

Yuchao Lin

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RESEARCH INTERESTS

Graph neural networks, 3D geometric graph learning, Equivariant network design.

EDUCATION

- Ph.D. **Texas A&M University**, College Station, TX, USA 2021-Present
Department of Computer Science & Engineering
Supervised by [Prof. Shuiwang Ji](#)
- B.S. **Nanjing University**, Nanjing, Jiangsu, China 2016-2020
Department of Software Engineering
Supervised by [Prof. Yang Yu](#)
Thesis: A Distributional Perspective on Self-Supervised Monocular Depth Estimation

PROFESSIONAL EXPERIENCE

- 2023 **Fujitsu Research of America, Inc.**, Santa Clara, CA, USA Jan 2023 - Apr 2023
Research Intern advised by Kanji Uchino
Work on molecular conformer generation & docking
- 2020 **Polixir Technologies**, Nanjing, China Jul 2020 - Aug 2020
Research Intern advised by [Prof. Yang Yu](#)
Work on extrinsic autocalibration and monocular depth estimation

PUBLICATIONS

- 2024 **Equivariance via Minimal Frame Averaging for More Symmetries and Efficiency.**
Yuchao Lin, Jacob Helwig, Shurui Gui, Shuiwang Ji. *Proceedings of the 41th International Conference on Machine Learning (ICML)*, 2024. **ICML Spotlight [Acceptance Rate 3.5%]**.
[\[PDF Link\]](#) [\[Code\]](#)
- 2024 **SineNet: Learning Temporal Dynamics in Time-Dependent Partial Differential Equations.** Xuan Zhang, Jacob Helwig, **Yuchao Lin**, Yaochen Xie, Cong Fu, Stephan Wojtowytsch, Shuiwang Ji. *Proceedings of the 41th International Conference on Machine Learning (ICLR)*, 2024. [\[PDF Link\]](#) [\[Code\]](#)
- 2024 **Genetic InfoMax: Exploring Mutual Information Maximization in High-Dimensional Imaging Genetics Studies.** Yaochen Xie, **Yuchao Lin**, Ziqian Xie, Sheikh Muhammad Saiful

- Islam, Degui Zhi, Shuiwang Ji. *Transactions on Machine Learning Research (TMLR)*, 2024. [\[PDF Link\]](#)
- 2023 **Large Scale Benchmark of Materials Design Methods.** Kamal Choudhary, Daniel Wines, Kangming Li, ..., Keqiang Yan, **Yuchao Lin**, Shuiwang Ji, ..., Adam J. Biacchi, Francesca Tavazza. *npj Computational Materials*. [\[PDF Link\]](#) [\[Website\]](#)
- 2023 **Artificial Intelligence for Science in Quantum, Atomistic, and Continuum Systems.** Xuan Zhang, Limei Wang, Jacob Helwig, Youzhi Luo, Cong Fu, Yaochen Xie, Meng Liu, **Yuchao Lin**, ..., Tess Smidt, Shuiwang Ji. *arXiv preprint arXiv:2307.08423 (2023)*. [\[PDF Link\]](#) [\[Code\]](#)
- 2023 **Efficient Approximations of Complete Interatomic Potentials for Crystal Property Prediction.** **Yuchao Lin**, Keqiang Yan, Youzhi Luo, Yi Liu, Xiaoning Qian, and Shuiwang Ji. *Proceedings of the 40th International Conference on Machine Learning (ICML)*, 2023. [\[PDF Link\]](#) [\[Code\]](#) [\[Math Overview\]](#)
- 2022 **ComENet: Towards Complete and Efficient Message Passing for 3D Molecular Graphs.** Limei Wang*, Yi Liu*, **Yuchao Lin**, Haoran Liu, and Shuiwang Ji. *The 36th Annual Conference on Neural Information Processing Systems (NeurIPS)*, 2022. [\[PDF Link\]](#) [\[Code\]](#)
- 2022 **Periodic Graph Transformers for Crystal Material Property Prediction.** Keqiang Yan, Yi Liu, **Yuchao Lin**, and Shuiwang Ji. *Thirty-sixth Conference on Neural Information Processing Systems (NeurIPS)*, 2022. [\[PDF Link\]](#) [\[Code\]](#)
- 2022 **Spherical Message Passing for 3D Molecular Graphs.** Yi Liu*, Limei Wang*, Meng Liu, **Yuchao Lin**, Xuan Zhang, Bora Oztekin, and Shuiwang Ji. *International Conference on Learning Representations (ICLR)*, 2022. [\[PDF Link\]](#) [\[Code\]](#)

SELECTED SCHOLARSHIPS, AWARDS, & HONORS

Travel Award , International Conference on Machine Learning (ICML)	2024
3rd Place of Open Catalyst Challenge	2021
National Scholarship , Nanjing University	2019

PROFESSIONAL SERVICES

Program Committee Member | Reviewer

The Conference on Neural Information Processing Systems (NeurIPS)	2023,2024
Proceedings of the International Conference on Learning Representations (ICLR)	2024,2025