

Heewoong Noh

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RESEARCH INTEREST

AI for Materials Discovery

My research focuses on developing AI and LLM-based agentic systems to accelerate materials design and synthesis, bridging computational prediction with experimental discovery.

- **Keywords:** AI-driven materials design and synthesis, LLM agents for scientific discovery

EDUCATION

KAIST, Daejeon, South Korea

- Ph.D. in Industrial & Systems Engineering Mar 2025 – Present
- M.S. in Industrial & Systems Engineering Mar 2023 – Feb 2025
 - Research Interest: Machine Learning, AI4Science, LLMs for Chemistry
 - Advisor: Prof. Chanyoung Park

Korea University, Seoul, South Korea

- B.S. in Industrial and Management Engineering GPA: 3.94/4.5 Mar 2017 – Feb 2023
- Leave of absence for military service (Aug.2018 - Mar.2020)

PUBLICATIONS

(†: Equal contribution)

CONFERENCES

- [C5] IR-Agent: Expert-Inspired LLM Agents for Structure Elucidation from Infrared Spectra
Heewoong Noh, Namkyeong Lee, GyoungS. Na, Kibum Kim, Chanyoung Park
International Conference on Learning Representations(**ICLR 2026**)
- [C4] Token-Efficient Item Representation via Images for LLM Recommender Systems
Kibum Kim, Sein Kim, Hongseok Kang, Jiwan Kim, **Heewoong Noh**, Yeonjun In, Kanghoon Yoon, Jinoh Oh, Chanyoung Park
International Conference on Learning Representations(**ICLR 2026**)
- [C3] 3D Interaction Geometric Pre-training for Molecular Relational Learning
Namkyeong Lee, Yunhak Oh, **Heewoong Noh**, Gyoung S. Na, Minkai Xu, Hanchen Wang, Tianfan Fu, Chanyoung Park
Conference on Neural Information Processing Systems (**NeurIPS 2025 Spotlight**)
- [C2] Retrieval-Retro: Retrieval-based Inorganic Retrosynthesis with Expert Knowledge
Heewoong Noh, Namkyeong Lee, GyoungS. Na*, Chanyoung Park*
Conference on Neural Information Processing Systems (**NeurIPS 2024**)
- [C1] Density of States Prediction of Crystalline Materials via Prompt-guided Multi-Modal Transformer
Namkyeong Lee†, **Heewoong Noh**†, Sungwon Kim, Dongmin Hyun, GyoungS. Na, Chanyoung Park
Conference on Neural Information Processing Systems (**NeurIPS 2023**)

WORKSHOPS

- [W3] MSP-LLM: A Unified Large Language Model Framework for Complete Material Synthesis Planning
Heewoong Noh, GyoungS. Na, Namkyeong Lee, Chanyoung Park
ICLR Workshop on AI4Mat: Accelerated Materials Design (**AI4Mat 2026**)
- [W2] Stoichiometry Representation Learning with Polymorphic Crystal Structures
Namkyeong Lee, **Heewoong Noh**, GyoungS. Na, Tianfan Fu, Jimeng Sun, Chanyoung Park
NeurIPS Workshop on AI for Scientific Discovery: From Theory to Practice (**AI4Science 2023**)
- [W1] Predicting Density of States via Multi-modal Transformer
Namkyeong Lee†, **Heewoong Noh**†, Sungwon Kim, Dongmin Hyun, GyoungS. Na, Chanyoung Park
ICLR Workshop on Machine Learning for Materials (**ML4Materials 2023**)

PREPRINTS

- [P1] MSP-LLM: A Unified Large Language Model Framework for Complete Material Synthesis Planning
Heewoong Noh, GyoungS. Na, Namkyeong Lee, Chanyoung Park

PROJECTS

Korea Research Institute of Chemical Technology (KRICT)

- Geometric Deep Learning for Molecular Interactions 2024
 - Retrosynthesis Analysis for Inorganic Materials 2023
- AWARDS & SCHOLARSHIPS**
- HAICon2021**, Korea Institute of Information Security & Cryptology (KIISC) Nov 2021
- Awarded 6th place among 177 participating teams (AI Competition)
 - Building an AI model for detecting security threats in industrial control systems (Time series anomaly detection)
- Industrial Engineering Project Competition**, Korean Institute of Industrial Engineers(KIIE) 2021
- Participation award in industrial engineering project competition
 - Building UAM dynamic corridor algorithm
- Veritas Scholarship**, Korea University 2021
- Research on the detection of anomalies in the manufacturing process
 - Advisor: Prof. Sungwon Han
- Certificate of Recognition**, National Police Agency Oct 2019
- Awarded when serving military service as an auxiliary police
- PROFESSIONAL SERVICES**
- Conference Reviews**
- Conference on Neural Information Processing Systems(NeurIPS) 2024 – Present
 - International Conference on Machine Learning (ICML) 2025 – Present
 - International Conference on Learning Representations (ICLR) 2025 – Present
 - Conference on Information and Knowledge Management (CIKM ADS) 2025
- Workshop Reviews**
- AI for Accelerated Materials Design(AI4Mat)@NeurIPS 2024 – Present
 - AI for Accelerated Materials Design(AI4Mat)@ICLR 2025 – Present
- TALKS AND SEMINARS**
- Density of States Prediction of Crystalline Materials via Prompt-guided Multi-Modal Transformer**
- TALK: Top Conference Session of Korea Software Congress(KSC) 2023
- Retrieval-Retro: Retrieval-based Inorganic Retrosynthesis with Expert Knowledge**
- TALK: Top Conference Session of Korea Computer Congress(KSC) 2025
- REFERENCES**
- **Prof. Chanyoung Park**, Associate Professor, KAIST
Email: cy.park@kaist.ac.kr

[CV compiled on 2026-03-22]