

# 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.
- 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.
- 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.
- 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.

## PROFESSIONAL EXPERIENCE

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

## SCHOLARSHIPS, AWARDS, & HONORS

- 2019     National Scholarship, Nanjing University