

# Yuchao Lin

Ph.D. Student  
Department of Computer Science & Engineering  
Texas A&M University

kruskallin@tamu.edu  
kruskallin.github.io

## RESEARCH INTERESTS

**Graph Deep Learning:** graph neural networks, graph transformer, equivariant network design.

**AI for Science:** molecule property prediction, material property prediction, protein-ligand docking.

## 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

- 2023 **Large Scale Benchmark of Materials Design Methods.** Kamal Choudhary, Daniel Wines, Kangming Li, ..., Keqiang Yan, **Yuchao Lin**, Shuiwang Ji, ..., Adam J. Bicchi, 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 (ICLR), 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

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

2020-21    Research Assistant at LAMDA, Nanjing University; Supervised By Prof. Yang Yu  
2022       Research Intern at Fujitsu Research of America, Inc.

## **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