

Zhenyu Lei

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Research Interests

My primary research interests lie at solving real-world challenges with **LLMs** (distillation, agents, RL, model editing), **AI for science** (AI for neural science, AI for chemistry), and **data mining** (graph machine learning, spatial-temporal models).

Education

University of Virginia, Charlottesville, VA, USA 2023.8-present

Ph.D. in ECE

Advisor: Jundong Li

Xi'an Jiaotong University, Xi'an, Shaanxi, China 2019.8-2023.6

B.S. in Physics

GPA: 89.46/100 (3.82/4.3) (**Transcript**)

Advisor: Minnan Luo

Industrial Experience

Applied Scientist Intern @ Bedminister, AT&T 2025.05 - 2025.08

Project: Improving LLM Reasoning with Model Editing and Mechanistic Interpretability

Host: Dr. Qiong Wu

Publications (* equal contribution)

[20] **Reforming the Mechanism: Editing Reasoning Patterns in LLMs with Circuit Reshaping**

Zhenyu Lei, Qiong Wu, Jianxiong Dong, Yinhan He, Emily Dodwell, Yushun Dong, Jundong Li

In submission

[19] **Editing Multimodal Molecule Language Models**

Zhenyu Lei, Patrick Soga, Yaochen Zhu, Yinhan He, Yushun Dong, Jundong Li

WSDM 2026 (Oral)

[18] **Learning from Diverse Reasoning Paths with Routing and Collaboration**

Zhenyu Lei, Zhen Tan, Song Wang, Yaochen Zhu, Zihan Chen, Yushun Dong, Jundong Li

EMNLP 2025

[17] **From Cross-Task Examples to In-Task Prompts: A Graph-Based Pseudo-Labeling Framework for In-context Learning**

Zihan Chen, Song Wang, Xingbo Fu, Chengshuai Shi, **Zhenyu Lei**, Cong Shen, Jundong Li

EMNLP 2025

[16] **A survey of scaling in large language model reasoning**

Zihan Chen, Song Wang, Zhen Tan, Xingbo Fu, **Zhenyu Lei**, Peng Wang, Huan Liu, Cong Shen, Jundong Li

Arxiv

[15] **Fairness-Aware Graph Learning: A Benchmark**

Yushun Dong, Song Wang, **Zhenyu Lei**, Zaiyi Zheng, Jing Ma, Chen Chen, Jundong Li

KDD 2025

[14] **Graph Prompting for Graph Learning Models: Recent Advances and Future Directions**

