# Chi Han

PhD Candidate in Computer Science · University of Illinois Urbana-Champaign

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## Research Summary

My long-term research goal is to develop a foundation for analyzing and reprogramming large language models (LLMs) to fundamentally bridge their gaps across domains, capabilities, and scientific disciplines. I seek to uncover the hidden laws governing LLMs' internal mechanisms, thereby suggesting a systematic framework for understanding and steering these seemingly black-box systems. My research roadmap aims to build a systematic framework that spans from foundational understanding to adaptation for scientific discovery. At the foundational level, I aim to develop a framework for LLMs that supports theoretical understanding and principled adaptation, simultaneously describing their internal mechanisms and guiding their structural reprogramming. Building upon this foundation, I leverage this framework as a driver of scientific discovery, bridging the architectural gap in LLMs for scientific discovery, such as drug candidate design, and ultimately extending it to broader scientific domains.

My research has been supported by IBM, Amazon AICE, and Mavis Future Faculty Ph.D. Fellowships. My research enabled the first zero-shot length generalization for LLMs, extending the capabilities of short LLMs to extremely long lengths, which was recognized by the NAACL 2024 Outstanding Paper award. One analysis of LLM representations provides a versatile toolkit for steering and interpreting LLM generations, receiving the ACL 2024 Outstanding Paper award. Our recent progress has developed the first synthesis-guaranteed drug design LLM capable of improving drugs and saving FDA-rejected "fallen angels", receiving the NSF SAIL 2025 Dest Demo Award.

## Education

**University of Illinois at Urbana-Champaign** — *Urbana, IL*
PhD in Computer Science — *2021 - present*
*Thesis Committee: Heng Ji (Advisor), Kyunghyun Cho, Dilek Hakkani-Tur, Christopher Manning, Kathleen McKeown, Tong Zhang*

**University of Illinois at Urbana-Champaign** — *Urbana, IL*
M.S. in Computer Science — *Awarded 2023*

**Massachusetts Institute of Technology** — *Boston, MA*
Visiting Student in Department of Brain and Cognitive Sciences — *2019*
*Advisors: Joshua Tenenbaum, Jiajun Wu, Chuang Gan, Jiayuan Mao*

**Tsinghua University** — *Beijing, China*
Undergraduate in Yao Class — *2016-2020*
*Thesis: Emergence of Hierarchy in Multi-Agent Systems*

## Awards & Honors

**Amazon AICE PhD Fellowship**, Amazon — *2025 - 2026*
**IBM PhD Fellowship**, IBM — *2024 - 2025*
**Outstanding Paper Award**, ACL — *2024*
**Outstanding Paper Award**, NAACL — *2024*

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| **Mavis Future Faculty Fellowship**, UIUC | *2025 - 2026* |
| **Best Demo Award (1st Place)**, Summit for AI Institutes Leadership, NSF | *2025* |
| **Community Service Award**, Tsinghua University | *2017 - 2019* |
| **Yao Class Scholarship**, Tsinghua University | *2016 - 2019* |
| **Second Prize, Freshman Scholarship**, Tsinghua University | *2016* |
| **Third Prize, 'Baidu Star of the Future' Scholarship**, Tsinghua University | *2016* |

## Publications

**Chi Han**, Qifan Wang, Wenhan Xiong, Yu Chen, Heng Ji, and Sinong Wang. "LM-Infinite: Zero-Shot Extreme Length Generalization for Large Language Models" *North American Chapter of the Association for Computational Linguistics* ***(NAACL Outstanding Paper Award)*** (2024)

**Chi Han**, Jialiang Xu, Manling Li, Yi Fung, Chenkai Sun, Nan Jiang, Tarek Abdelzaher, and Heng Ji. "Word Embeddings Are Steers for Language Models" *Association for Computational Linguistics* ***(ACL Outstanding Paper Award)*** (2024)

Edwards, Carl*, **Chi Han***, Gawon Lee, Thao Nguyen, Bowen Jin, Chetan Kumar Prasad, Sara Szymkuć, Bartosz A. Grzybowski, Ying Diao, Jiawei Han, Ge Liu, Hao Peng, Martin D. Burke, and Heng Ji. "mCLM: A Function-Infused and Synthesis-Friendly Modular Chemical Language Model" *In Proceedings of the Fourteenth International Conference on Learning Representations* (ICLR 2026 **(Oral Presentation)**)

