# Haiyang Yu

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

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## RESEARCH AREAS

My research interests are graph deep learning, AI for science, and trustworthy AI. I am one of the authors of SubgraphX explaining the GNNs to human and GraphFM applying GNNs on large-scale graphs containing massive nodes and edges. Additionally, I am the author of QHNet and QH9, which facilitate the usage of machine learning model, particularly equivariant networks, for density functional theory (DFT). I am also one of the authors of Seq2Exp using LLM, a framework that uses large language models (LLM) to capture the causal relationships between DNA and epigenomic data for gene-expression prediction, which is an oral paper from the ICLR.

## EDUCATION

**TEXAS A&M University (TAMU)**                                    *Augest 2020 - Present*
Ph.D. in Computer Science Engineering; Advisor: Prof. Shuiwang Ji

**University of Science and Technology of China (USTC)**          *September 2016 - July 2020*
B.S. in Electronic and Information Engineering

## EXPERIENCE

**TEXAS A&M University (TAMU)**                                    *Augest 2024 - December 2024*
Graduate Assistant Lecturer
CSCE 421-503: Machine Learning (course for undergraduate students)

**Amazon Web Service (AWS)**          *June 2023 - Augest 2023 and June 2024 - Augest 2024*
Applied Scientist Intern, Graph Machine Learning Team
Mentor: Dr. Xiang Song                                            Santa Clara, CA, USA

**University of Sydney (USYD)**                                   *July 2019 - September 2019*
Visiting Student
Advisor: Dr. Jing Zhang, Prof. Dacheng Tao                        Sydney, Australia

## PUBLICATIONS

* indicates equal contribution

Xingyu Su*, **Haiyang Yu**\*, Degui Zhi and Shuiwang Ji. **Learning to discover regulatory elements for gene expression prediction.** *International Conference on Learning Representations* (**ICLR 2025 Oral**).

Karish Grover, **Haiyang Yu**, Xiang Song, Qi Zhu, Han Xie, Vassilis N. Ioannidis, Christos Faloutsos. **Spectro-Riemannian Graph Neural Networks.** *International Conference on Learning Representations* (**ICLR 2025**).

Zhao Xu*, **Haiyang Yu**\*, Montgomery Bohde, and Shuiwang Ji. **Equivariant Graph Network Approximations of High-Degree Polynomials for Force Field Prediction.** Transactions on Machine Learning Research (**TMLR Featured**), 2024.

Meng-Chieh Lee, **Haiyang Yu**, Jian Zhang, Vassilis N. Ioannidis, Xiang Song, Soji Adeshina, Da Zheng and Christos Faloutsos. **NetInfoF Framework: Measuring and Exploiting Network Usable Information.** *International Conference on Learning Representations* (**ICLR 2024 Spotlight**).

Meng Liu, **Haiyang Yu**, and Shuiwang Ji. **Your Neighbors Are Communicating: Towards Powerful and Scalable Graph Neural Networks.** Transactions on Machine Learning Research (**TMLR**), 2024.

**Haiyang Yu\***, Meng Liu\*, Youzhi Luo, Alex Strasser, Xiaofeng Qian, Xiaoning Qian, and Shuiwang Ji. **QH9: A Quantum Hamiltonian Prediction Benchmark for QM9 Molecules.** *Neural Information Processing Systems, Datasets and Benchmarks Track* (**NeurIPS 2023**).

**Haiyang Yu**, Zhao Xu, Xiaofeng Qian, Xiaoning Qian, Shuiwang Ji. **Efficient and Equivariant Graph Networks for Predicting Quantum Hamiltonian.** *International Conference on Machine Learning* (**ICML 2023**).

Hao Yuan, **Haiyang Yu**, Shurui Gui, Shuiwang Ji. **Explainability in Graph Neural Networks: A Taxonomic Survey.** IEEE Transactions on Pattern Analysis and Machine Intelligence (**TPAMI**), 2022.

