

Yuchao Lin

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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 University**, Department of Software Engineering, 2016-2020
Supervised By Prof. Yang Yu

PUBLICATIONS

- 2022 **Efficient Approximations of Complete Interatomic Potentials for Crystal Property Prediction.** Yuchao Lin, Keqiang Yan, Youzhi Luo, Yi Liu, Xiaoning Qian, and Shuiwang Ji. Under review on ICLR 2023. PDF Link.
- 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