Zhining Zhang, Wentao Zhu, Chi Han, Yizhou Wang, Heng Ji. "Neural Synchrony Between Socially Interacting Language Models" *In Proceedings of the Fourteenth International Conference on Learning Representations* (ICLR 2026)

**Chi Han**, Ziqi Wang, Han Zhao, and Heng Ji. "Understanding In-Context Learning from a Kernel Regression Perspective" *Transactions on Machine Learning Research* (2025)

**Chi Han**. "Can Language Models Follow Multiple Turns of Entangled Instructions?" *The 2025 Conference on Empirical Methods in Natural Language Processing Findings* (2025)

**Chi Han** and Heng Ji. "Computation Mechanism Behind LLM Position Generalization" *Association for Computational Linguistics* (2025)

Ziqi Wang, Hanlin Zhang, Xiner Li, Kuan-Hao Huang, **Chi Han**, Shuiwang Ji, Sham M. Kakade, Hao Peng, and Heng Ji. "Eliminating Position Bias of Language Models: A Mechanistic Approach" *The Thirteenth International Conference on Learning Representations* (2025)

**Chi Han**, Hengzhi Pei, Xinya Du, and Heng Ji. "Zero-Shot Classification by Logical Reasoning on Natural Language Explanations" *Findings of the Association for Computational Linguistics* (2023)

Qian, Cheng, **Chi Han**, Yi R. Fung, Yujia Qin, Zhiyuan Liu, and Heng Ji. "CREATOR: Disentangling Abstract and Concrete Reasonings of Large Language Models through Tool Creation" *Findings of the Association for Computational Linguistics* (2023)

Wang, Ziqi, **Chi Han**, Wenxuan Bao, and Heng Ji. "Understanding the Effect of Data Augmentation on Knowledge Distillation" *arXiv preprint arXiv:2305.12565.* (2023)

**Chi Han**, Qizheng He, Charles Yu, Xinya Du, Hanghang Tong, and Heng Ji. "Logical Entity Representation in Knowledge-Graphs for Differentiable Rule Learning" *The Eleventh International Conference on Learning Representations* (2022)

**Chi Han**, Mingxuan Wang, Heng Ji, and Lei Li. "Learning Shared Semantic Space for Speech-to-Text Translation" *Findings of the Association for Computational Linguistics* (2021)

**Chi Han**, Jiayuan Mao, Chuang Gan, Josh Tenenbaum, and Jiajun Wu. "Visual Concept-Metaconcept Learning" *Advances in Neural Information Processing Systems 32* (2019)

## Invited Talks

**Constructing and Reconstructing A "Brain Atlas" for Large Language Models**
Invited Talk, University of Chicago, 2025

**The Quest for A Science of LMs**
Tutorial (Single-Speaker), AAAI, 2025

**The Lifecycle of Knowledge in Large Language Models: Memorization, Editing, and Beyond**
Tutorial, AAAI, 2025

**Towards A Physiology of Language Models: Elucidating and Utilizing Hidden Language Representation**
Guest Lecture, Northeastern University, 2025

**Towards A Physiology of Language Model Representations**
Guest Lecture, Case Western Reserve University, 2024

**The Quest for A Science of LMs**
Guest Lecture, University of Illinois at Urbana-Champaign CS546 Course, 2024

**Towards A Physiology of Language Model Representations**
Invited Talk, University of Illinois at Urbana-Champaign ML Seminar, 2024

**Enabling AI to Perceive and Translate Texts and Speech Uniformly**
Invited Talk, The Jiangmen Talk Series, 2021

**Letting Neural Networks Translate Speech and Texts Uniformly**
Invited Talk, TechBeat Talk Series, 2021

## Media Coverage

**CS PhD student Chi Han diagnoses language models**
University of Illinois at Urbana-Champaign CS News, 2024

**2024 IBM Ph.D. Fellowship Announcement: Chi Han et al. Are Selected**
The Heart of Machines, 2025

**The first author of the NAACL 2024 Outstanding Paper Award, Han Chi from UIUC, gives a lecture.**
AI Time, 2024

**ACL 2024 Outstanding Paper Award: Chi Han's Lecture | LM-Steer: Word Vectors Are Steering Wheels of Language Models**
AI Time, 2024

## Professional Service

**Tutorials**
"The Quest for A Science of Language Models", **Chi Han**, Heng Ji, AAAI 2025 Tutorial
"The Lifecycle of Knowledge in Large Language Models: Memorization, Editing, and Beyond", Manling Li, **Chi Han**, et al., AAAI 2025 Tutorial