Shuiwang Ji\*, Meng Liu\*, Liu, Yi\*, Youzhi Luo\*, Limei Wang\*, Yaochen Xie\*, Zhao Xu\*, **Haiyang Yu\***. **Frontiers of Graph Neural Networks with DIG.** *ACM SIGKDD International Conference on Knowledge Discovery and Data Mining* (**SIGKDD 2022 Hands-on Tutorial**).

**Haiyang Yu\***, Limei Wang\*, Bokun Wang\*, Meng Liu, Tianbao Yang, and Shuiwang Ji. **GraphFM: Improving Large-Scale GNN Training via Feature Momentum.** *International Conference on Machine Learning* (**ICML 2022**), 25684–25701.

Meng Liu\*, Youzhi Luo\*, Limei Wang\*, Yaochen Xie\*, Hao Yuan\*, Shurui Gui\*, **Haiyang Yu\***, Zhao Xu, Jingtun Zhang, Yi Liu, Keqiang Yan, Haoran Liu, Cong Fu, Bora Oztekin, Xuan Zhang, and Shuiwang Ji. **DIG: A Turnkey Library for Diving into Graph Deep Learning Research.** Journal of Machine Learning Research (**JMLR**), 22(240): 1-9, 2021.

Hao Yuan, **Haiyang Yu**, Jie Wang, Kang Li, Shuiwang Ji. **On explainability of graph neural networks via subgraph explorations.** *International Conference on Machine Learning* (**ICML 2021**), 12241-12252

## PREPRINTS

Xuan Zhang\*, Limei Wang\*, Jacob Helwig\*, Youzhi Luo\*, Cong Fu\*, Yaochen Xie\*, Meng Liu, Yuchao Lin, Zhao Xu, Keqiang Yan, Keir Adams, Maurice Weiler, Xiner Li, Tianfan Fu, Yucheng Wang, **Haiyang Yu**, YuQing Xie, Xiang Fu, Alex Strasser, Shenglong Xu, Yi Liu, Yuanqi Du, Alexandra Saxton, Hongyi Ling, Hannah Lawrence, Hannes Stärk, Shurui Gui, Carl Edwards, Nicholas Gao, Adriana Ladera, Tailin Wu, Elyssa F. Hofgard, Aria Mansouri Tehrani, Rui Wang, Ameya Daigavane, Montgomery Bohde, Jerry Kurtin, Qian Huang, Tuong Phung, Minkai Xu, Chaitanya K. Joshi, Simon V. Mathis, Kamyar Azizzadenesheli, Ada Fang, Alán Aspuru-Guzik, Erik Bekkers, Michael Bronstein, Marinka Zitnik, Anima Anandkumar, Stefano Ermon, Pietro Liò, Rose Yu, Stephan Günnemann, Jure Leskovec, Heng Ji, Jimeng Sun, Regina Barzilay, Tommi Jaakkola, Connor W. Coley, Xiaoning Qian, Xiaofeng Qian, Tess Smidt, Shuiwang Ji. **Artificial Intelligence for Science in Quantum, Atomistic, and Continuum Systems.** 2023. Paper Link: https://arxiv.org/abs/2307.08423

## SELECTED AWARDS

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|---|---:|
| ICML Travel Grant | *2022* |
| Institute of electronics, Chinese Academy of Science Scholarship | *2019* |
| Outstanding Student Scholarship (Golden), USTC | *2018* |

## SERVICES | PROGRAM COMMITTEE MEMBER | REVIEWER

International Conference on Machine Learning (**ICML**) *2022, 2023, 2024*

International Conference on Learning Representations (**ICLR**) *2023, 2024, 2025*

Annual Conference on Neural Information Processing Systems (**NeurIPS**) *2023, 2024*

Learning on Graphs Conference (**LoG**) *2022, 2023*

Student volunteer on Knowledge Discovery and Data Mining (**KDD**) *2022*

IEEE Transactions on Pattern Analysis and Machine Intelligence (**TPAMI**)