Namkyeong Lee

E-mail • Homepage • Google Scholar • Github • LinkedIn

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 — Mar 2023 – Feb 2026 (Expected)
- M.S. in Industrial and Systems Engineering — Mar 2021 – Feb 2023
  - Research Interest: Large Language Models, LLM Agents, AI4Science
  - GPA: 3.68/4.3
  - Advisor: Prof. Chanyoung Park

Korea University

- B.S. in Industrial Management Engineering — Mar 2015 – Feb 2021
  - GPA: 3.9/4.5
  - Dean's List (Spring 2019)

POSITIONS

Genentech, South San Francisco, CA, USA

- Research Intern — Oct 2025 – Dec 2025
  - Mentors: Dr. Hanchen Wang and Prof. Aviv Regev
  - Project: LLM Agents for Biological Perturbation
- Research Intern — Sep 2024 – Nov 2024
  - Mentors: Dr. Edward De Brouwer, Dr. Ehsan Hajiramezanali, and Dr. Gabriele Scalia
  - Project: LLM Agents for Drug Discovery

University of Illinois at Urbana-Champaign, Urbana, IL, USA — Sep 2023 – Feb 2024

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

NAVER, Seongnam, Korea — Dec 2022 – Feb 2023

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

AISoftKorea, Seoul, Korea — Jun 2020 – Mar 2021

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

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)

[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**)
and ACL 2024 Workshop on Language and Molecules

[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**)

AWARDS & SCHOLARSHIPS

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
- 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 GSAI Open Seminar — 2025

Learning Multiple Modalities of Molecules: from GNNs to LLM Agents

- Genentech — 2025

Conditional Graph Information Bottleneck for Molecular Relational Learning

- Learning on Graphs and Geometry (LoGG) Reading Group — 2024

Relational Self-Supervised Learning on Graphs

- Top Conference Session of Korea Software Congress (KSC) — 2022

Augmentation-Free Self-Supervised Learning on Graphs

- Top Conference Session of Korea Computer Congress (KCC) — 2022

REFERENCES

Prof. Chanyoung Park
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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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