Sikun Guo

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Education

- **University of Virginia** — Charlottesville, VA
  PhD in Computer Science; GPA: 4.000 — *08/2023 – Present*
  - **Research Focus** Reasoning with Large Language Models, Theories of Large Language Model's In-context Learning Ability, Foundation Models for Scientific Discovery, Advisor: Prof. Aidong Zhang
- **University of Virginia** — Charlottesville, VA
  Master of Science in Computer Science; GPA: 3.918 — *08/2021 – 12/2022*
  - **MS Thesis:** Robust Graph Neural Networks via Adaptive Aggregator Selection and Long-range Dependency Modeling, Advisor: Prof. Hongning Wang
- **Nankai University** — Tianjin, China
  Bachelor of Science in Electronic Information Science and Technology; GPA: Top 33% — *08/2017 – 06/2021*
  - **BS Thesis:** The Study of Low Pass Filter Based on Ferromagnetic Substance Powder, Advisor: Prof. Lu Ji

Publications and Patent

Conference and Journal Papers

[1] **Sikun Guo** and Aidong Zhang, "Knowing the Clue, Missing the Answer: Causal Evidence for Knowledge Recruitment Failures in Language Models", under review in *The Fortieth Annual Conference on Neural Information Processing Systems (**NeurIPS** 2026)*

[2] **Sikun Guo**, Di Wang, Xiaohan Fan, Albert Huang, and Aidong Zhang, "Curiosity-Driven Questioning for Engine-Agnostic LLM Research Ideation", in *Proceedings of the ACM SIGKDD Conference on Knowledge Discovery and Data Mining (**KDD** 2026)*

[3] **Sikun Guo**, Amir Hassan Shariatmadari, Jiuqi Wang, Albert Huang, Stefan Bekiranov, Shangtong Zhang, and Aidong Zhang, "InfRL: Inference-time Reinforcement Learning for Research Idea Optimization", in *Proceedings of the ACM SIGKDD Conference on Knowledge Discovery and Data Mining (**KDD** 2026)*

[4] Amir Hassan Shariatmadari, **Sikun Guo**, Nathan C Sheffield, Aidong Zhang, and Kishlay Jha, "HyHG: A Temporal Hypergraph Contrastive Learning Framework for Biomedical Hypothesis Generation", in *Proceedings of the IEEE ICDM 2025 The world's premier research conference in Data Mining (**ICDM** 2025)* ***Best Paper Award***

[5] Amir Hassan Shariatmadari, Alireza Jafari, **Sikun Guo**, Sneha Srinivasan, Nathan C Sheffield, Aidong Zhang, and Kishlay Jha, "ConceptDrift: leveraging spatial, temporal and semantic evolution of biomedical concepts for hypothesis generation", in ***Bioinformatics** 2025)*

[6] **Sikun Guo**, Amir Hassan Shariatmadari, Peng Wang, Albert Huang, and Aidong Zhang, "InfAL: Inference Time Adversarial Learning for Improving Research Ideation", in *Proceedings of the 2025 Conference on Empirical Methods in Natural Language Processing (**EMNLP** 2025)*

[7] **Sikun Guo**, Amir Hassan Shariatmadari, Guangzhi Xiong, Albert Huang, Myles Kim, Corey Williams, Stefan Bekiranov, and Aidong Zhang, "IdeaBench: Benchmarking Large Language Models for Research Idea Generation", in *Proceedings of the ACM SIGKDD Conference on Knowledge Discovery and Data Mining (**KDD** 2025)*

[8] Guangzhi Xiong, Eric Xie, Corey Williams, Myles Kim, Amir Hassan Shariatmadari, **Sikun Guo**, Stefan Bekiranov, and Aidong Zhang, "Toward Reliable Biomedical Hypothesis Generation: Evaluating Truthfulness and Hallucination in Large Language Models", in *Proceedings of the International Joint Conference on Artificial Intelligence (**IJCAI** 2025)*

[9] **Sikun Guo**, Guangzhi Xiong and Aidong Zhang, "Optimizing External and Internal Knowledge of Foundation Models for Scientific Discovery", in *Proceedings of the SIAM International Conference on Data Mining (**SDM** 2025)*

[10] **Sikun Guo**, Amir Hassan Shariatmadari, Guangzhi Xiong, and Aidong Zhang, " Embracing Foundation Models for Advancing Scientific Discovery", in *Proceedings of the 2024 IEEE International Conference on Big Data (**IEEE BigData** 2024)*

[11] Guangzhi Xiong, Eric Xie, Amir Hassan Shariatmadari, **Sikun Guo**, Stefan Bekiranov, and Aidong Zhang, "Improving Scientific Hypothesis Generation with Knowledge Grounded Large Language Models", arxiv preprint.

