Yuchao Lin

Ph.D. Student
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RESEARCH INTERESTS

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

EDUCATION

Ph.D.   **Texas A&M University**, Department of Computer Science & Engineering, 2021-Present

Supervised By Prof. Shuiwang Ji

B.S.   **Nanjing Univerty**, Department of Software Engineering, 2016-2020

Supervised By Prof. Yang Yu

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.

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. *arXiv preprint arXiv:2306.11688 (2023)*. PDF Link.

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.

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.

SCHOLARSHIPS, AWARDS, & HONORS

2021　3rd Place of Open Catalyst Challenge

2019　National Scholarship, Nanjing University

PROFESSIONAL EXPERIENCE

01/2023-04/2023　Research Intern at Fujitsu Research of America, Inc.

07/2020-08/2020　Research Intern at Polixir Technologies, Supervised by Dr. Yang Yu.

PROFESSIONAL SERVICES

Program Committee Member | Reviewer

2024　The 38th Conference on Neural Information Processing Systems (NeurIPS), 2024

2024　Proceedings of the 12th International Conference on Learning Representations (ICLR), 2024

2023　The 37th Conference on Neural Information Processing Systems (NeurIPS), 2023