Dr. Yunchao (Lance) Liu

CONTACT INFORMATION

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GitHub: https://github.com/LanceKnight
Google Scholar: http://scholar.google.com/citations?user=oFtlWfwAAAAJ&hl=en

BIOGRAPHY

Dr. Yunchao (Lance) Liu, is currently a Computational Scientist at the Broad Institute of MIT and Harvard. His research aims at developing novel state-of-the-art geometric deep learning models for understanding genomics. He received his PhD from the Vanderbilt University, where he ws advised by Dr. Jens Meiler and Dr. Tyler Derr. His Ph.D research focused on the development of AI models for drug discovery applications.

For more detailed information, please see below or visit his website at https://www.LiuYunchao.com.

EDUCATION

Vanderbilt University — May 2025
- Doctor of Philosophy (**Ph.D.**) in Computer Science
- Advisors: Dr. Jens Meiler, Dr. Tyler Derr
- Dissertation: Geometric Deep Learning in Drug Discovery
- Cumulative GPA: 3.918 / 4.00

University of Texas at Dallas — May 2015
- Master of Science (**M.S.**) in Computer Science

Beijing University of Posts and Telecommunications — Sep 2013
- Bachelor of Science (**B.S.**) in Management

RESEARCH EXPERIENCE

Broad Institute of MIT and Harvard — May 2020 – Present
Computational Scientist I
- Supervisor: Dr. Victoria Popic
- Research Interests: Structural Variation, Sequence Analysis

Network and Data Science Lab, Vanderbilt University — Sep 2020 – May 2025
PhD Student, Computer Science Department
- Advisor: Dr. Tyler Derr
- Research Interests: Topological/Geometric Deep Learning, Generative Models, Self-Supervised Learning

Meiler Lab, Vanderbilt University — Sep 2018 – May 2025
PhD Student, Computer Science Department
- Advisor: Dr. Jens Meiler
- Research Interests: AI for Drug Design, Small Molecules, Proteins

Learning in Virtual Environments Lab, Vanderbilt University — Sep 2018 – Sep 2020
PhD Student, Computer Science Department
- Advisor: Dr. Bobby Bodenheimer
- Research Interests: Citizen Science for Drug Discovery

State Key Laboratory of Intelligent Technology and Systems, Tsinghua University — Jul 2012 – Mar 2013
Research Assistant, Department of Computer Science and Technology
- Advisor: Dr. Xiaolin Hu
- Research Interests: Visual Saliency for Road Sign Detection

HONORS & AWARDS

- Nvidia Academic Grant (6*RTX A6000 Ada) — Dec 2024
- 1st Place with DiffWater poject @ AI Showcase at Vanderbilt University — Apr 2024
- 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

PUBLICATIONS

Please note the following symbols below to signify certain author types in this and next section:

*	denotes co-first authors
†	denotes *student mentored* by Dr. Yunchao (Lance) Liu

[PU09] 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 . Journal of Chemical Information and Modeling **(JCIM)**, 2025. (IF: 5.9)

[PU08] Xiaobo Lin, Zhaoqian Su, Yunchao Liu, Jingxian Liu, Xiaohan Kuang, Peter T Cummings, Jesse Spencer-Smith, Jens Meiler. SuperMetal: A Generative AI Framework for Rapid and Precise Metal Ion Location Prediction in Proteins . Journal of Cheminformatics **(JCIM)**, 2025. (IF: 8.5)

[PU07] 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. (Acceptance Rate: 17.4%)

[PU06] 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. (Acceptance Rate: 25.3%)

[PU05] 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. (IF: 2.0)

[PU04] 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. (Acceptance Rate: 31%)

[PU03] 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. (IF: 7.2)

[PU02] 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. (Acceptance Rate: 19.6%)

[PU01] 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. (Acceptance Rate: Unknown)

UNDER REVIEW & PREPRINTS

[PR02] Shan Jiang, Zhaoqian Su, Nathaniel Bloodworth, Yunchao Liu, Cristina Martina, David G. Harrison, Jens Meiler. Machine learning application to predict binding affinity between peptide containing noncanonical amino acids and HLA0201 , **Under Review** @ **PLOS ONE** , 2024.

[PR01] Xiaohan Kuang*†, Zhaoqian Su*, Yunchao Liu, Xiaobo Lin, Jesse Spencer-Smith, Tyler Derr, Yinghao Wu, Jens Meiler. SuperWater: Predicting Water Molecule Positions on Protein Structures by Generative AI , **Under Revision** @ **Nature Communication**, 2024.

