

# Wendi Yu

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## EDUCATION

- Sep 2023–Present**      **Texas A&M University**  
*Ph.D. student in Computer Science · Advisor: Prof. Shuiwang Ji*
- Sep 2019–June 2023**      **Tongji University**  
*Bachelor of Software Engineering (Machine Intelligence) · GPA: 91.25/100*

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## RESEARCH EXPERIENCE

- 2025–Present**      **Texas A&M University — Ph.D. Research, Advisor: Prof. Shuiwang Ji**  
*Diffusion LMs: efficient parallel decoding (project lead, in preparation)*  
*LLM agents: multi-agent theory (NeurIPS 2026, first author, agents for scientific discovery)*  
*AI for science: E(3)-equivariant GNNs (NeurIPS 2026)*
- 2022–2023**      **North Carolina State University — Research Intern, Advisor: Prof. Xiaorui Liu**  
*Spectral GNNs: automated polynomial filter learning (IEEE BigData 2024, first author)*

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## PUBLICATIONS

### Selected Publications (\* equal contribution)

- Wendi Yu\***, Lianhao Zhou\*, Xiangjue Dong, Sai Sudarshan Barath, Declan Staunton, Byung-Jun Yoon, Xiaoning Qian, James Caverlee, Shuiwang Ji. *When Do Multi-Agent Systems Help? An Information Bottleneck Perspective.*      **NeurIPS, 2026**
- Chenxing Liang, Yuchao Lin, Andrii Kryvenko, **Wendi Yu**, Chuan Li, Jianwen Xie, Xiaofeng Qian, Shuiwang Ji. *Spin-Weighted Spherical Harmonics Enable Complete and Scalable E(3)-Equivariant Networks.*      **NeurIPS, 2026**
- Lianhao Zhou, **Wendi Yu**, Brady Nguyen, Declan Staunton, Sai Sudarshan Barath, Shuiwang Ji. *Multi-Agent Asymmetric Memory Evolution for Algorithm Design.*      **Manuscript, 2026**
- Lianhao Zhou, Hongyi Ling, Cong Fu, Yepeng Huang, Michael Sun, **Wendi Yu**, Xiaoxuan Wang, Xiner Li, Xingyu Su, Junkai Zhang, Xiusi Chen, Chenxing Liang, Xiaofeng Qian, Heng Ji, Wei Wang, Marinka Zitnik, Shuiwang Ji. *Autonomous Agents for Scientific Discovery: Orchestrating Scientists, Language, Code, and Physics.*      **Preprint, arXiv:2510.09901, 2025**
- Wendi Yu**, Zhichao Hou, Xiaorui Liu. *Automated Polynomial Filter Learning for Graph Neural Networks.*      **IEEE BigData, 2024**
- Gang Li, **Wendi Yu**, Yao Yao, Wei Tong, Yingbin Liang, Qihang Lin, Tianbao Yang. *Model Developmental Safety: A Safety-Centric Method and Applications in Vision-Language Models.*      **NeurIPS AFM Workshop, 2024**

## Other Publications

Lianhao Zhou, Raj S Roy, Zachary Krueger, **Wendi Yu**, Byung-Jun Yoon, Xiaoning Qian, Shuiwang Ji. EvoAntigen: An Evolving Agent for Antigen Design. **NeurIPS AgenticLS Workshop, 2026**

Xiner Li, Xingyu Su, Yuchao Lin, Chenyu Wang, Yijia Xiao, Tianyu Liu, Chi Han, Michael Sun, Montgomery Bohde, Anna Hart, **Wendi Yu**, Masatoshi Uehara, Gabriele Scalia, Xiao Luo, Carl Edwards, Wengong Jin, Jianwen Xie, Ehsan Hajiramezanali, Edward De Brouwer, Qing Sun, Byung-Jun Yoon, Xiaoning Qian, Marinka Zitnik, Heng Ji, Hongyu Zhao, Wei Wang, Shuiwang Ji. Generative Artificial Intelligence for Biology: Toward Unifying Models, Algorithms, and Modalities. **ChemRxiv preprint, 2026**

Xuelin Tang, Yan Chen, Yongfei Ren, Wanli Yang, **Wendi Yu**, Yu Zhou, Jingyan Guo, Jiali Hu, Xi Chen, Yuqi Gu, Chuyi Wang, Yi Dong, Hong Yang, Christine Sato, Ji He, Dongsheng Fan, Linya You, Lorne Zinman, Ekaterina Rogaeva, Yelin Chen, Ming Zhang. Deep learning analyses of splicing variants identify the link of PCP4 with amyotrophic lateral sclerosis. **Brain, 2025**

Cong Fu, Yuchao Lin, Zachary Krueger, **Wendi Yu**, Xiaoning Qian, Byung-Jun Yoon, Raymundo Arróyave, Xiaofeng Qian, Toshiyuki Maeda, Maho Nakata, Shuiwang Ji. A Benchmark for Quantum Chemistry Relaxations via Machine Learning Interatomic Potentials. **Preprint, arXiv:2506.23008, 2025**

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## HONORS AND AWARDS

|                  |                                                                |
|------------------|----------------------------------------------------------------|
| <b>2025–2026</b> | TAMIDS Graduate Research Fellow                                |
| <b>2023</b>      | Outstanding Graduation Thesis, Tongji University               |
| <b>2023</b>      | Outstanding Graduate, Tongji University                        |
| <b>2019–2022</b> | Cyrus Tang Scholarship, Tongji University                      |
| <b>2021</b>      | Meritorious Winner, Mathematical Contest in Modeling (MCM/ICM) |
| <b>2019–2023</b> | Outstanding Student Scholarship, Tongji University             |

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## SERVICE

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|---------------------------|---------------------------------------------------------------|
| <b>Reviewer</b>           | ACM Computing Surveys                                         |
| <b>Teaching Assistant</b> | CSCE 421 Machine Learning, CSCE 313 Intro to Computer Systems |