

Namkyeong Lee

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RESEARCH INTEREST

Artificial Intelligence for Science

By leveraging the power of Artificial Intelligence, I'm interested in bringing insights and advancements to various scientific fields, including biology, chemistry, and more, ultimately benefiting human society through scientific discovery.

- Large Language Models for Science
- LLM Agents for Science
- Graph Neural Networks for Science

EDUCATION

KAIST (Korea Advanced Institute of Science and Technology)

- Ph.D. in Industrial and Systems Engineering
- M.S. in Industrial and Systems Engineering
 - Research Interest: Large Language Models, LLM Agents, AI4Science
 - GPA: 3.73/4.3
 - Advisor: [Prof. Chanyoung Park](#)

Mar 2023 – Feb 2026

Mar 2021 – Feb 2023

Korea University

- B.S. in Industrial Management Engineering
 - GPA: 3.9/4.5
 - Dean's List (Spring 2019)

Mar 2015 – Feb 2021

POSITIONS

Genentech, South San Francisco, CA, USA

- Senior Machine Learning Scientist
 - Manager: [Dr. Gabriele Scalia](#)
- Research Intern
 - Mentors: [Dr. Hanchen Wang](#) and [Prof. Aviv Regev](#)
 - Project: LLM Agents for Biological Perturbation
- Research Intern
 - Mentors: [Dr. Edward De Brouwer](#), [Dr. Ehsan Hajiramezani](#), and [Dr. Gabriele Scalia](#)
 - Project: LLM Agents for Drug Discovery

Mar 2026 – Present

Oct 2025 – Dec 2025

Sep 2024 – Nov 2024

University of Illinois at Urbana-Champaign, Urbana, IL, USA

- Visiting Scholar in Computer Science Department
 - Host: [Prof. Jimeng Sun](#)
 - Project: Large Language Models for Drug Discovery

Sep 2023 – Feb 2024

NAVER, Seongnam, Korea

- Research Intern
 - Mentors: [Dr. Donghyun Kim](#) and [Dr. Min-Chul Yang](#)
 - Project: Learning Continual User Representation for Recommendation

Dec 2022 – Feb 2023

AIsoftKorea, Seoul, Korea

- Co-founder of an AI-based Legal Counseling Startup Company
 - Building AI model for providing qualified answers to Korean legal questions

Jun 2020 – Mar 2021

SELECTED PUBLICATIONS

RAG-Enhanced Collaborative LLM Agents for Drug Discovery

Namkyeong Lee, *et al.*, Gabriele Scalia

AAAI Conference on Artificial Intelligence (AAAI 2026)

3D Interaction Geometric Pre-training for Molecular Relational Learning

Namkyeong Lee, *et al.*, Chanyoung Park

Conference on Neural Information Processing Systems (NeurIPS 2025 Spotlight)

Conditional Graph Information Bottleneck for Molecular Relational Learning

Namkyeong Lee, *et al.*, Chanyoung Park

International Conference on Machine Learning (ICML 2023)

Augmentation-Free Self-Supervised Learning on Graphs

Namkyeong Lee, *et al.*, Chanyoung Park

AAAI Conference on Artificial Intelligence (AAAI 2022)

