Nayoung Kim

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Education

Ph.D. **Korea Advanced Institute of Science and Technology (KAIST)**, Graduate School of Artificial Intelligence — Seoul, South Korea, Feb 2025 – present
- Advisor: Sungsoo Ahn

M.S. **Korea Advanced Institute of Science and Technology (KAIST)**, Graduate School of Artificial Intelligence — Daejeon, South Korea, Feb 2022 – Aug 2024
- Advisor: Jinkyoo Park

B.S. **Korea Advanced Institute of Science and Technology (KAIST)**, Chemical and Biomolecular Engineering — Daejeon, South Korea, Aug 2017 – Feb 2022
- GPA: 4.14/4.30 (Summa Cum Laude)

Experience

Pohang University of Science and Technology (POSTECH), Researcher — Pohang, South Korea, Sept 2024 – Jan 2025
- Advisor: Sungsoo Ahn
- Topic: Generative model for metal-organic frameworks

Korea Advanced Institute of Science and Technology (KAIST), M.S — Daejeon, South Korea, Feb 2022 – Aug 2022
- Advisor: Jay Hyung Lee
- Topic: Thermodynamic and kinetic modeling of electric vacuum swing adsorption (EVSA) cycle for efficient direct air capture (DAC)

Korea Advanced Institute of Science and Technology (KAIST), Research Intern — Daejeon, South Korea, June 2021 – Aug 2021
- Advisor: Jay Hyung Lee
- Topic: Modeling polarization in electrochemical processes

Korea Advanced Institute of Science and Technology (KAIST), Research Intern — Daejeon, South Korea, Dec 2020 – Feb 2021
- Advisor: Jinwoo Lee
- Topic: Analyzing mechanism of potassium-ion batteries (KIB)
- Topic: Intercalation-conversion hybrid cathode using V5S8 in lithium-sulfur battery to improve energy density

SK Hynix, Intern — Icheon, South Korea, Dec 2019 – Feb 2020
- Topic: Modeling the relationship between zone 1 and zone 2 in CMP head for accurate prediction of removal rate (Excellence Award)

Publications

Machine Learning Hamiltonians are Accurate Energy-Force Predictors 2026
Seongsu Kim, Chanhui Lee, Yoonho Kim, Seongjun Yun, Honghui Kim, ***Nayoung Kim***, Changyoung Park, Sehui Han, Sungbin Lim, Sungsoo Ahn
arxiv.org/abs/2602.16897 (arXiv)

AtomMOF: All-Atom Flow Matching for MOF-Adsorbate Structure Prediction 2026
Nayoung Kim, Honghui Kim, Sihyun Yu, Minkyu Kim, Seongsu Kim, Sungsoo Ahn
arxiv.org/abs/2602.07351 (arXiv)

CatFlow: Co-generation of Slab-Adsorbate Systems via Flow Matching 2026
Minkyu Kim, ***Nayoung Kim***, Honghui Kim, Sungsoo Ahn
arxiv.org/abs/2602.05372 (arXiv)

Flexible MOF Generation with Torsion-Aware Flow Matching 2025
Nayoung Kim, Seongsu Kim, Sungsoo Ahn
arxiv.org/abs/2505.17914 (NeurIPS)

High-order Equivariant Flow Matching for Density Functional Theory Hamiltonian Prediction 2025
Seongsu Kim, ***Nayoung Kim***, Sungsoo Ahn
arxiv.org/abs/2505.18817 (NeurIPS)
Spotlight Presentation (688/21575=3.19%)

MOFFlow: Flow Matching for Structure Prediction of Metal-Organic Frameworks 2025
Nayoung Kim, Seongsu Kim, Minsu Kim, Jinkyoo Park, Sungsoo Ahn
arxiv.org/abs/2410.17270 (ICLR, NeurIPS AIDrugX Workshop)

Decoupled Sequence and Structure Generation for Realistic Antibody Design 2025
Nayoung Kim, Minsu Kim, Sungsoo Ahn, Jinkyoo Park
arxiv.org/abs/2402.05982 (TMLR)

Awards & Honors

Korea National Research Foundation (NRF) Ph.D. Fellowship Sept 2025 – Aug 2027

SK Hynix Internship Excellence Award Feb 2021

Korea National Science & Technology Scholarship 2019 – 2021
Awarded in Fall 2019, Spring 2020, Fall 2020, and Spring 2021

Dean's List of College of Engineering, KAIST 2019 – 2021
Awarded in Spring 2019, Fall 2019, and Spring 2021

Academic Excellence Scholarship of Chemical and Biomolecular Engineering, KAIST 2019 – 2020
Awarded in Spring 2019 and Fall 2020

Projects

Deep Generative Models for Simulation and Design of Metal-Organic Frameworks Mar 2025 – Sept 2025
NVIDIA Academic Grant Program Award

Talks

MOFFlow: Flow Matching for Structure Prediction of Metal-Organic Frameworks Nov 2024
KAIST-MILA Prefrontal AI Research Center

Reviewer

Conference
ICLR 2025, NeurIPS 2025, ICLR 2026

Skills

Languages: Korean (native), English (fluent), Chinese (basic)