Yuchao Lin

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Department of Computer Science & Engineering
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RESEARCH INTERESTS

Graph Deep Learning: graph neural networks, graph transformer.

AI for Science: 3D molecule generation, protein-ligand docking, material property prediction.

Generative Modeling: diffusion modeling, score-based generative modeling.

EDUCATION

Ph.D.   **Texas A&M University**, Department of Computer Science & Engineering, 2021-
Supervised By Prof. Shuiwang Ji

B.S.   **Nanjing Univerty**, Department of Software Engineering, 2016-2020
Supervised By Prof. Yang Yu

PUBLICATIONS

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*.

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

2020   Research Intern at Polixir Technologies; Supervised By Prof. Yang Yu

2020-21   Research Assistant at LAMDA, Nanjing University; Supervised By Prof. Yang Yu

SCHOLARSHIPS, AWARDS, & HONORS

2021   3rd Place of Open Catalyst Challenge

2019   National Scholarship, Nanjing University