TEACHING

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

MENTORING

Network and Data Science Lab, Vanderbilt University

- Xin (Allen) Wang, M.S. Computer Science, Vanderbilt University — 2024 Fall
  -Co-First-Authored on [PU06]
  -Participated BioML challenge (Results Pending)
- Leyao (Laura) Wang, B.S. Computer Science & Math, Vanderbilt University — 2024 Spring
  -2024-2025 CRA Outstanding Undergraduate Research Award
- Qinwen Ge, M.S. Computer Science, Vanderbilt University — 2023 Fall
  -Vanderbilt Engineering Graduate Fellowship Award

Meiler Lab, Vanderbilt University 2023 Summer

- Ha Dong, B.S. Neuroscience & Physics, Amherst College
  -Co-First-Authored on [PU06]
  -Visiting Undergraduate Student Program @ Harvard 2025
  -Break Through Tech AI Fellow @MIT 2024

Data Science Institute, Vanderbilt University

- Hexuan (Hillbert) Fan, M.S. Data Science, Vanderbilt University 2024 Fall
  -Contributed to Nvidia Hardware Grant Proposal Writing
- Yuhao Zhang, M.S. Data Science, Vanderbilt University 2024 Spring
- Xiaohan Kuang, M.S. Data Science, Vanderbilt University 2023 Fall
  -Co-Authored on [PR01]
  -Team Member of DiffWater Project That Won 1st Place @ AI Showcase at Vanderbilt University
  -Nvidia GTC 2025 Poster Presentation

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

- Xiaohan Kuang*, Zhaoqian Su*, Yunchao Liu, Xiaobo Lin, Jesse Spencer-Smith, Tyler Derr, Yinghao Wu, Jens Meiler. SuperWater: Predicting Water Molecule Positions on Protein Structures by Generative AI *@ Nvidia GTC* 2025.
- Xiaobo Lin*, Zhaoqian Su*, Yunchao Liu, 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.
- 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 *Learning on Graphs Conference (LoG)* 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 *Summer RosettaCon* 2022.

SERVICES

Journel Reviewer

- PLOS Computational Biology, IF: 3.8 2024 – Present
- ACM Computing Surveys, IF: 23.8 2024 – Present
- International Journal of Electrical and Computer Engineering **(IJECE)**, IF: unknown 2024 – Present
- Information Fusion, IF: 14.8 2023 – Present
- Journal of Computational Biophysics and Chemistry **(JCBC)**, IF: 2.0 2023 – Present
- ACM Transactions on Knowledge Discovery from Data **(TKDD)**, IF: 4.0 2023 – Present
- Big Data Research, IF: 3.5 2022 – Present

Chairship

- Organizer at 2025 Midwest AI for Drug Discovery and Development **(AI4D3)** 2025
- Publicity Chair at Machine Learning on Graphs **(MLoG)@ICDM23** 2023
- Publicity Chair at Machine Learning on Graphs **(MLoG)@WSDM23** 2023
- Session Chair at Association for the Advancement of Artificial Intelligence **(AAAI)** 2023
- Session Chair at ACM International Conference on Web Search and Data Mining **(WSDM)** 2022

Program Committee

- 39th Conference on Neural Information Processing Systems (**NeurIPS**) 2025
- Generative AI and Biology Workshop (GenBio) @ ICML 2025
- Frontiers in Probabilistic Inference: Sampling Meets Learning **(FPI) @ ICLR** 2025
- 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)@ NeurIPS** 2023
- **AI4Science@NeurIPS** 2023
- Generative AI and Biology **(GenBio)@NeurIPS** 2023
- Structured Probabilistic Inference & Generative Modeling **(SPIGM)@ICML** 2023
- **AI4Science@ICML** 2023
- Graph Techniques for Adversarial Activity Analytics **(GTA3)@IEEE Big Data Conference** 2023
- **AI4Science@NeurIPS** 2022
- **AI4Science@ICML** 2022
- Deep Generative Models for Highly Structured Data **(DGM4HSD)@ICLR** 2022
- Graph Techniques for Adversarial Activity Analytics **(GTA3)@ IEEE Big Data Conference** 2022

Conference Sub-Reviewer

- SIAM International Conference on Data Mining **(SDM)** 2023
- Machine Learning on Graphs @ ACM International Conference on Web Search and Data Mining **(WSDM)** 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
- 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

Volunteering

- Volunteer at New Frontiers of AI for Drug Discovery and Development **(AI4D3)@NeurIPS** 2023
- Volunteer at Association for the Advancement of Artificial Intelligence **(AAAI)** 2023
- Volunteer at International Conference on Learning Representations **(ICLR)** 2022

COMPETITIONS

- BioML Challenge 2024: Bits to Binders
- Merck Datathon 2023

REFERENCES Available Upon Request

[*CV compiled on 2025-05-29*]