# 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 2021)

## WORK EXPERIENCE

**NAVER** — Dec 2022 – Feb 2023

Seongnam, Korea

- Research Intern
- Project: Learning Continual User Representation for Recommendation

**AISoftKorea** — Jun 2020 – Mar 2021

Seoul, Korea

- Co-founder of an AI-based legal counseling startup company.
- AI model for providing qualified answers to Korean legal questions.

## PUBLICATIONS

(†: Equal contribution)

### CONFERENCES

[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)

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

**WORKSHOPS**

[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**[†], Heewoong Noh[†], Sungwon Kim, Dongmin Hyun, Chanyoung Park
ICLR Workshop on Machine Learning for Materials (**ML4Materials 2023**)

**PROJECTS**

**Retrosynthesis Analysis for Inorganic Materials** May 2023 – Present
- Collaboration with Korea Research Institute of Chemical Technology (KRICT)

**Learning Continual Universal User Representation for Recommendation** Jul 2022 – Jun 2023
- Collaboration with NAVER Shopping

**Predicting Molecular Properties after Chemical Interaction** Mar 2022 – Dec 2022
- Collaboration with Korea Research Institute of Chemical Technology (KRICT)

**Predicting Density of States based on the Structure of Materials** May 2021 – Mar 2022
- Collaboration with Korea Research Institute of Chemical Technology (KRICT)

**Sentence Similarity Model for Korean Legal Sentences** June 2020 – Dec 2020
- 1st Awarded project at Seoul R&D research center (2020)

**AWARDS & SCHOLARSHIPS**

**CIKM Travel Award** Sep 2022
- SIGIR student travel grants for CIKM 2022.

**Grand Prize at Seoul Innovation Challenge 2020**, Seoul Business Agency Jan 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

**Certificate**, Korea National Police Agency Fall 2018
- An exemplary auxiliary police.

**TEACHING EXPERIENCE**

**Teaching Assistant**
- IE343: Statistical Machine Learning Spring 2021, 2022, 2023
- CoE202: Basics of Artificial Intelligence Fall 2021

## PROFESSIONAL SERVICES

### Conference Reviews

- Conference on Neural Information Processing Systems (NeurIPS), 2023
- AAAI Conference on Artificial Intelligence (AAAI), 2023

### Journal Reviews

- ACM Transactions on Knowledge Discovery from Data (TKDD)
- IEEE Transactions on Neural Networks and Learning Systems (TNNLS)
- World Wide Web

### Workshop Reviews

- Computational Biology (WCB) @ ICML 2023
- Structured Probabilistic Inference & Generative Modeling (SPIGM) @ ICML 2023

## TALKS AND SEMINARS

### 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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