Seongsu Kim

Ph.D. candidate
Graduate School of Artificial Intelligence   🌐 seongsukim-ml.github.io ↗   ✉ seongsu.kim@kaist.ac.kr ↗

EDUCATION

9/2025 - current
Ph.D. candidate, Korea Advanced Institute of Science and Technology (KAIST), Korea
Graduate School of Artificial Intelligence
Topic 1. *Accelerating the ab-initio calculation with Artificial Intelligence*
Topic 2. *Machine Learning for Solid States Physics and Quantum Chemistry*
Topic 3. *Generative Model for Material and Molecular Science*
Adivisor: Sungsoo Ahn

2/2023 - 8/2025
M.S., Pohang University of Science and Technology (POSTECH), Korea
Graduate School of Artificial Intelligence
Adivisor: 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 session study abroad program
Courses: *Quantum Physics*, *Data Structures and Algorithms*

PUBLICATIONS & CONFERENCES

High-order Equivariant Flow Matching for Density Functional Theory Hamiltonian Prediction
<u>Seongsu Kim</u>, Nayoung Kim, Dongwoo Kim,and Sungsoo Ahn
Neural Information Processing Systems (NeurIPS) **Spotlight**, **2025**, PDF ↗

Flexible MOF Generation with Torsion-Aware Flow Matching
Nayoung Kim, <u>Seongsu Kim</u>, and Sungsoo Ahn
Neural Information Processing Systems (NeurIPS), **2025**, PDF ↗

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

Gaussian Plane-wave Neural Operator for Electron Density Estimation
<u>Seongsu Kim</u> and Sungsoo Ahn
International Conference on Machine Learning (ICML), **2024**, PDF ↗ CODE ↗

EXPERIENCE

2/2025 - current
2/2023 - 2/2025
Structure and Probabilistic Machine Learning (SPML) Lab, Korea   Student researcher
KAIST, *Korea Advanced Institute of Science and Technology* (Advisor: Prof. Sungsoo Ahn)
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

6/2023 – 7/2023
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

5/6/2025	**Accelerating the *ab-initio* Calculation with the Machine Learning** KAIST-MILA Prefrontal AI Workshop	**Talks**
15/7/2024	**Gaussian Plane-wave Neural Operator for Electron Density Estimation** KAIST-POSTECH joint AI Workshop	**Presentation**

HONORS & AWARDS

11/2022	**International Collegiate Programming Contest (ICPC)** Participated in the Seoul Regional (main contest of Korea) as a college representative	**Contest**
3/2016 - 2/2023	**Government-Sponsored Tuition Scholarship** Received scholarship 8 times	**Scholarship**
3/2016 - 2/2017	**Government-Sponsored Presidential Science Scholarship** Received scholarship 2 times	**Scholarship**

REVIEWER OF

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

Languages	**Python (Proficient)**, C++, C, Java
Python Library	PyTorch, Lightning, Hydra, PyG, WandB, Numpy, Scikit-learn, Matplotlib
Software, OS, etc.	Version control (Git and GitHub), Linux, Vim, Slurm, Docker
DFT tools	VASP, Quantum Espresso, Castep
CSP tools	GULP, USPEX, CrySPY