**Area Chair**
EMNLP Demo Track (2024-2025)
ACL Rolling Review(2025)

**Panelist**
Leadership & Career Development Panelist at 2025 Summit for AI Institutes Leadership (SAIL)

**Journal Reviewer**
IEEE Transactions on Circuits and Systems for Video Technology (IEEE TCSVT)
IEEE Transactions on Neural Networks and Learning Systems (IEEE TNNLS)
Transactions on Intelligent Systems and Technology (TIST)

**Organizer**
UIUC-NLP Seminar (2023-2025)
Molecule Maker Lab Institute (MMLI) Student and Postdoc Student Council (2025-2026)
UIUC Data and Information Systems (DAIS) Cross-Lab Annual Gathering (2023)
UIUC Artificial Intelligence (AI) Cross-Lab Annual Gathering (2024)

**Program Committee Member**
ACL (2023-now)
EMNLP (2023-now)
NAACL (2023-now)
EMNLP Demo (2024)
ICLR (2025)
AISTATS (2025)
TMLR (2025)

## Internships

**University of Illinois at Urbana-Champaign** *Urbana, IL*
Research Assistant *Aug 2024 - present*

**Amazon AI** *Seattle, WA*
Applied Scientist Intern *2024*

- Project: A Comprehensive Benchmark for Large Language Model Multi-Turn Capabilities
- Advisor: Xin Liu, Qingyu Yin

**Meta GenAI** *Bellevue, WA*
Research Scientist Intern *2023*

- Project: LM-Infinite: Zero-Shot Extreme Length Generalization for Large Language Models (NAACL 2024 Outstanding Paper)
- Advisor: Sinong Wang, Qifan Wang, Wenhan Xiong, Yu Chen

**ByteDance AI Lab** *Shanghai, China*
Research Intern on Natural Language Processing *2020-2021*

- Project: Learning Shared Semantic Space for Speech-to-Text Translation. (ACL 2021 Findings)
- Advisor: Prof. Lei Li (now Assistant Professor at CMU)

## Funding Projects Worked on

**Capital One-Illinois ASKS Center Seedling Fund** *2025-Present*

**IBM-Illinois Discovery Accelerator Institute (IIDAI) Center** *2025-Present*

**DoE Center for Advanced Bioenergy and Bioproducts Innovation** *2022-Present*

- Co-authored paper in protein language modeling and protein property prediction.

**NSF MMLI: Molecule Maker Lab Institute** *2020-Present*

- Led the mCLM backbone model design and contributed to the writing for the MMLI proposal and renewal.

**DARPA Seedling Fund: Miriam - News Event Simulator** *2023-2024*

**DARPA INCAS: Influence Campaign Awareness and Sensemaking** *2021–2025*

- System was selected in annual **DARPA research highlights** as a major milestone in trustworthy AI research
- Delivery paper received **ACL Outstanding Paper Award** 2024
- Led live demo design showcased at the **DARPA transition meetings** for message source attribution and stance analysis
- the system was selected by DARPA to be delivered to the **Department of State** as a transition product, supporting speech draft proofreading.

**DARPA MIPS: Modeling Influence Pathways** *2022-2024*

## Teaching and Mentoring

### Teaching

**Teaching Assistant**, with a guest lecture "Towards A Science of Language Models", UIUC CS546 *2024*

### Mentored Students and Publications

**Zhining Zhang**, Inter-Brain Synchrony in LLMs **(In Submission to ICLR 2026)**, CS Undergrad@PKU → CS Ph.D.@UC-Berkeley *2025*

**Xuehang Guo**, SyncMind: Measuring Agent Out-of-Sync Recovery **(ICML 2025)**, CS MS@UPitt → CS Ph.D@William & Mary *2024*

**Cheng Li**, Diagnosis and Treatment of Mental Health Disorders (in progress), MSRA→CS Ph.D.@UW *2024*

**Ziyi Gao**, Curing direct preference learning (in progress), CS Undergrad@THU → Deepseek AI *2023*

**Jialiang Xu**, Flexible control of language models **(ACL 2024)**, CS Undergrad@UIUC → CS MS@Stanford *2022*

**Cheng Qian**, Tool creation for disentangling abstract and concrete reasoning of large language models **(EMNLP 2023 Findings)**, CS Undergrad@THU → CS Ph.D.@UIUC *2022*