

YANQIAO ZHU

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Education

Doctor of Philosophy (2022 – present)

Department of Computer Science, University of California, Los Angeles



Advisors: Professors [Wei Wang](#) and [Yizhou Sun](#)

Master of Engineering (2019 – 2022)

Institute of Automation, Chinese Academy of Sciences



Advisors: Professors [Tieniu Tan](#) and [Shu Wu](#)

Thesis: *Self-Supervised Representation Learning on Graph-Structured Data*

Committee: [Xilin Chen](#) (Chair), [Zhouchen Lin](#), [Ji-Rong Wen](#), [Jiwen Lu](#), [Peng Cui](#), and [Shiming Xiang](#)

Research Experience

Research Assistant

NSF Center for Computer Assisted Synthesis (C-CAS)

(2022 – present)

Los Angeles, CA, USA

Research Assistant

Institute of Automation, Chinese Academy of Sciences

(2019 – 2022)

Beijing, China

Selected Publications



▷ Citations: 4406

▷ h-index: 20

▷ i10-index: 29

Conference Papers

[c11] Learning Over Molecular Conformer Ensembles: Datasets and Benchmarks

[Yanqiao Zhu](#), [Jeehyun Hwang](#), [Keir Adams](#), [Zhen Liu](#), [Bozhao Nan](#), [Brock Stenfors](#), [Yuanqi Du](#), [Jatin Chauhan](#), [Olaf Wiest](#), [Olexandr Isayev](#), [Connor W. Coley](#), [Yizhou Sun](#), and [Wei Wang](#)
ICLR 2024

[c10] Uncovering Neural Scaling Laws in Molecular Representation Learning

[Dingshuo Chen](#)^{*}, [Yanqiao Zhu](#)^{*}, [Jieyu Zhang](#), [Yuanqi Du](#), [Qiang Liu](#), and [Shu Wu](#)
NeurIPS 2023 (Datasets and Benchmarks)

[c9] A Systematic Survey of Chemical Pre-trained Models

[Jun Xia](#)^{*}, [Yanqiao Zhu](#)^{*}, [Yuanqi Du](#)^{*}, and [Stan Z. Li](#)
IJCAI 2023 (Survey)

[c8] Code Recommendation for Open Source Software Developers

[Yiqiao Jin](#), [Yunsheng Bai](#), [Yanqiao Zhu](#), [Yizhou Sun](#), and [Wei Wang](#)
WWW 2023

- [c7] **A Survey on Deep Graph Generation: Methods and Applications**
Yanqiao Zhu*, Yuanqi Du*, Yinkai Wang*, Yichen Xu, Jieyu Zhang, Qiang Liu, and Shu Wu
LoG 2022
- [c6] **Interpretable Graph Neural Networks for Connectome-Based Brain Disorder Analysis**
Hejie Cui, Wei Dai, Yanqiao Zhu, Xiaoxiao Li, Lifang He, and Carl Yang
MICCAI 2022 (Oral Presentation)
- [c5] **An Empirical Study of Graph Contrastive Learning**
Yanqiao Zhu, Yichen Xu, Qiang Liu, and Shu Wu
NeurIPS 2021 (Datasets and Benchmarks)
- [c4] **Mining Latent Structures for Multimedia Recommendation**
Jinghao Zhang*, Yanqiao Zhu*, Qiang Liu, Shu Wu, Shuhui Wang, and Liang Wang
ACMMM 2021 (Oral Presentation)
- [c3] **Graph Contrastive Learning with Adaptive Augmentation**
Yanqiao Zhu*, Yichen Xu*, Feng Yu, Qiang Liu, Shu Wu, and Liang Wang
WWW 2021
- [c2] **TAGNN: Target Attentive Graph Neural Networks for Session-based Recommendation**
Feng Yu*, Yanqiao Zhu*, Qiang Liu, Shu Wu, Liang Wang, and Tieniu Tan
SIGIR 2020 (Short Paper)
- [c1] **Session-based Recommendation with Graph Neural Networks**
Shu Wu, Yuyuan Tang, Yanqiao Zhu, Liang Wang, Xing Xie, and Tieniu Tan
AAAI 2019 (Oral Presentation)

