

# 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 chemistry, biology, and more.

- Graph Neural Networks for Chemistry and Biology
- Graph Representation Learning

## EDUCATION

### KAIST (Korea Advanced Institute of Science and Technology)

- Ph.D. in Industrial and Systems Engineering Mar 2023 – Present
  - Research Interest: Graph Representation Learning, AI4Science
  - Advisor: [Prof. Chanyoung Park](#)

### KAIST (Korea Advanced Institute of Science and Technology)

- M.S. in Industrial and Systems Engineering Mar 2021 – Feb 2023
  - GPA: 3.85/4.3
  - Research Interest: Graph Representation Learning, Graph Mining
  - 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)

## WORK EXPERIENCE

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

Sep 2023 – Present

- 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

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

#### WORKSHOPS

- [W3] Stoichiometry Representation Learning with Polymorphic Crystal Structures  
**Namkyeong Lee**, Heewoong Noh, Gyoung S. Na, Tianfan Fu, Jimeng Sun, Chanyoung Park  
NeurIPS Workshop on AI for Scientific Discovery: From Theory to Practice (**AI4Science 2023**)
- [W2] Deep Single-cell RNA-seq data Clustering with Graph Prototypical Contrastive Learning  
Junseok Lee, Sungwon Kim, Dongmin Hyun, **Namkyeong Lee**, Yejin Kim, Chanyoung Park  
ICML Workshop on Computational Biology (**WCB 2023**)
- [W1] Predicting Density of States via Multi-modal Transformer  
**Namkyeong Lee**<sup>†</sup>, Heewoong Noh<sup>†</sup>, Sungwon Kim, Dongmin Hyun, Gyoung S. Na, Chanyoung Park  
ICLR Workshop on Machine Learning for Materials (**ML4Materials 2023**)

#### PROJECTS

- Retrosynthesis Analysis for Inorganic Materials** 2023
  - Collaboration with Korea Research Institute of Chemical Technology (KRICT)
- Learning Continual Universal User Representation for Recommendation** 2022
  - Collaboration with NAVER Shopping
- Predicting Molecular Properties after Chemical Interaction** 2022
  - Collaboration with Korea Research Institute of Chemical Technology (KRICT)
- Predicting Density of States based on the Structure of Materials** 2021
  - Collaboration with Korea Research Institute of Chemical Technology (KRICT)
- Sentence Similarity Model for Korean Legal Sentences** 2020
  - 1st Awarded project at Seoul R&D research center

#### 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
  - 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"> <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>Certificate</b> , Korea National Police Agency	2018
	<ul style="list-style-type: none"> <li>▪ An exemplary auxiliary police.</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 - 2023 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>▪ International Conference on Machine Learning (ICML)</li> <li>▪ International Conference on Learning Representations (ICLR)</li> <li>▪ Learning on Graphs Conference (LoG)</li> <li>▪ Conference on Neural Information Processing Systems (NeurIPS)</li> </ul> <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> </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 - 2024 2024 2024 2023 2023  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> <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> <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>	2024  2022 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 2024-01-06]