

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)

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

- [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**)
- [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

- [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[†], Heewoong Noh[†], 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

- 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 2018

- An exemplary auxiliary police.

**TEACHING
EXPERIENCE**

Teaching Assistant

- IE343: Statistical Machine Learning Spring 2021 - 2023
- CoE202: Basics of Artificial Intelligence Fall 2021

**PROFESSIONAL
SERVICES**

Conference Reviews

- AAAI Conference on Artificial Intelligence (AAAI) 2023 - 2024
- International Conference on Machine Learning (ICML) 2024
- International Conference on Learning Representations (ICLR) 2024
- Learning on Graphs Conference (LoG) 2023
- Conference on Neural Information Processing Systems (NeurIPS) 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

- 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

**TALKS AND
SEMINARS**

Conditional Graph Information Bottleneck for Molecular Relational Learning

- Learning on Graphs and Geometry (LoGG) Reading Group 2024

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

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

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