Seongsu Kim

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Ph.D. Student
Graduate School of Artificial Intelligence
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RESEARCH INTEREST

My research interests include integrating AI into scientific research and using AI to uncover scientific facts. Additionally, I am interested in physical and chemical concepts such as **solid state physics** *[C1]*, **molecular science** *[C1,C4,P2]*, **density functional theory (DFT)** *[C1,C4,P2]*, and **structure prediction** and **material generation** on structured materials like MOF *[C2,C3,P1]*.

EDUCATION

9/2025 - current **Ph.D. Student, Korea Advanced Institute of Science and Technology (KAIST), Korea**
Graduate School of Artificial Intelligence
Advisor: Sungsoo Ahn

2/2023 - 8/2025 **M.S., Pohang University of Science and Technology (POSTECH), Korea**
Graduate School of Artificial Intelligence
Advisor: Sungsoo Ahn, and Dongwoo Kim

3/2016 - 2/2023 **B.S., Gwangju Institute of Science and Technology (GIST), Korea**
Majored in *Physics*
Minored in *Mathematics*, *Computer Science*, *Aritificial Intelligence*

7/2017 - 8/2017 **University of California, Berkeley**
Summer study abroad program

PUBLICATIONS

[C] Conference
[P] Preprint

[P2] Machine Learning Hamiltonians are Accurate Energy-Force Predictors
Seongsu Kim, Chanhui Lee, Yoonho Kim, Seongjun Yun, Honghui Kim, Nayoung Kim, Changyong Park, Sehui Han, Sungbin Lim, and Sungsoo Ahn
Preprint 2026, PDF

[P1] ATOMMOF: All-Atom Flow Matching for MOF-Adsorbate Structure Prediction
Nayoung Kim, Honghui Kim, Sihyun Yu, Minkyu Kim, Seongsu Kim, and Sungsoo Ahn
Preprint 2026, PDF

[C4] High-order Equivariant Flow Matching for Density Functional Theory Hamiltonian Prediction
Seongsu Kim, Nayoung Kim, Dongwoo Kim, and Sungsoo Ahn
Neural Information Processing Systems ***(NeurIPS)***, **2025**, PDF CODE SLIDE
Spotlight ***(3.1%≈688/21575)***

[C3] Flexible MOF Generation with Torsion-Aware Flow Matching
Nayoung Kim, Seongsu Kim, and Sungsoo Ahn
Neural Information Processing Systems ***(NeurIPS)***, **2025**, PDF

[C2] MOFFlow: Flow Matching for Structure Prediction of Metal-Organic Frameworks
Nayoung Kim, Seongsu Kim, Minsu Kim, Jinkyu Park, and Sungsoo Ahn
International Conference on Learning Representations ***(ICLR)***, **2025**, PDF
NeurIPS AIDrugX Workshop, **2024**

[C1] Gaussian Plane-wave Neural Operator for Electron Density Estimation
Seongsu Kim, and Sungsoo Ahn
International Conference on Machine Learning ***(ICML)***, **2024**, PDF CODE

EXPERIENCE

Structure and Probabilistic Machine Learning (SPML) Lab, Korea **Student researcher**
2/2025 - current ***KAIST***, *Korea Advanced Institute of Science and Technology* (Advisor: Prof. Sungsoo Ahn)
2/2023 - 2/2025 ***POSTECH***, *Pohang University of Science and Technology*
- Machine learning for Scientific Research
- Project 1: Accelerating the Density Functional Theory
- Project 2: Designing Metal-Organic Framework

9/2021 - 2/2023 **Computational Many-body Physics (CMBP) Lab, Korea** **Research Intern**
***GIST**, Gwangju Institute of Science and Technology* (Advisor: Prof. Donghee Kim)
- Computer-simulated thermodynamics of *solid states physics*
- Investigated the phase transition of physical models using the Monte Carlo method
- Investigated the critical phenomena in the 2D long-range antiferromagnetic Ising model with anisotropy
- Wrote the simulation code with C++, MPI and CUDA programming

6/2022 – 7/2022 **Statistical Artificial Intelligence (SAIL) Lab, Korea** **Research Intern**
***KAIST**, Korea Advanced Institute of Science and Technology* (Advisor: Prof. Jaesik Choi)
- Investigated the various techniques of *explainable A.I.* including LIMES, LRP, CRP, and GRAD-CAM.

12/2019 – 2/2020 **Quantum Field & Gravity Theory Group, Korea** **Research Intern**
***GIST**, Gwangju Institute of Science and Technology* (Advisor: Prof. Keunyoung Kim)
- Investigated the correspondence of deep learning and the Ads/CFT

TALKS & PRESENTATION

10/31/2025 **QHFlow: Accelerating DFT with Equivariant Flow Matching** **Invited Talk**
NVIDIA BioNeMo Team (Hosted by Youhan Lee) SLIDE

5/6/2025 **Accelerating the *ab-initio* Calculation with the Machine Learning** **Invited Talk**
KAIST-MILA Prefrontal AI Research Center

15/7/2024 **Gaussian Plane-wave Neural Operator for Electron Density Estimation** **Presentation**
KAIST-POSTECH joint AI Workshop

HONORS & AWARDS

2016 - 2023 **Government-Sponsored Tuition Scholarship** **Scholarship**
Received scholarship 8 times ($20,000)

2016 - 2017 **Government-Sponsored Presidential Science Scholarship** **Scholarship**
Received scholarship 2 times ($1,400)

REVIEWER

AAAI (2023), **ICML** (2024), **ICLR** (2025 Notable reviewer), **NeurIPS** (2025)

WORK EXPERIENCE

1/2020 - 8/2021 **Republic of Korea Army, Korea**
Mandatory military service

LANGUAGES

English - Professional Working, **Korean** - Native

SKILLS

Backgrounds	Computational physics, Quantum mechanics, Statistical physics
Languages	**Python (Proficient)**, C++, C, Java
Python Libraries	PyTorch, Lightning, Hydra, PyG, WandB, Numpy, Scikit-learn, Matplotlib
Softwares, etc.	Version control (Git and GitHub), Linux-based environment, Vim, Slurm, Docker
DFT tools	PySCF, ORCA, VASP, Quantum Espresso, Castep
CSP tools	GULP, USPEX, CrySPY