

# Namkyeong Lee

[namkyeong96@kaist.ac.kr](mailto:namkyeong96@kaist.ac.kr) • [Homepage](#) • [Google Scholar](#) • [Github](#)

## 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

### 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

- [C11] Molecule Language Model with Augmented Pairs and Expertise Transfer  
**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**<sup>†</sup>, Heewoong Noh<sup>†</sup>, 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, 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**)
- [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
- Predicting the Density of States based on the Structure of Materials 2021

##### NAVER Shopping

- Learning Continual Universal User Representation for Recommendation 2022

##### AISoftKorea

- Sentence Similarity Model for Korean Legal Sentences 2020
  - 1st Awarded project at Seoul R&D research center among 444 teams

#### AWARDS & SCHOLARSHIPS

**NeurIPS Scholar Award** 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
	<ul style="list-style-type: none"> <li>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> </li> </ul>	
	<b>Dean's List</b> , Korea University	Spring 2019
	<ul style="list-style-type: none"> <li>Academic Excellence Award for attaining a semester GPA of 4.5 / 4.5</li> </ul>	
	<b>Special Scholarship for the Student Affairs Office</b> , Korea University	Fall 2019, Spring 2020
	<b>Veritas Scholarship</b> , Korea University	Spring 2020
	<ul style="list-style-type: none"> <li>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> </li> </ul>	
<b>TEACHING EXPERIENCE</b>	<b>Teaching Assistant</b>	
	<ul style="list-style-type: none"> <li>IE343: Statistical Machine Learning</li> <li>CoE202: Basics of Artificial Intelligence</li> </ul>	Spring 2021 - 2024 Fall 2021
<b>PROFESSIONAL SERVICES</b>	<b>Conference Reviews</b>	
	<ul style="list-style-type: none"> <li>AAAI Conference on Artificial Intelligence (AAAI)</li> <li>Conference on Neural Information Processing Systems (NeurIPS)</li> <li>International Conference on Learning Representations (ICLR)</li> <li>International Conference on Machine Learning (ICML)</li> <li>Learning on Graphs Conference (LoG)</li> </ul>	2023 - 2025 2023 - 2024 2024 2024 2023 - 2025
	<b>Journal Reviews</b>	
	<ul style="list-style-type: none"> <li>ACM Transactions on Knowledge Discovery from Data (TKDD)</li> <li>IEEE Transactions on Neural Networks and Learning Systems (TNNLS)</li> <li>World Wide Web</li> <li>Information Sciences</li> </ul>	
	<b>Workshop Reviews</b>	
	<ul style="list-style-type: none"> <li>New Frontiers of AI for Drug Discovery and Development (AI4D3) @ NeurIPS</li> <li>Computational Biology (WCB) @ ICML</li> <li>Structured Probabilistic Inference &amp; Generative Modeling (SPIGM) @ ICML</li> </ul>	2023 2023 2023
<b>TALKS AND SEMINARS</b>	<b>Conditional Graph Information Bottleneck for Molecular Relational Learning</b>	
	<ul style="list-style-type: none"> <li>Learning on Graphs and Geometry (LoGG) Reading Group</li> </ul>	2024
	<b>Relational Self-Supervised Learning on Graphs</b>	
	<ul style="list-style-type: none"> <li>Top Conference Session of Korea Software Congress (KSC)</li> </ul>	2022
	<b>Augmentation-Free Self-Supervised Learning on Graphs</b>	
	<ul style="list-style-type: none"> <li>Top Conference Session of Korea Computer Congress (KCC)</li> </ul>	2022
<b>REFERENCES</b>	<b>Prof. Chanyoung Park</b>	
	Assistant Professor, Korea Advanced Institute of Science and Technology (KAIST)	
	E-mail: <a href="mailto:cy.park@kaist.ac.kr">cy.park@kaist.ac.kr</a>	
	<b>Prof. Jimeng Sun</b>	
	Health Innovation Professor, University of Illinois at Urbana-Champaign (UIUC)	
	E-mail: <a href="mailto:jimeng@illinois.edu">jimeng@illinois.edu</a>	
	<b>Prof. Tianfan Fu</b>	
	Assistant Professor, Rensselaer Polytechnic Institute (RPI)	
	E-mail: <a href="mailto:fut2@rpi.edu">fut2@rpi.edu</a>	

[CV compiled on 2024-07-16]