Yuchao Lin

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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. Submitted to *Proceedings of the 41th International Conference on Machine Learning (ICML), 2024*.

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.

PROFESSIONAL EXPERIENCE

2023   Research Intern at Fujitsu Research of America, Inc.

2020   Research Intern at Polixir Technologies

SCHOLARSHIPS, AWARDS, & HONORS

2021   3rd Place of Open Catalyst Challenge

2019   National Scholarship, Nanjing University

PROFESSIONAL SERVICES

Program Committee Member | Reviewer

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

2023   Proceedings of the 41th International Conference on Learning Representations (ICLR), 2024