- [C18] IR-Agent: Expert-Inspired LLM Agents for Structure Elucidation from Infrared Spectra
 Heewoong Noh, **Namkyeong Lee**, Gyoung S. Na, Kibum Kim, Chanyoung Park
 International Conference on Learning Representations (**ICLR 2026**)
- [C17] RAG-Enhanced Collaborative LLM Agents for Drug Discovery
Namkyeong Lee, Edward De Brouwer, Ehsan Hajiramezanali, Tommaso Biancalani, Chanyoung Park, Gabriele Scalia
 AAAI Conference on Artificial Intelligence (**AAAI 2026**)
- [C16] 3D Interaction Geometric Pre-training for Molecular Relational Learning
Namkyeong Lee, Yunhak Oh, Heewoong Noh, Gyoung S. Na, Minkai Xu, Hanchen Wang, Tianfan Fu, Chanyoung Park
 Conference on Neural Information Processing Systems (**NeurIPS 2025 Spotlight**)
- [J3] MolTextQA: A Curated Question-Answering Dataset and Benchmark for Molecular Structure-Text Relationship Learning
 Siddhartha Laghuvarapu, **Namkyeong Lee**, Chufan Gao, Jimeng Sun
 Journal of Data-centric Machine Learning Research (**DMLR**)
- [C15] Global Context-aware Representation Learning for Spatially Resolved Transcriptomics
 Yunhak Oh[†], Junseok Lee[†], Yeongmin Kim, Sangwoo Seo, **Namkyeong Lee**, Chanyoung Park
 International Conference on Machine Learning (**ICML 2025**)
- [C14] Thickness-aware E(3)-Equivariant Mesh Neural Networks
 Sungwon Kim, **Namkyeong Lee**, Yunyoung Doh, Seungmin Shin, Guimok Cho, Seung-Won Jeon, Sangkook Kim, Chanyoung Park
 International Conference on Machine Learning (**ICML 2025**)
- [C13] Subgraph Federated Learning for Local Generalization
 Sungwon Kim, Yoonho Lee, Yunhak Oh, **Namkyeong Lee**, Sukwon Yun, Junseok Lee, Sein Kim, Carl Yang, Chanyoung Park
 International Conference on Learning Representations (**ICLR 2025 Oral Presentation**)
- [C12] Retrieval-Retro: Retrieval-based Inorganic Retrosynthesis with Expert Knowledge
 Heewoong Noh, **Namkyeong Lee**, Gyoung S. Na, Chanyoung Park
 Conference on Neural Information Processing Systems (**NeurIPS 2024**)
- [C11] Vision Language Model is NOT All You Need: Augmentation Strategies for Molecule Language Models
Namkyeong Lee, Siddhartha Laghuvarapu, Chanyoung Park, Jimeng Sun
 ACM International Conference on Information and Knowledge Management (**CIKM 2024**)
- [C10] Debaised Graph Poisoning Attack via Contrastive Surrogate Objective
 Kanghoon Yoon, Yeonjun In, **Namkyeong Lee**, Kibum Kim, Chanyoung Park
 ACM International Conference on Information and Knowledge Management (**CIKM 2024**)
- [W1] Compositional Representation of Polymorphic Crystalline Materials
Namkyeong Lee, Heewoong Noh, Gyoung S. Na, Jimeng Sun, Tianfan Fu, Marinka Zitnik, Chanyoung Park
 AI4Science Workshop at NeurIPS 2023 (**AI4Science 2023**)
- [C9] Density of States Prediction of Crystalline Materials via Prompt-guided Multi-Modal Transformer
Namkyeong Lee[†], Heewoong Noh[†], Sungwon Kim, Dongmin Hyun, Gyoung S. Na, Chanyoung Park
 Conference on Neural Information Processing Systems (**NeurIPS 2023**)
- [C8] Shift-Robust Molecular Relational Learning with Causal Substructure
Namkyeong Lee, Kanghoon Yoon, Gyoung S. Na, Sein Kim, Chanyoung Park
 ACM SIGKDD Conference on Knowledge Discovery and Data Mining (**KDD 2023**)
- [C7] Task Relation-aware Continual User Representation Learning
 Sein Kim, **Namkyeong Lee**, Donghyun Kim, Min-Chul Yang, Chanyoung Park
 ACM SIGKDD Conference on Knowledge Discovery and Data Mining (**KDD 2023**)
- [C6] Task-Equivariant Graph Few-shot Learning
 Sungwon Kim, Junseok Lee, **Namkyeong Lee**, Wonjoong Kim, Seungyoon Choi, Chanyoung Park
 ACM SIGKDD Conference on Knowledge Discovery and Data Mining (**KDD 2023**)