Journal Papers

- [j4] **Molecular Contrastive Pretraining with Collaborative Featurizations**
Yanqiao Zhu*, Dingshuo Chen*, Yuanqi Du*, Yingze Wang, Qiang Liu, and Shu Wu
J. Chem. Inf. Model. 64(4)
- [j3] **Latent Structure Mining with Contrastive Modality Fusion for Multimedia Recommendation**
Jinghao Zhang, Yanqiao Zhu, Qiang Liu, Mengqi Zhang, Shu Wu, and Liang Wang
IEEE Trans. Knowl. Data Eng. 35(9)
- [j2] **Unsupervised Graph Representation Learning with Cluster-Aware Self-Training and Refining**
Yanqiao Zhu*, Yichen Xu*, Feng Yu, Qiang Liu, and Shu Wu
ACM Trans. Intell. Syst. Technol. 14(5)
- [j1] **BrainGB: A Benchmark for Brain Network Analysis with Graph Neural Networks**
Hejie Cui, Wei Dai, Yanqiao Zhu, Xuan Kan, Antonio Aodong Chen Gu, Joshua Lukemire, Liang Zhan, Lifang He, Ying Guo, and Carl Yang
IEEE Trans. Med. Imaging 42(2)

Workshop Papers

- [w1] **Deep Graph Contrastive Representation Learning**
Yanqiao Zhu*, Yichen Xu*, Feng Yu, Qiang Liu, Shu Wu, and Liang Wang
GRL+@ICML 2020

Preprints

- [p2] **SciBench: Evaluating College-Level Scientific Problem-Solving Abilities of Large Language Models**
Xiaoxuan Wang*, Ziniu Hu*, Pan Lu*, Yanqiao Zhu*, Jieyu Zhang, Satyen Subramaniam, Arjun R. Loomba, Shichang Zhang, Yizhou Sun, and Wei Wang
arXiv: [2307.10635](https://arxiv.org/abs/2307.10635) [cs.CL]
- [p1] **A Survey on Graph Structure Learning: Progress and Promise**
Yanqiao Zhu, Shichang Zhang, Yuanqi Du, Jieyu Zhang, Yizhou Sun, and Wei Wang
arXiv: [2103.03036](https://arxiv.org/abs/2103.03036) [cs.LG]

Academic Services

» Conference Organizers

- Organizing Committee Member, Learning on Graphs Conference (LoG) 2022~2024

» Conference Program Committee Members

- International Joint Conference on Artificial Intelligence (IJCAI), Survey Track 2024
- ACM SIGKDD Conference on Knowledge Discovery and Data Mining (KDD) 2022~2024
- International Conference on Machine Learning (ICML) 2021~2024
- The Web Conference (WWW) 2021, 2024
- International Conference on Learning Representations (ICLR) 2021~2024
- Conference on Neural Information Processing Systems (NeurIPS) 2020~2023
- AAAI Conference on Artificial Intelligence (AAAI) 2021, 2022

» Journal Reviewers

- IEEE Transactions on Pattern Analysis and Machine Intelligence
- IEEE Transactions on Medical Imaging
- IEEE Transactions on Neural Networks and Learning Systems
- IEEE Transactions on Knowledge and Data Engineering
- IEEE Transactions on Signal and Information Processing over Networks
- IEEE Computational Intelligence Magazine
- ACM Transactions on Information Systems

Selected Honors and Awards

- NeurIPS Scholar Award 2023
- Graduate Dean's Scholar Award, University of California, Los Angeles 2022
- National Scholarship, The Ministry of Education of China 2017, 2021
- NeurIPS Outstanding Reviewer Award 2021
- SIGMM Student Travel Grant Award 2021
- SIGIR Student Travel Award 2021
- ICML Participation Grant 2021
- Outstanding Student of University of Chinese Academy of Sciences 2020, 2021
- AAAI Student Scholarship 2019