

Yunchao “Lance” Liu

CONTACT INFORMATION

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

EDUCATION

Vanderbilt University

- **Doctor of Philosophy (Ph.D.)** student in Computer Science
- Advisors: Dr. Jens Meiler, Dr. Tyler Derr, Dr. Bobby Bodenheimer
- 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 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. 2022. bioRxiv

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

HONORS & AWARDS

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)

POSTER PRESENTATION

Interpretable Chirality-Aware Graph Neural Network for Quantitative Structure Activity Relationship Modeling in Drug Discovery

Aug 2022

Summer RosettaCon

Sleeping Lady Mountain Resort, Leavenworth, WA

SERVICES

Journal Reviewer

- Big Data Research

2022

Conference Reviewer

- Association for the Advancement of Artificial Intelligence (AAAI)
- ACM International Conference on Web Search and Data Mining (WSDM)
- Machine Learning on Graphs @ International Conference on Data Mining (ICDM)
- AI4Science @ Conference on Neural Information Processing Systems (NeurIPS)
- AI4Science @ International Conference on Machine Learning (ICML)

2023

2023

2022

2022

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

Volunteering

- 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
	<ul style="list-style-type: none"> • 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
	<ul style="list-style-type: none"> • Developed visulization software for remotely monitoring optical signals 	
	University of Texas at Dallas, Dallas, TX, USA	
	Website Developer Intern	Jun 2014 – Dec 2014
	<ul style="list-style-type: none"> • Developed websites for the international center 	

PROJECTS	Foldit Drug Design (FolditDD) Usability Study	2020
	<ul style="list-style-type: none"> • Used the think-aloud method to conduct a usability study on FolditDD • Compared the expert scientists and citizen scientists for their scientific problem solving skill in a game setting 	
	FolditDD Interface Revamp	2019
	<ul style="list-style-type: none"> • Customized Foldit interface to meet the need for drug design • Introduced a preset function to quickly set the interface to drug design settings 	
	Geometric Objects Rendering with Ray Tracing Technique	2019
	<ul style="list-style-type: none"> • Used C++ and OpenGL library to render objects using ray tracing technique • Achieved optical effects including reflection, diffusion, (overlapping) shadows 	
	Geographical Data Visualization for UFO reports	2018
	<ul style="list-style-type: none"> • Visualized geographic data of USO reports in the USA • Designed interactive UI with features including zooming/panning/subplot 	
	Visualizing Protein Flexibility using the Visualization Toolkit (VTK)	2018
	<ul style="list-style-type: none"> • Developed a C++ program using VTK library to show the distance of two conformations of a protein • Designed visulization scheme to show color coded flexibility on different parts of the protein 	
	IFS Enterprise Resource Planning (ERP) Deployment	2016– 2018
	<ul style="list-style-type: none"> • Designed the workflows for purchase order, inventory management, sales order, invoice, shop order, work order in the IFS ERP system • Extracted data using SQL and designed auto-generated financial reports including balance sheet, income statement, cost analysis etc. 	
	Library Management System	2015
	<ul style="list-style-type: none"> • Designed and developed a library management system usng Java and SQL • Features including book lookup, return, overdue fine calculation, fine payment etc. 	

Full-time Curricular Practical Training (CPT) calculator

2014

- Developed a web-based full-time CPT calculator at the international center at UT Dallas to help international students avoid overtime working

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**

American Chemical Society's Division of Computers In Chemistry

Member

2022

LANGUAGES

English: Fluent (speaking, reading, writing).

Chinese: Native language.

REFERENCES

Available Upon Request

[CV compiled on 2022-10-25]