA**, M.S. in Electrical and Computer Engineering Sept 2020 - May 2023
- GPA: 4.0/4.0
- Sun Yat-sen University, China**, B.S. in Physics Sept 2016 - May 2020
- GPA: 4.3/5.0, Rank: 1/83

## Research Interests

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**Geometric Deep Learning:** graph neural networks, equivariant neural networks

**Generative Models:** diffusion model/flow matching for spatio-temporal data

**AI for Science:** apply geometric-aware/generative AI models for scientific discovery, forecasting and decision-making/control

## Research Experience

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- Research Assistant**, Georgia Institute of Technology Sept 2023 –
- Developed stable and expressive positional encodings for undirected and directed graphs (ICLR 2024-2025)
  - Developed a differentially private training algorithm for relational learning with rigorous entity-level privacy guarantees (NeurIPS 2025)
  - Developing efficient diffusion and flow-matching models for online forecasting and decision-making (ongoing)
- Research Intern**, Peking University Feb 2022 – Sept 2022
- Revealed fundamental limitations of subgraph neural networks in capturing graph substructures, and developed an efficient node labeling method to enhance their expressive power (ICLR 2023)
- Research Intern**, Beijing Institute for General Artificial Intelligence Sept 2021 – Feb 2022
- Developed E(3)-equivariant generative models that incorporate molecular geometry for drug discovery (ICML 2022, Oral)

## Publications

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- [1] 3DLinker: An E(3) Equivariant Variational Autoencoder for Molecular Linker Design  
**Yinan Huang**, Xingang Peng, Jianzhu Ma, Muhan Zhang  
*International Conference on Machine Learning (ICML), 2022 (Oral)*.
- [2] Boosting the Cycle Counting Power of Graph Neural Networks with I<sup>2</sup>-GNNs  
**Yinan Huang**, Xingang Peng, Jianzhu Ma, Muhan Zhang  
*International Conference on Learning Representations (ICLR), 2023*.
- [3] On the Stability of Expressive Positional Encodings for Graphs  
**Yinan Huang\***, William Lu\*, Joshua Robinson, Yu Yang, Muhan Zhang, Stefanie Jegelka, Pan Li  
*International Conference on Learning Representations (ICLR), 2024*.
- [4] What Are Good Positional Encodings for Directed Graphs?  
**Yinan Huang**, Haoyu Wang, Pan Li  
*International Conference on Learning Representations (ICLR), 2025*.
- [5] Is Distance Matrix Enough for Geometric Deep Learning?

Zian Li, Xiyuan Wang, **Yinan Huang**, Muhan Zhang  
*Advances in Neural Information Processing Systems (NeurIPS), 2023.*

- [6] Differentially Private Relational Learning with Entity-level Privacy Guarantees  
**Yinan Huang\***, Haoteng Yin\*, Eli Chien, Rongzhe Wei, Pan Li  
*Advances in Neural Information Processing Systems (NeurIPS), 2025.*
- [7] GenAI Copyright Evidence with Operational Meaning  
Eli Chien, Amit Saha, **Yinan Huang**, Pan Li  
*ICML Workshop on Reliable and Responsible Foundation Models, 2025*
- [8] Powers of Magnetic Graph Matrix: Fourier Spectrum, Walk Compression, and Applications  
**Yinan Huang**, David F Gleich, Pan Li  
*The Proceedings of the National Academy of Sciences (PNAS), 2026*

## Preprints

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- [1] Accelerated Sequential Flow Matching: A Bayesian Filtering Perspective  
**Yinan Huang**, Hans Hao-Hsun Hsu, Junran Wang, Bo Dai, Pan Li  
<https://arxiv.org/abs/2602.05319>
- [2] What Can We Learn from State Space Models for Machine Learning on Graphs?  
**Yinan Huang\***, Siqu Miao\*, Pan Li  
<https://arxiv.org/abs/2406.05815>
- [3] A Benchmark on Directed Graph Representation Learning in Hardware Designs  
Haoyu Wang, **Yinan Huang**, Nan Wu, Pan Li  
<https://arxiv.org/abs/2410.06460>

## Honors and Awards

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- Travel Award for ICLR 2025
- Georgia Tech ECE Fellowship 2023
- China National Scholarship 2017

## Professional Service

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- Reviewer for International Conference on Machine Learning (ICML) 2023-2025
- Reviewer for International Conference on Learning Representations (ICLR) 2024-2025
- Reviewer for Advances in Neural Information Processing Systems (NeurIPS) 2023-2026
- Program Committee for Association for the Advancement of Artificial Intelligence (AAAI) 2026
- Reviewer for Association for Computing Machinery's Special Interest Group on Knowledge Discovery and Data Mining (KDD) 2026
- Teaching Assistant: ECE 3077 Introduction to Probability and Statistics, ECE 6250 Advanced Digital Signal Processing

## Skills

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- Programming languages and frameworks: Python, Pytorch, Pytorch Geometric, Matlab, C