

# 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 (LLMs) for Science
- LLM Agents for Science
- Foundation Models 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 Hajiramezanali](#), 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**)

**FULL  
PUBLICATIONS**  
 C: CONFERENCE  
 J: JOURNAL  
 W: WORKSHOP  
 (†: Equal contribution)

- [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] Debiased 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**)

- [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**)
- [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**)
- [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)
- [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**)
- [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**)
- [J1] Self-Supervised Graph Representation Learning via Positive Mining  
**Namkyeong Lee**, Junseok Lee, Chanyoung Park  
**Information Sciences** (2022)
- [C1] Augmentation-Free Self-Supervised Learning on Graphs  
**Namkyeong Lee**, Junseok Lee, Chanyoung Park  
 AAAI Conference on Artificial Intelligence (**AAAI 2022**)

<b>AWARDS &amp; SCHOLARSHIPS</b>	<b>KAIST Presidential Best Ph.D. Thesis Award</b>	2026
	▪ Thesis Title: Understanding Science through the Lens of AI	
	<b>NeurIPS Top Reviewer</b>	2025
	<b>Best Paper Award</b>	2024
	▪ KDD 2024 Workshop on Federated Learning for Data Mining and Graph Analytics	
	<b>NeurIPS Scholar Award</b>	2023
	<b>KDD Travel Award</b>	2023
	<b>CIKM Travel Award</b>	2022
	<b>Grand Prize at Seoul Innovation Challenge 2020</b> , Seoul Business Agency	2021
	▪ Building AI model for providing quantified answers to Korean legal questions <ul style="list-style-type: none"> <li>• Awarded for the best team among 444 teams</li> </ul>	
	<b>Dean's List</b> , Korea University	Spring 2019
	▪ Academic Excellence Award for attaining a semester GPA of 4.5 / 4.5	
	<b>Special Scholarship for the Student Affairs Office</b> , Korea University	Fall 2019, Spring 2020
	<b>Veritas Scholarship</b> , Korea University	Spring 2020
	▪ Research on optimize drone routing with trucks for on-demand services <ul style="list-style-type: none"> <li>• Advisor: <a href="#">Prof. Taesu Cheong</a></li> </ul>	
<b>TEACHING EXPERIENCE</b>	<b>Teaching Assistant</b>	
	▪ IE343: Statistical Machine Learning	Spring 2021 - 2024
	▪ CoE202: Basics of Artificial Intelligence	Fall 2021
<b>PROFESSIONAL SERVICES</b>	<b>Conference Reviews</b>	
	▪ 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

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