

Namkyeong Lee

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RESEARCH INTEREST

Applied Machine Learning

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

- Graph Neural Networks for Biology and Chemistry
- Multi-Modal Large Language Model for Biology and Chemistry
- Graph Representation Learning

EDUCATION

KAIST (Korea Advanced Institute of Science and Technology)

- Ph.D. in Industrial and Systems Engineering
- Research Interest: Graph Representation Learning, AI4Science
- Advisor: [Prof. Chanyoung Park](#)

Mar 2023 – Present

KAIST (Korea Advanced Institute of Science and Technology)

- M.S. in Industrial and Systems Engineering
- GPA: 3.85/4.3
- Research Interest: Graph Representation Learning, Graph Mining
- Advisor: [Prof. Chanyoung Park](#)

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

- Research Intern
- Mentors: [Dr. Ehsan Hajiramezanali](#), [Dr. Edward De Brouwer](#), and [Dr. Gabriele Scalia](#)
- Project: LLM Agents for Drug Discovery

Sep 2024 – Nov 2024

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

- Visiting Scholar in Computer Science Department
- Host: [Prof. Jimeng Sun](#)
- Project: Uncertainty Quantification for Polymorphic Crystalline Materials
- 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

PUBLICATIONS

C: CONFERENCE
J: JOURNAL

(†: Equal contribution)

- [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**)
and KDD 2024 Workshop on Federated Learning for Data Mining and Graph Analytics (**FedKDD**)
- [C12] Implicit Precursor Extraction with Expert Retriever for Inorganic Retrosynthesis
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**)
- [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**)
and ICLR 2023 Workshop on Machine Learning for Materials (**ML4Materials**)
- [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, Seungyeon 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)
and ICML 2023 Workshop on Computational Biology (**WCB**)
- [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 Scholar Award	2023
KDD Travel Award	2023
CIKM Travel Award	2022
Grand Prize at Seoul Innovation Challenge 2020 , Seoul Business Agency	2021
<ul style="list-style-type: none"> ▪ 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
<ul style="list-style-type: none"> ▪ 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

Spring 2020

- ## TEACHING EXPERIENCE

Spring 2021 - 2024
Fall 2021

- IE343: Statistical Machine Learning
- CoE202: Basics of Artificial Intelligence

PROFESSIONAL SERVICES

2023 - Present
2023 - Present
2024 - Present
2024 - Present
2023 - Present

- AAAI Conference on Artificial Intelligence (AAAI)
- Conference on Neural Information Processing Systems (NeurIPS)
- International Conference on Learning Representations (ICLR)
- International Conference on Machine Learning (ICML)
- Learning on Graphs Conference (LoG)

- 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

- 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

- Student Organizer at MLGenX Workshop @ ICLR 2025

TALKS AND SEMINARS

2024

- Learning on Graphs and Geometry (LoGG) Reading Group

2022

- Top Conference Session of Korea Software Congress (KSC)

2022

- Top Conference Session of Korea Computer Congress (KCC)

REFERENCES

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

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

Associate Professor, Nanjing University
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