Yunchao "Lance" Liu

CONTACT INFORMATION	Office: 5144G Medical Rearch Building III Homepage: http://www.LiuYunchao.com 465 21st Ave S LinkedIn: http://www.linkedin.com/in/YunchaoLiu/ Nashville, TN 37212 GitHub: https://github.com/LanceKnight E-mail: lanceknight26@gmail.com Google Scholar: http://scholar.google.com/citations?user=oFtlWfwAAAAJ&hl=en

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EDUCATION

Vanderbilt University
- **Doctor of Philosophy (Ph.D.)** student in Computer Science   Aug 2018 – Present
- Advisors: Dr. Jens Meiler, Dr. Tyler Derr, Dr. Bobby Bodenheimer
- 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 Student, Computer Science Department   Sep 2018 – Present
- Advisors: Dr. Jens Meiler, Dr. Tyler Derr, Dr. Bobby Bodenheimer
- Research Areas: Computer-Aided Drug Discovery, Geometric Deep Learning, Self-Supervised Learning

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 areas: Visual Saliency for Road Sign Detection

PUBLICATIONS

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.

HONORS & AWARDS

- AAAI2023 student scholarship and volunteer program travel award   Dec 2022
- Reviewer Award @ ICML-AI4Science   Jun 2022
- Nvidia Hardware Grant (RTX A6000)   Mar 2022

INVITED TALKS

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)

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

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

PRESENTATIONS & POSTERS	<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)*, Poster 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*, Poster 2022.
	<u>Yunchao Liu</u>, Rocco Moretti, Bobby Bodenheimer, Jens Meiler. Foldit Drug Design Game Usability Study: Comparison of Citizen and Expert Scientists, *ACM SIGGRAPH Conference on Motion, Interaction and Games (MIG)*, Presentation, 2020.

SERVICES

Journel Reviewer
- Big Data Research   2022

Conference Reviewer
- 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
- 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 at WSDM'23   2023

Program Committee
- Graph Techniques for Adversarial Activity Analytics @ IEEE Big Data Conference   2022

Volunteering
- 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

OTHER WORK EXPERIENCE

American Wonder Porcelain LLC., Nashville, TN, USA
IT Specialist   Sep 2015 – Jan 2018
- Administrated IFS ERP system: user right control, workflow design and etc.
- Analyzed sales data with Power BI
- Planned internet layout
- Provided other technical support

Xtera Communicatons Inc., Allen, TX, USA
Software Engineer Intern   Jan 2015 – Jul 2015
- Developed visulization software for remotely monitoring optical signals

University of Texas at Dallas, Dallas, TX, USA
Website Developer Intern   Jun 2014 – Dec 2014
  • Developed websites for the international center

SKILLS Proficient with: Python, LaTeX
Coded using: C, C++, C#, Java, Visual Basic, HTML, Javascript, MATLAB, R
Operating Systems: CentOS, Ubuntu, and Windows

PROFESSIONAL AFFILIATIONS & ACTIVITIES **Association for the Advancement of Artificial Intelligence (AAAI)**
Member   2022
American Chemical Society's Division of Computers In Chemistry (ACS COMP)
Member   2022

LANGUAGES English: Fluent (speaking, reading, writing).
Chinese: Native language.

REFERENCES Available Upon Request

[CV compiled on 2023-04-30]