

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*
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, Artificial Intelligence*

7/2017 - 8/2017 **University of California, Berkeley**
Summer session study abroad program
Courses: *Quantum Physics, Data Structures and Algorithms*

PUBLICATIONS & CONFERENCES

[C] Conference **[W] Workshop** **[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](#) [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, W1] 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 AI DrugX 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

2/2025 - current **Structure and Probabilistic Machine Learning (SPML) Lab, Korea** Student researcher
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 NVIDIA BioNeMo Team	Invited Talk
5/6/2025	Accelerating the <i>ab-initio</i> Calculation with the Machine Learning KAIST-MILA Prefrontal AI Research Center	Invited Talk
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

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

WORK EXPERIENCE

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