

# Yunchao (Lance) Liu

## CONTACT INFORMATION

Office: 5154G Medical Research Building III  
465 21st Ave S  
Nashville, TN 37212  
E-mail: [yunchao.liu@vanderbilt.edu](mailto:yunchao.liu@vanderbilt.edu)

Homepage: <http://www.LiuYunchao.com>  
LinkedIn: <http://www.linkedin.com/in/YunchaoLiu/>  
GitHub: <https://github.com/LanceKnight>  
Google Scholar: <http://scholar.google.com/citations?user=oFtWfwAAAAJ&hl=en>

## EDUCATION

### Vanderbilt University

- **Doctor of Philosophy (Ph.D.)** student in Computer Science
- Advisors: Dr. Jens Meiler, Dr. Tyler Derr
- Cumulative GPA: 3.92 / 4.00

Aug 2018 – Present

### University of Texas at Dallas

- **Master of Science (M.S.)** in Computer Science
- Cumulative GPA: 3.85 / 4.0

May 2015

### Beijing University of Posts and Telecommunications

- **Bachelor of Science (B.S.)** in Management

Sep 2013

## RESEARCH EXPERIENCE

### Meiler Lab, Vanderbilt University

PhD Candidate, Computer Science Department

Sep 2018 – Present

- Advisors: Dr. Jens Meiler, Dr. Tyler Derr, Dr. Bobby Bodenheimer
- Research Interests: AI for Drug Design, Topological/Geometric Deep Learning, Generative Models, Self-Supervised Learning, Small Molecules/Proteins

### State Key Laboratory of Intelligent Technology and Systems, Tsinghua University

Research Assistant, Department of Computer Science and Technology

Jul 2012 – Mar 2013

- Advisor: Dr. Xiaolin Hu
- Research Interests: Visual Saliency for Road Sign Detection

## PUBLICATIONS

Grace Zhang, Xiaohan Kuang, Yuhao Zhang, **Yunchao Liu**, Zhaoqian Su, Tom Zhang, Yinghao Wu. Machine-learning-based structural analysis of interactions between antibodies and antigens. *BioSystems*, 2024.

Yu Wang, Tong Zhao, Yuying Zhao, **Yunchao Liu**, Xueqi Cheng, Neil Shah, Tyler Derr. A Topological Perspective on Demystifying GNN-Based Link Prediction Performance. *Proceedings of the 12th International Conference on Learning Representations (ICLR)*, 2024.

Yuying Zhao, Yu Wang, **Yunchao Liu**, Xueqi Cheng, Charu Aggarwal, Tyler Derr. Fairness and Diversity in Recommender Systems: A Survey. *ACM Transactions on Intelligent Systems and Technology*, 2024.

**Yunchao Liu**, Yu Wang, Oanh Vu, Rocco Moretti, Bobby Bodenheimer, Jens Meiler and Tyler Derr. Interpretable Chirality-Aware Graph Neural Network for Quantitative Structure Activity Relationship Modeling in Drug Discovery. *Proceedings of the 37th Association for the Advancement of Artificial Intelligence (AAAI)*, 2023.

**Yunchao Liu**, Rocco Moretti, Bobby Bodenheimer and Jens Meiler. Foldit Drug Design Game Usability Study: Comparison of Citizen and Expert Scientists. *Proceedings of the 13th Annual ACM SIGGRAPH Conference on Motion, Interaction and Games (MIG)*, 2020.

## PREPRINTS

**Yunchao Liu**, Rocco Moretti, Yu Wang, Ha Dong, Bailu Yan, Bobby Bodenheimer, Tyler Derr and Jens Meiler. Advancements in Ligand-Based Virtual Screening through the Synergistic Integration of Graph Neural Networks and Expert-Crafted Descriptors *bioRxiv*, 2023.

Yuying Zhao, Yu Wang, **Yunchao Liu**, Xueqi Cheng, Charu Aggarwal, Tyler Derr Fairness and Diversity in Recommender Systems: A Survey *arXiv*, 2023.

## SERVICES

### Journal Reviewer

- ACM Computing Surveys 2024
- Information Fusion 2024
- Big Data Research 2024
- International Journal of Electrical and Computer Engineering (IJECE) 2024
- Information Fusion 2023
- Journal of Computational Biophysics and Chemistry 2023
- ACM Transactions on Knowledge Discovery from Data (TKDD) 2023
- Big Data Research 2022

### Conference Reviewer

- 46th Annual International Conference of the IEEE Engineering in Medicine and Biology Society (EMBC) 2024
- New Frontiers of AI for Drug Discovery and Development (AI4D3) @ Conference on Neural Information Processing Systems (NeurIPS) 2023
- AI4Science @ Conference on Neural Information Processing Systems (NeurIPS) 2023
- Generative AI and Biology (GenBio) @ Conference on Neural Information Processing Systems (NeurIPS) 2023
- Structured Probabilistic Inference & Generative Modeling (SPIGM) @ International Conference on Machine Learning (ICML) 2023
- SIAM International Conference on Data Mining (SDM) 2023
- Machine Learning on Graphs @ ACM International Conference on Web Search and Data Mining (WSDM) 2023
- AI4Science @ International Conference on Machine Learning (ICML) 2023
- ACM SIGKDD Conference on Knowledge Discovery and Data Mining (KDD) 2023
- Association for the Advancement of Artificial Intelligence (AAAI) 2023
- ACM International Conference on Web Search and Data Mining (WSDM) 2023
- Machine Learning on Graphs @ International Conference on Data Mining (ICDM) 2022
- AI4Science @ Conference on Neural Information Processing Systems (NeurIPS) 2022
- AI4Science @ International Conference on Machine Learning (ICML) 2022
- Deep Generative Models for Highly Structured Data (DGM4HSD) @ International Conference on Learning Representations (ICLR) 2022
- Conference on Neural Information Processing Systems (NeurIPS) 2022
- Machine Learning on Graphs (MLOG) @ ACM International Conference on Web Search and Data Mining (WSDM) 2022
- ACM The Web Conference (TheWebConf) 2022
- International Conference on Learning Representations (ICLR) 2022
- ACM International Conference on Web Search and Data Mining (WSDM) 2022
- ACM International Conference on Information and Knowledge Management (CIKM) 2021
- ACM SIGKDD Conference on Knowledge Discovery and Data Mining (KDD) 2021
- AI4Science @ Conference on Neural Information Processing Systems (NeurIPS) 2021

