

Hyukjun Lim

 Personal Website
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  GitHub
  LinkedIn

Research Interest

Keywords: AI for Chemistry, Molecular Modeling, Materials Discovery

- Incorporating **physics-informed inductive biases** into AI models for molecular science.
- Modeling **molecular interactions and dynamics** using geometric and generative AI.
- Leveraging **Machine Learning Interatomic Potentials (MLIPs)** for materials property prediction.
- Accelerating **materials discovery** via AI to discover high-performance, low-cost materials.

Education

Seoul National University

M.S./Ph.D. in Chemical and Biological Engineering (PI: Yousung Jung)

Mar 2026 – Present

GPA: 4.0/4.3

B.S. in Materials Science and Engineering & Artificial Intelligence

Mar 2022 – Feb 2026

GPA: 4.09/4.3

- *Summa Cum Laude*, Ranked 3/67 in the department

Publications

Learning Reaction-Condition Plausibility for Evaluation and Self-Curation Under Noisy and Non-Unique Supervision

Hyukjun Lim, Yousung Jung

ICML Workshop on AI for Science, 2026 [\[Paper\]](#)

Angular Relational Knowledge Distillation of Machine Learning Interatomic Potentials for Scalable Catalyst Exploration

Hyukjun Lim*, Seokhyun Choung*, Jinuk Moon, Jeong Woo Han

npj Computational Materials, 2026 [\[Paper\]](#)

A Priori Sampling of Transition States with Guided Diffusion

Hyukjun Lim*, Soojung Yang*, Lucas Pinede*, Miguel Steiner, Yuanqi Du, Rafael Gómez-Bombarelli

NeurIPS Workshop on Frontiers in Probabilistic Inference, 2025 [\[Paper\]](#)

Real-Time Prediction of TSV Thermal Fatigue Reliability in HBM Using FEA-Guided U-Net-Based Deep Learning Framework

Hyukjun Lim, Joonseok Bang, Chanhyung Lee, Junhyeong Park, Juhyeong Shin, Hyeongseo Kim, Myoung-Gyu Lee

International Symposium on Microelectronics and Packaging (ISMP), 2025, **Oral Presentation**

CheapNet: Cross-attention on Hierarchical representations for Efficient protein-ligand binding Affinity Prediction

Hyukjun Lim, Sun Kim, Sangseon Lee

ICLR, 2025 [\[Paper\]](#)

* Equal contribution

Research Experience

Learning Matter Lab (PI: Rafael Gómez-Bombarelli)

Jul 2025 – Aug 2025

DMSE, MIT, Visiting Student

- Developed **ASTRA**, A Priori Sampling of **TR**ANSITION States with Guided Diffusion, eliminating the need for explicit knowledge of transition state samples.
- Enabled *a priori* sampling using **Score-Based Interpolation** and **Score-Aligned Ascent**.
- Benchmarked ASTRA on various systems, demonstrating generalizability across complex chemical spaces.

Computational Catalysis & Emerging Materials Lab (PI: Jeong Woo Han)

Mar 2025 – Jun 2025

DMSE, SNU, Intern

- Proposed **ARK**, Angular relational knowledge distillation of machine learning interatomic potentials, a framework for efficiently training MLIPs.
- Directly transfers first-order interaction from a high-fidelity teacher model to a compact student model, by formalizing **relational vectors** and **InfoNCE-based contrastive objective**.
- Achieved state-of-the-art performance in various datasets compared to baselines.

Bio & Health Informatics Lab (PI: Sun Kim)

Mar 2024 – Dec 2024

CSE, SNU, Intern

- Developed **CheapNet** [\[GitHub\]](#), a GNN model for protein-ligand binding affinity prediction.
- Proposed **cluster-attention mechanism**, which dynamically groups atoms based on embeddings and refines biologically meaningful interactions using cross-attention mechanism.
- Achieved state-of-the-art results, and evaluated CheapNet's **interpretability** and **memory efficiency**.

Scholarship

Presidential Science Scholarship for Graduate Students

Mar 2026 – Feb 2028

25,000 USD, living stipend

AI Seoul Tech Scholarship

Mar 2026 – Feb 2027

15,000 USD, living stipend

Kwanjeong Educational Foundation

Mar 2024 – Feb 2026

12,000 USD, living stipend

KIAT, Semiconductor Specialized University Semiconductor Track

Nov 2023 – Feb 2026

14,000 USD

Korea Student Aid Foundation

Mar 2022 – Feb 2026

13,500 USD, full tuition

Bodam Scholarship Foundation

Mar 2023 – Feb 2024

4,500 USD, full tuition

Skills

Languages: Python (advanced), C++ (intermediate), C (intermediate), MATLAB (intermediate)

Technologies: Pytorch, Pytorch-Geometric, Deep Graph Library, RDKit, PyMOL

English: TOEFL – 96 (03/29/2025), TEPS – 416 (02/04/2024)

Reviewer

ICML Workshop on AI for Science, 2026

4 submissions

ICLR Workshop on AI with Recursive Self-Improvement, 2026

1 submission

NeurIPS Workshop on AI for Science, 2025

4 submissions

NeurIPS Workshop on Frontiers in Probabilistic Inference, 2025

3 submissions

Teaching Experience

Basic Computing: First Adventures in Computing

Sep 2025 – Dec 2025

Sep 2024 – Dec 2024

Mar 2024 – Jun 2024

College Writing 2: Writing in Science & Technology

Mar 2023 – Jun 2023

Awards

Young Scientist Award

Nov 2025

International Symposium on Microelectronics and Packaging (ISMP), 2025

Excellence Award, Deep Learning-based Product Recognition AI Competition

Jul 2025

Digital Innovation Sharing University