Yunchao (Lance) Liu

CONTACT INFORMATION	Office: 5154G Medical Rearch Building III 465 21st Ave S Nashville, TN 37212 E-mail: 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=oFtlWfwAAAAJ&hl=en

EDUCATION

Vanderbilt University
- **Doctor of Philosophy (Ph.D.)** student in Computer Science   Aug 2018 – Present
- Advisors: Dr. Jens Meiler, Dr. Tyler Derr
- Cumulative GPA: 3.92 / 4.00

University of Texas at Dallas
- **Master of Science (M.S.)** in Computer Science   May 2015
- Cumulative GPA: 3.85 / 4.0

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

Xueqi Cheng, Yu Wang, **Yunchao Liu**, Yuying Zhao, Charu C Aggarwal, Tyler Derr. Edge Classification on Graphs: New Directions in Topological Imbalance. Proceedings of the ACM 18th International Conference on Web Search and Data Mining (**WSDM**), 2025.

Yunchao Liu, Ha Dong, Xin Wang, Rocco Moretti, Yu Wang, Zhaoqian Su, Jiawei Gu, Bobby Bodenheimer, Charles Weaver, Jens Meiler, Tyler Derr. WelQrate: Defining the Gold Standard in Small Molecule Drug Discovery Benchmarking. Proceedings of the 38th Conference on Neural Information Processing Systems (**NeurIPS**), 2024.

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 (**TIST**), 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. Preceedings 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. Preceedings 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.

SERVICES	**Journel Reviewer**	

SERVICES

Journel Reviewer
- PLOS Computational Biology — 2024
- 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

HONORS & AWARDS	• 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

TEACHING	• Guest Speaker @ DS 3891: Intro to Generative Artificial Intelligence Models	Mar 2024
	• RFdiffusion @ Rosetta Workshop	Dec 2023

MENTORING	**Data Science Institute**, Vanderbilt University	
	• LeyaoWang (Laura) Wang, B.S. Computer Science, from Vanderbilt University	2024 Spring
	Data Science Institute, Vanderbilt University	
	• Xiaohan Kuang, M.S. Computer Science, from Vanderbilt University	2023 Fall
	• Yuhao Zhang, M.S. Computer Science, from Vanderbilt University	2023 Fall
	Network and Data Science Lab, Vanderbilt University	
	• Meilin Guo, M.S. Computer Science, from Columbia University	2023 Summer
	Meiler Lab, Vanderbilt University	
	• Ha Dong, B.S. Neuroscience & Physics, from Amherst College	2023 Summer

INVITED TALKS	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)	

POSTERS	• Xiaobo Lin, Zhaoqian Su, <u>Yunchao Liu</u>, Jingxian Liu, Xiaohan Kuang, Jesse Spencer-Smith. SuperMetal: A Generative AI Framework for Rapid and Precise Metal Ion Location Prediction in Proteins *Machine Learning in Structural Biology (MLSB) @ NeurIPS* 2024. • <u>Yunchao Liu</u>, 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 *Learning on Graphs Conference (LoG)* 2022. • <u>Yunchao Liu</u>, 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 *Summer RosettaCon* 2022.

REFERENCES	Available Upon Request

[CV compiled on 2024-10-26]