- Xingbo Fu, Zehong Wang, Zihan Chen, Jiazheng Li, Yaochen Zhu, **Zhenyu Lei**, Cong Shen, Yanfang Ye, Chuxu Zhang, Jundong Li
KDD 2025
- [13] **Energy-Based Models for Predicting Mutational Effects on Proteins**
Patrick Soga, **Zhenyu Lei**, Yinhan He, Camille Bilodeau, Jundong Li
KDD 2025
- [12] **Harnessing Large Language Models for Disaster Management: A Survey**
Zhenyu Lei, Yushun Dong, Weiyu Li, Rong Ding, Qi Wang, Jundong Li
ACL 2025
- [11] **BrainMAP: Learning Multiple Activation Pathways in Brain Networks**
Song Wang*, **Zhenyu Lei***, Zhen Tan, Jiaqi Ding, Xinyu Zhao, Yushun Dong, Guorong Wu, Tianlong Chen, Chen Chen, Aiyang Zhang, Jundong Li
AAAI'25 (Oral)
- [10] **ST-FiT: Inductive Spatial-Temporal Forecasting with Limited Training Data**
Zhenyu Lei, Yushun Dong, Jundong Li, Chen Chen
AAAI'25 (Oral)
- [9] **Deep Interactions for Multimodal Molecular Property Prediction**
Patrick Soga, **Zhenyu Lei**, Camille Bilodeau, and Jundong Li
PAKDD'25
- [8] **Idea: A flexible framework of certified unlearning for graph neural networks**
Yushun Dong, Binchi Zhang, **Zhenyu Lei**, Na Zou, Jundong Li
KDD'24
- [7] **PyGDebias: A Python Library for Debiasing in Graph Learning**
Yushun Dong, **Zhenyu Lei**, Zaiyi Zheng, Song Wang, Jing Ma, Alex Jing Huang, Chen Chen, Jundong Li
WWW'24
- [6] **LMBot: Distilling Graph Knowledge into Language Model for Graph-less Deployment in Twitter Bot Detection**
Zijian Cai, Zhaoxuan Tan, **Zhenyu Lei**, Hongrui Wang, Zifeng Zhu, Qinghua Zheng, Minnan Luo
WSDM'24
- [5] **HOFA: Twitter Bot Detection with Homophily-Oriented Augmentation and Frequency Adaptive Attention**
Sen Ye, Zhaoxuan Tan, **Zhenyu Lei**, Ruijie He, Hongrui Wang, Qinghua Zheng, Minnan Luo
arXiv'23
- [4] **Twibot-22: Towards graph-based Twitter bot detection**
Shangbin Feng, Zhaoxuan Tan, Herun Wan, Ningnan Wang, Zilong Chen, Binchi Zhang, Qinghua Zheng, Wenqian Zhang, **Zhenyu Lei**, Shujie Yang, Xinshun Feng, Qingyue Zhang, Hongrui Wang, Yuhao Liu, Yuyang Bai, Heng Wang, Zijian Cai, Yanbo Wang, Lijing Zheng, Zihan Ma, Jundong Li, Minnan Luo
NeurIPS'23
- [3] **KALM: Knowledge-Aware Integration of Local, Document, and Global Contexts for Long Document Understanding**
Shangbin Feng, Zhaoxuan Tan, Wenqian Zhang, **Zhenyu Lei**, Yulia Tsvetkov
ACL'23
- [2] **BIC: Twitter Bot Detection with Text-Graph Interaction and Semantic Consistency**

Zhenyu Lei*, Herun Wan*, Wenqian Zhang, Shangbin Feng, Jundong Li, Qinghua Zheng, Minnan Luo
ACL'23

[1] **KCD: Knowledge Walks and Textual Cues Enhanced Political Perspective Detection in News Media**

Wenqian Zhang, Shangbin Feng, Zilong Chen, **Zhenyu Lei**, Jundong Li, Minnan Luo
NAACL'22

Honors and Awards

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| UVA Presidential Fellowship in Collaborative Neuroscience | 2025 |
| UVA Precision Health Initiative Trainee Travel Stipend | 2025 |
| UVA Engineering Academic Commitment to Excellence (ACE) Fellowship | 2024 |
| Scholarship for Outstanding Sichuan Students | 2021 |
| Provincial First Prize, CUMCM | 2020 |
| Dean's List, Xi'an Jiao Tong University | 2020, 2021 |

Services

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| Reviewer for CIKM | 2025 |
| Reviewer for COLM | from 2024 |
| Reviewer for KDD | from 2024 |
| Reviewer for ACL Rolling Review | from 2023, Dec |
| Reviewer for NeurIPS | from 2023 |

Mentorship

Sen Ye → first author in 1*WSDM 2024 submission, PhD student @ Peking University
Zijian Cai → first author in 1*WSDM, MS student @ The Institute of Automation, CAS

Teaching

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| Teaching Assistant of Convex Optimization, University of Virginia | 2025 Fall |
| Teaching Assistant of CS 3501 Foundation of Data Analysis, University of Virginia | 2024 Spring |

Skills

- Programming Skills: Python, PyTorch, MATLAB, C/C++, bash, HTML/CSS, \LaTeX
- Language Skills: Mandarin (native), English (TOEFL 101: R 29, L 29, S 22, W 21)