Seongsu Kim

Ph.D. candidate
Graduate School of Artificial Intelligence

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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
Preprint, **2025**, PDF 🔗

Flexible MOF Generation with Torsion-Aware Flow Matching
Nayoung Kim, <u>Seongsu Kim</u>, and Sungsoo Ahn
Preprint, **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

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

Computational Many-body Physics (CMBP) Lab, Korea   **Research Intern**
9/2021 - 2/2023 *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

Statistical Artificial Intelligence (SAIL) Lab, Korea   **Research Intern**
6/2023 – 7/2023 *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.

Quantum Field & Gravity Theory Group, Korea   **Research Intern**
12/2019 – 2/2020 *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** | Talks |
| | KAIST-MILA Prefrontal AI Workshop | |

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

PROJECTS

9/2023 - 11/2023   **Multiple Canonicalizations for Model Agnostic Equivariance**
Wrote short paper on the multiple canonicalizations for reduced sensitivity to data deformation

HONORS & AWARDS

| 11/2022 | **International Collegiate Programming Contest (ICPC)** | Contest |
| | Participated in the Seoul Regional (main contest of Korea) as a college representative | |

| 3/2016 - 2/2023 | **Government-Sponsored Tuition Scholarship** | Scholarship |
| | Received scholarship 8 times | |

| 3/2016 - 2/2017 | **Government-Sponsored Presidential Science Scholarship** | Scholarship |
| | Received scholarship 2 times | |

REVIEWER OF

2026   Conference on Neural Information Processing Systems (**NeurIPS**)

2025   International Conference on Learning Representations (**ICLR**, Notable reviewer)

2024   International Conference on Machine Learning (**ICML**)

2023   Association for the Advancement of Artificial Intelligence (**AAAI**)

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