

# Zhenyu Lei

University of Virginia

Phone: +1 4349877068

Email: vjd5zr@virginia.edu

Webpage: <https://lzyfischer.github.io>

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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] **MolEdit: Knowledge Editing for 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

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

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

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,  $\text{\LaTeX}$
- Language Skills: Mandarin (native), English (TOEFL 101: R 29, L 29, S 22, W 21)