[12] Guimin Dong, Mingyue Tang, Zhiyuan Wang, Jiechao Gao, **Sikun Guo**, Lihua Cai, Robert Gutierrez, Bradford Campbel, Laura E Barnes, and Mehdi Boukhechba, "Graph neural networks in IoT: A survey" in *ACM Transactions on Sensor Networks*

[13] **Sikun Guo**, "A Survey on GAT-like Graph Neural Networks" in *2020 IEEE International Conference on Communications, Information System and Computer Engineering (CISCE 2020)*

Patents

[1] Lu Ji, **Sikun Guo**, Jinli Zhang, Yu Zhao, Xingyue Sun, and Yu'ang Huang, "A Low Pass Filter for Cryogenic Quantum Experiments Based on Ferromagnetic Substance Powder", Patent Number: CN111540984B

Industry Experience

- **Autoscience Institute** — San Francisco, CA
  Research Scientist Intern at Autoscience Institute — *07/2025 – 08/2025*
  - **Automated Scientific Ideation Rating with LLMs.** Built an agentic LLM system for automatic scientific ideation rating.

Community Service

- **Reviewer:** NeurIPS 2026, KDD 2026, ICDM 2025, KDD 2025
- **Student Volunteer:** IEEE BigData 2024

Teaching Experience

- **University of Virginia** — Charlottesville, VA
  Teaching Assistant
  - Spring 2026, Artificial Intelligence (CS4710)

Research Experience

- **University of Virginia** — Charlottesville, VA
  Research Assistant at Dr.Zhang's RealAI Lab — *01/2024 – now*
  - **The Study of Advancing Scientific Discovery with Foundation Models**
    - Released IdeaBench, a benchmarking system for testing LLM's ability of research ideation.
    - Formulated zero-shot in-context agentic adversarial learning and reinforcement learning for improving research ideation.
    - Categorized challenges and opportunities of embracing foundation models for scientific discovery.
    - Proposed an approach to enable curiosity in LLMs for scientific ideation.
    - Revealed knowledge recruitment failure in LLMs during scientific reasoning.

- **University of Virginia** — Charlottesville, VA
  Research Assistant at Information and Language Processing Lab — *08/2023 – 12/2023*
  - **The Study of Large Language Models' Hallucination Mechanisms**
    - Designed an inter-layer token probability total-variation-based decoding strategy for inducing hallucination of Large Language Models.

- **University of Virginia** Charlottesville, VA
  Research Assistant at Human-Centric Data Mining Group *01/2022 – 08/2023*
  - **The Study of Adversarial Robustness on Graph Neural Networks**
    * Designed a graph neural network GalNN using PyTorch and PyG, robust to poisoning adversarial structure attack with 0 to 25% edges attack budget, and it outperforms other defense baselines across the whole homophily spectrum.

- **University of Virginia** Charlottesville, VA
  Research Assistant at Sensing Systems for Health Lab *01/2022 – 06/2022*
  - **RadioSleep: Non-Contact Sleep Monitoring using Radio Waves for Patients with Sleep Disorders**
    * Published Graph Neural Networks in IoT: A Survey with collaborators.
    * Monitored patients' vital signs with UWB radar sensors and analyzed the data to detect sleep disorder using machine learning.

- **Nankai University** Tianjin, China
  Research Assistant at Radio Frequency Electromagnetic Waves and Superconductor Lab *08/2018 – 06/2021*
  - **The Study of Low Pass Filter Based on Ferromagnetic Substance Powder**
    * Published the patent A Low Pass Filter for Cryogenic Quantum Experiments Based on Ferromagnetic Substance Powder as the 2nd inventor.
    * Led a team consisting of 4 undergraduate researchers and won the 1st Prize in National Undergraduates' Innovation and Entrepreneurship Training Program.
    * Designed the filter's structure using SolidWorks and AutoCAD; analyzed experiment data using Origin.
    * Maintained the collaboration with researchers at Aalto University, Finland, and our filters helped them conduct cryogenic quantum experiments successfully; administered financial work for the team.
  - **The Study of Macroscopic Quantum Tunneling in High Temperature Superconductors**
    * Assisted make Josephson Junction based on $TlBa_2Ca_2Cu_3O_9$ superconductor thin film.
    * Succeeded calculating probability density curves of macroscopic quantum tunneling in intrinsic Josephson junctions under certain experimental conditions using Mathematica and MATLAB.

Programming Skills

- **Languages:** Python, MATLAB, C/C++, Java
- **Technologies:** OpenClaw Agentic AI System, TensorFlow2(Google certified developer), PyTorch, scikit-learn, pandas, AWS, Docker, Git

Awards and Honors

- ICDM 2025 Best Paper Award
- 2024 IEEE International Conference on Big Data Student Travel Award
- Third-class Scholarship in LinkedIn China's Workplace Trainee Boot Camp Season One
- Excellent Undergraduate Thesis (Top 3% at Nankai University)
- 1st Prize in National Undergraduates' Innovation and Entrepreneurship Training Program(3/110)
- 2nd Prize in Tianjin and No.2 at Nankai University of 10th National University Students Ecommerce "Innovation, Creativity, and Entrepreneurship" Competition

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