

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
- Graph Representation Learning
- Multi-modal Learning for Scientific Discovery

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

Sep 2024 – Present

- Research Intern
- Mentors: [Dr. Ehsan Hajiramezanali](#) and [Dr. Gabriele Scalia](#)
- Project: Large Language Models 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: Uncertainty Quantification for Polymorphic Crystalline Materials
- 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

PUBLICATIONS

(†: Equal contribution)

CONFERENCES

- [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] 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**)

- [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**)
- [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**)
- [C1] Augmentation-Free Self-Supervised Learning on Graphs
Namkyeong Lee, Junseok Lee, Chanyoung Park
AAAI Conference on Artificial Intelligence (**AAAI 2022**)

JOURNALS

- [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**)
- [J1] Self-Supervised Graph Representation Learning via Positive Mining
Namkyeong Lee, Junseok Lee, Chanyoung Park
Information Sciences (2022)

WORKSHOPS

- [W2] Subgraph Federated Learning for Local Generalization
Sungwon Kim, Yoonho Lee, Carl Yang, Yunhak Oh, **Namkyeong Lee**, Sukwon Yun, Junseok Lee, Sein Kim, Chanyoung Park
KDD 2024 Workshop on Federated Learning for Data Mining and Graph Analytics (**FedKDD**)
- [W1] Stoichiometry Representation Learning with Polymorphic Crystal Structures
Namkyeong Lee, Heewoong Noh, Gyoung S. Na, Tianfan Fu, Jimeng Sun, Chanyoung Park
NeurIPS 2023 Workshop on AI for Scientific Discovery: From Theory to Practice (**AI4Science**)

PROJECTS

Korea Research Institute of Chemical Technology (KRICT)

- Geometric Deep Learning for Molecular Interactions 2024
- Retrosynthesis Analysis for Inorganic Materials 2023
- Predicting Molecular Properties after Chemical Interaction 2022

	<ul style="list-style-type: none"> ▪ Predicting the Density of States based on the Structure of Materials 	2021
	NAVER Shopping	
	<ul style="list-style-type: none"> ▪ Learning Continual Universal User Representation for Recommendation 	2022
	AISoftKorea	
	<ul style="list-style-type: none"> ▪ Sentence Similarity Model for Korean Legal Sentences • 1st Awarded project at Seoul R&D research center among 444 teams 	2020
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
	Veritas Scholarship , Korea University	Spring 2020
	<ul style="list-style-type: none"> ▪ Research on optimize drone routing with trucks for on-demand services • Advisor: Prof. Taesu Cheong 	
TEACHING EXPERIENCE	Teaching Assistant	
	<ul style="list-style-type: none"> ▪ IE343: Statistical Machine Learning ▪ CoE202: Basics of Artificial Intelligence 	Spring 2021 - 2024 Fall 2021
PROFESSIONAL SERVICES	Conference Reviews	
	<ul style="list-style-type: none"> ▪ AAAI Conference on Artificial Intelligence (AAAI) 	2023 - 2025
	<ul style="list-style-type: none"> ▪ Conference on Neural Information Processing Systems (NeurIPS) 	2023 - 2024
	<ul style="list-style-type: none"> ▪ International Conference on Learning Representations (ICLR) 	2024 - 2025
	<ul style="list-style-type: none"> ▪ International Conference on Machine Learning (ICML) 	2024
	<ul style="list-style-type: none"> ▪ Learning on Graphs Conference (LoG) 	2023 - 2025
	Journal Reviews	
	<ul style="list-style-type: none"> ▪ ACM Transactions on Knowledge Discovery from Data (TKDD) 	
	<ul style="list-style-type: none"> ▪ IEEE Transactions on Neural Networks and Learning Systems (TNNLS) 	
	<ul style="list-style-type: none"> ▪ World Wide Web 	
	<ul style="list-style-type: none"> ▪ Information Sciences 	
	Workshop Reviews	
	<ul style="list-style-type: none"> ▪ New Frontiers of AI for Drug Discovery and Development (AI4D3) @ NeurIPS 	2023
	<ul style="list-style-type: none"> ▪ Computational Biology (WCB) @ ICML 	2023
	<ul style="list-style-type: none"> ▪ Structured Probabilistic Inference & Generative Modeling (SPIGM) @ ICML 	2023
TALKS AND SEMINARS	Conditional Graph Information Bottleneck for Molecular Relational Learning	
	<ul style="list-style-type: none"> ▪ Learning on Graphs and Geometry (LoGG) Reading Group 	2024
	Relational Self-Supervised Learning on Graphs	
	<ul style="list-style-type: none"> ▪ Top Conference Session of Korea Software Congress (KSC) 	2022
	Augmentation-Free Self-Supervised Learning on Graphs	
	<ul style="list-style-type: none"> ▪ Top Conference Session of Korea Computer Congress (KCC) 	2022
REFERENCES	Prof. Chanyoung Park	
	Assistant 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

Assistant Professor, Rensselaer Polytechnic Institute (RPI)

E-mail: fut2@rpi.edu

[CV compiled on 2024-09-26]