	<p>[C5] Conditional Graph Information Bottleneck for Molecular Relational Learning Namkyeong Lee, Dongmin Hyun, Gyoung S. Na, Sungwon Kim, Junseok Lee, Chanyoung Park International Conference on Machine Learning (ICML 2023)</p> <p>[C4] Heterogeneous Graph Learning for Multi-modal Medical Data Analysis Sein Kim, Namkyeong Lee, Junseok Lee, Dongmin Hyun, Chanyoung Park AAAI Conference on Artificial Intelligence (AAAI 2023 Oral Presentation)</p> <p>[J2] Deep Single-cell RNA-seq data Clustering with Graph Prototypical Contrastive Learning Junseok Lee, Sungwon Kim, Dongmin Hyun, Namkyeong Lee, Yejin Kim, Chanyoung Park Bioinformatics (2023)</p> <p>[C3] Relational Self-Supervised Learning on Graphs Namkyeong Lee, Dongmin Hyun, Junseok Lee, Chanyoung Park ACM International Conference on Information and Knowledge Management (CIKM 2022)</p> <p>[C2] GraFN: Semi-Supervised Node Classification on Graph with Few Labels via Non-Parametric Distribution Assignment Junseok Lee, Yunhak Oh, Yeonjun In, Namkyeong Lee, Dongmin Hyun, Chanyoung Park ACM SIGIR Conference on Research and Development in Information Retrieval (SIGIR 2022 Short Paper)</p> <p>[J1] Self-Supervised Graph Representation Learning via Positive Mining Namkyeong Lee, Junseok Lee, Chanyoung Park Information Sciences (2022)</p> <p>[C1] Augmentation-Free Self-Supervised Learning on Graphs Namkyeong Lee, Junseok Lee, Chanyoung Park AAAI Conference on Artificial Intelligence (AAAI 2022)</p>	
AWARDS & SCHOLARSHIPS	KAIST Presidential Best Ph.D. Thesis Award	2026
	NeurIPS Top Reviewer	2025
	Best Paper Award	2024
	▪ KDD 2024 Workshop on Federated Learning for Data Mining and Graph Analytics	
	NeurIPS Scholar Award	2023
	KDD Travel Award	2023
	CIKM Travel Award	2022
	Grand Prize at Seoul Innovation Challenge 2020 , Seoul Business Agency	2021
	▪ Building AI model for providing quantified answers to Korean legal questions	
	• Awarded for the best team among 444 teams	
	Dean's List , Korea University	Spring 2019
	▪ Academic Excellence Award for attaining a semester GPA of 4.5 / 4.5	
	Special Scholarship for the Student Affairs Office , Korea University	Fall 2019, Spring 2020
	Veritas Scholarship , Korea University	Spring 2020
	▪ Research on optimize drone routing with trucks for on-demand services	
	• Advisor: Prof. Taesu Cheong	
TEACHING EXPERIENCE	Teaching Assistant	
	▪ IE343: Statistical Machine Learning	Spring 2021 - 2024
	▪ CoE202: Basics of Artificial Intelligence	Fall 2021
PROFESSIONAL SERVICES	Conference Reviews	
	▪ AAAI Conference on Artificial Intelligence (AAAI)	2023 - Present
	▪ Conference on Neural Information Processing Systems (NeurIPS)	2023 - Present
	▪ International Conference on Learning Representations (ICLR)	2024 - Present
	▪ International Conference on Machine Learning (ICML)	2024 - Present
	▪ Learning on Graphs Conference (LoG)	2023 - Present

Journal Reviews

- IJSE Transactions
- ACM Transactions on Knowledge Discovery from Data (TKDD)
- IEEE Transactions on Neural Networks and Learning Systems (TNNLS)
- IEEE Transactions on Artificial Intelligence (TAI)
- World Wide Web
- Information Sciences
- The Journal of Supercomputing

Workshop Reviews

- Machine Learning for Genomics Explorations (MLGenX) @ ICLR 2025
- AI for New Drug Modalities (AIDrugX) @ NeurIPS 2024
- New Frontiers of AI for Drug Discovery and Development (AI4D3) @ NeurIPS 2023
- Computational Biology (WCB) @ ICML 2023
- Structured Probabilistic Inference & Generative Modeling (SPIGM) @ ICML 2023

Event Organizations

- Student Organizer at MLGenX Workshop @ ICLR 2025

TALKS AND SEMINARS

Artificial Intelligence for Molecular Science

- UNIST IE Research Seminar
- UNIST AIGS Open Seminar

Feb 2026
Oct 2025

Learning Multiple Modalities of Molecules: from GNNs to LLM Agents

- Genentech

Oct 2025

Conditional Graph Information Bottleneck for Molecular Relational Learning

- Learning on Graphs and Geometry (LoGG) Reading Group

Feb 2024

Relational Self-Supervised Learning on Graphs

- Top Conference Session of Korea Software Congress (KSC)

Dec 2022

Augmentation-Free Self-Supervised Learning on Graphs

- Top Conference Session of Korea Computer Congress (KCC)

Jun 2022

REFERENCES

Prof. Chanyoung Park

Associate Professor, Korea Advanced Institute of Science and Technology (KAIST)
E-mail: cy.park@kaist.ac.kr

Prof. Jimeng Sun

Health Innovation Professor, University of Illinois at Urbana-Champaign (UIUC)
E-mail: jimeng@illinois.edu

Prof. Tianfan Fu

Associate Professor, Nanjing University
E-mail: futianfan@gmail.com

[CV compiled on 2026-02-10]