Cong Fu

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

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Research Interests and Highlights

- My research interests are **deep learning** and **machine learning**. I am currently working on specific topics including **AI for science**, **geometric deep learning**, and **generative modeling for drug discovery (diffusion, language model)**.
- In general, my research aims to advance deep learning techniques within scientific fields like **biology** and **physics**. Within these domains, I have designed deep learning models tailored for **small molecule generation**, **protein generation**, **partial differential equations**, and **quantum many-body problems**.
- Our team won the **runner-up award at KDD Cup 2021 on molecular property prediction**, where I made the main contribution.

Education

Texas A&M University, College Station, TX, USA — Jan 2021 - Dec 2025 (Expect)
Ph.D., Department of Computer Science & Engineering
GPA: 4.0/4.0
Advisor: Prof. Shuiwang Ji

University of Michigan, Ann Arbor, MI, USA — Aug 2016 – Apr 2018
M.S., Department of Mechanical Engineering
GPA: 3.92/4.0

Harbin Institute of Technology, Harbin, CHINA — Aug 2012 – Jul 2016
B.S., Department of Mechanical Engineering
GPA: 3.88/4.0

Professional Experiences

Uber, Sunnyvale, CA, USA — Jun 2024 – Aug 2024
PhD Software Engineer Intern
Work on improving ETA prediction accuracy

Fujitsu Research of America, Sunnyvale, CA, USA — Jul 2022 – Dec 2022
Research Intern
Work on developing SE(3) equivariant latent diffusion model for protein backbone generation

DMAI, Los Angeles, CA, USA — Jun 2018 – Mar 2020
Robotics Engineer
Work on developing mobile robot autonomous navigation systems and building bipedal robotics system

Selected Publications [Google Scholar]

* indicates equal contribution.

[ICLR 2024] **Complete and Efficient Graph Transformers for Crystal Material Property Prediction**
Keqiang Yan, **Cong Fu**, Xiaofeng Qian, Xiaoning Qian, Shuiwang Ji
*International Conference on Learning Representations (**ICLR**), 2024*

[ICLR 2024] **SineNet: Learning Temporal Dynamics in Time-Dependent Partial Differential Equations**
Xuan Zhang*, Jacob Helwig*, Yuchao Lin, Yaochen Xie, **Cong Fu**, Stephan Wojtowytsch, Shuiwang Ji
*International Conference on Learning Representations (**ICLR**), 2024*

[LoG 2023] **A Latent Diffusion Model for Protein Structure Generation**

Cong Fu*, Keqiang Yan*, Limei Wang, Wing Yee Au, Michael McThrow, Tao Komikado, Koji Maruhashi, Kanji Uchino, Xiaoning Qian, Shuiwang Ji
*Learning on Graphs Conference (**LoG**), 2023*

[LoG 2023] **Semi-Supervised Learning for High-Fidelity Fluid Flow Reconstruction**
Cong Fu, Jacob Helwig, Shuiwang Ji
*Learning on Graphs Conference (**LoG**), 2023*

[SDM 2023] **Lattice Convolutional Networks for Learning Ground States of Quantum Many-body Systems**
Cong Fu*, Xuan Zhang*, Huixin Zhang, Hongyi Ling, Shenglong Xu, Shuiwang Ji
*SIAM International Conference on Data Mining (**SDM**), 2023*

[ICML 2023] **Group Equivariant Fourier Neural Operators for Partial Differential Equations**
Jacob Helwig*, Xuan Zhang*, **Cong Fu**, Jerry Kurtin, Stephan Wojtowytsch, Shuiwang Ji
*International Conference on Machine Learning (**ICML**), 2023*

[NeurIPS-W 2021] **Fast Quantum Property Prediction via Deeper 2D and 3D Graph Networks**
Meng Liu*, **Cong Fu***, Xuan Zhang, Limei Wang, Yaochen Xie, Hao Yuan, Youzhi Luo, Zhao Xu, Shenglong Xu, and Shuiwang Ji
***AI4Science Workshop at NeurIPS**, 2021*
Awardee of KDD Cup 2021 on OGB-LSC

[JMLR] **DIG: A Turnkey Library for Diving into Graph Deep Learning Research**
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
*Journal of Machine Learning Research (**JMLR**), 2021*

[Preprint] **Fragment and Geometry Aware Tokenization of Molecules for Structure-Based Drug Design Using Language Models**
Cong Fu, Xiner Li, Blake Olson, Heng Ji, Shuiwang Ji

[Preprint] **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, 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

Professional Services

Program Committee Member | Reviewer

International Conference on Machine Learning (**ICML**)	2022, 2023, 2024
Annual Conference on Neural Information Processing Systems (**NeurIPS**)	2022, 2023, 2024
NeurIPS Track Datasets and Benchmarks	2023, 2024
International Conference on Learning Representations (**ICLR**)	2023, 2024
ACM International Conference on Information and Knowledge Management (**CIKM**)	2023, 2024
Structured Probabilistic Inference & Generative Modeling Workshop @ ICML2023	2023
New Frontiers of AI for Drug Discovery and Development Workshop @ NeurIPS2023	2023
Generative AI and Biology Workshop @ NeurIPS2023	2023
AI4Science Workshop @ NeurIPS2022, @ NeurIPS2023	2022, 2023
ACM Transactions on Knowledge Discovery from Data	

Teaching Assistant

Machine Learning	CSCE 421, TAMU, 2023

Scholarships, Awards, & Honors

Travel Grant, CSE@TAMU	2023
Travel Award, AI4Science Workshop @ NeurIPS	2021

Runner-up Award, KDD Cup on Open Graph Benchmark Large-Scale Challenge (OGB-LSC) 2021
National Scholarship, China 2014

Programming Language & Tool

Python, C++, PyTorch, PyTorch Geometric, SQL

News Coverage

Ji and his team earn top showing at premier data mining competition TAMU News