Hyukjun Lim

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Research Interest

Keywords: `AI for Materials Science`, `Molecular Modeling`, `Materials Discovery`

- Incorporating **physically inspired inductive biases** into AI models
- Leveraging **machine learning potentials** for materials property prediction
- Accelerating **materials discovery** via AI to discover high-performance, low-cost materials

Education

Seoul National University *Anticipated Graduation: Feb 2026*
GPA: 4.07/4.3

B.S. in Materials Science and Engineering *Mar 2022 – Current*

Interdisciplinary Major in Artificial Intelligence *Sep 2023 – Current*

Publication

Hyukjun Lim, Sun Kim, and Sangseon Lee†. CheapNet: Cross-attention on Hierarchical representations for Efficient protein-ligand binding Affinity Prediction. In The Thirteenth International Conference on Learning Representations, 2025. († indicates corresponding author) [Paper] [Project Page]

Research Experience

Computational Catalysis & Emerging Materials Lab (PI: Jeong Woo Han) *Mar 2025 – Current*
MSE, SNU, Intern

- Proposed a **latent space-driven screening pipeline** for fuel cell cathode materials leveraging the equivariant graph neural network, EquiformerV2.
- Introduced a metric quantifying **structural novelty** and **prediction uncertainty**, guiding balanced exploration and exploitation of candidate materials.

Materials Data & Informatics Lab (PI: Seungwu Han) *Jan 2025 – Feb 2025*
MSE, SNU, Intern

- Developed **SevenNet-dFS** [GitHub], a GNN interatomic potential model for materials property prediction, incorporating **direct output head** for predicting force and stress.
- Ensured stable direct output for force and stress, by leveraging the derivation of energy as guidance.
- Achieved a **250x** speedup in molecular dynamics (MD) simulations while maintaining accuracy.

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**.

Neuromorphic Materials & Devices Lab (PI: Sangbum Kim) *Jul 2023 – Nov 2023*
MSE, SNU, Intern

- Enhanced MNIST Accuracy of **SNN-RBM** Simulation from 85% (baseline) to 97.5% using **transfer learning**.
- Demonstrated feature extracting properties of SNN-RBM simulation by a **count-spike** method.

Scholarship

Kwanjeong Educational Foundation *Mar 2024 – Current*
3,000 USD/semester, living stipend

Korea Student Aid Foundation *Mar 2024 – Current*
2,250 USD/semester, full tuition *Mar 2022 – Feb 2023*

KIAT, Semiconductor Specialized University Semiconductor Track *Nov 2023 – Current*
1500 USD

Bodam Scholarship Foundation *Mar 2023 – Feb 2024*
2,250 USD/semester, full tuition

Skills

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

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

English: TOEFL – 93 (02/15/2025), TEPS – 416 (02/04/2024)

Teaching Experience

Basic Computing: First Adventures in Computing *Sep 2024 – Dec 2024*
Mar 2024 – Jun 2024

College Writing 2: Writing in Science & Technology *Mar 2023 – Jun 2023*

Awards

Outstanding Tutor in College Writing Tutoring Program *Aug 2023*
Faculty of Liberal Education, SNU

Excellence Award, National Public Safety Slogan Competition *Feb 2025*
KORAIL NETWORKS (Ranked 2nd among 2,327 participants)

Extracurricular Activities

IPESK, Next-Generation Engineer *Dec 2024*

NAEK, Young Engineers Honor Society *Nov 2023*

Attendee, 17th International Conference on Scintillating Materials and their Applications (SCINT 2024) *Jul 2024*
University of Milano – Bicocca

Practice of Semiconductor Manufacturing Process *Jan 2024*
Inter-University Semiconductor Research Center

Samsung Shining Star *Jan 2023*
Samsung, Seoul