### Chairship

- Publicity Chair at Machine Learning on Graphs (MLOG) Workshop at ICDM'23 2023
- Publicity Chair at Machine Learning on Graphs (MLOG) Workshop at WSDM'23 2023

### Program Committee

- Graph Techniques for Adversarial Activity Analytics (GTA3) @ IEEE Big Data Conference 2023
- Graph Techniques for Adversarial Activity Analytics (GTA3) @ IEEE Big Data Conference 2022

### Volunteering

- Volunteer at New Frontiers of AI for Drug Discovery and Development (AI4D3) @ NeurIPS 2023
- Session Chair at Association for the Advancement of Artificial Intelligence (AAAI) 2023
- Volunteer at Association for the Advancement of Artificial Intelligence (AAAI) 2023
- Volunteer at International Conference on Learning Representations (ICLR) 2022
- Session Manager at ACM International Conference on Web Search and Data Mining (WSDM) 2022

<b>HONORS &amp; AWARDS</b>	• Finalist of Vanderbilt Three Minute Thesis Competition	Nov 2023
	• AAAI2023 student scholarship travel award	Dec 2022
	• Reviewer Award @ ICML-AI4Science	Jun 2022
	• Nvidia Hardware Grant (RTX A6000)	Mar 2022
<hr/>		
<b>TEACHING</b>	• Guest Speaker @ DS 3891: Intro to Generative Artificial Intelligence Models	Mar 2024
	• RFdiffusion @ Rosetta Workshop	Dec 2023
<hr/>		
<b>MENTORING</b>	<b>Data Science Institute</b> , Vanderbilt University	
	• LeyaoWang (Laura) Wang, B.S. Computer Science, from Vanderbilt University	2024 Spring
	<b>Data Science Institute</b> , Vanderbilt University	
	• Xiaohan Kuang, M.S. Computer Science, from Vanderbilt University	2023 Fall
	• Yuhao Zhang, M.S. Computer Science, from Vanderbilt University	2023 Fall
	<b>Network and Data Science Lab</b> , Vanderbilt University	
	• Meilin Guo, M.S. Computer Science, from Columbia University	2023 Summer
	<b>Meiler Lab</b> , Vanderbilt University	
	• Ha Dong, B.S. Neuroscience & Physics, from Amherst College	2023 Summer
<hr/>		
<b>INVITED TALKS</b>	Molecular-Kernel Graph Neural Network for Drug Discovery	Jun 2023
	• Max Planck Institute for Mathematics in the Sciences	
	• Leipzig, Germany	
	Interpretable Chirality-Aware Graph Neural Network for Quantitative Structure Activity Relationship Modeling in Drug Discovery.	Mar 2023
	• Molecular Modeling & Drug Discovery Talks (Organized by Mila & Valence Discovery)	
	• Virtual Event	
	Interpretable Chirality-Aware Graph Neural Network for Quantitative Structure Activity Relationship Modeling in Drug Discovery.	Feb 2023
	• The 37th AAAI conference on artificial intelligence	
	• Walter E. Washington Convention Center, Washington, DC, USA	
	Foldit Drug Design Game Usability Study: Comparison of Citizen and Expert Scientists	Oct 2020
	• ACM SIGGRAPH Conference on Motion, Interaction and Games (MIG)	
	• Zucker Family Graduate Education Center (virtual due to COVID-19)	
<hr/>		
<b>PRESENTATIONS &amp; POSTERS</b>	Yunchao Liu, Yu Wang, Oanh Vu, Rocco Moretti, Bobby Bodenheimer, Jens Meiler and Tyler Derr. Interpretable Chirality-Aware Graph Neural Network for Quantitative Structure Activity Relationship Modeling in Drug Discovery <i>Learning on Graphs Conference (LoG)</i> , Poster 2022.	
	Yunchao Liu, Yu Wang, Oanh Vu, Rocco Moretti, Bobby Bodenheimer, Jens Meiler and Tyler Derr. Interpretable Chirality-Aware Graph Neural Network for Quantitative Structure Activity Relationship Modeling in Drug Discovery <i>Summer RosettaCon</i> , Poster 2022.	
	Yunchao Liu, Rocco Moretti, Bobby Bodenheimer, Jens Meiler. Foldit Drug Design Game Usability Study: Comparison of Citizen and Expert Scientists, <i>ACM SIGGRAPH Conference on Motion, Interaction and Games (MIG)</i> , Presentation, 2020.	
<hr/>		
<b>REFERENCES</b>	Available Upon Request	