

# Seongsu Kim

Last updated: Oct. 31, '25

Ph.D. candidate

Graduate School of Artificial Intelligence

 [seongsukim-ml.github.io](https://github.com/seongsukim-ml)

 [seongsu.kim@kaist.ac.kr](mailto: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*  
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 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

- 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	<b>QHFlow: Accelerating DFT with Equivariant Flow Matching</b> NVIDIA BioNeMo Team	Invited Talk
5/6/2025	<b>Accelerating the <i>ab-initio</i> Calculation with the Machine Learning</b> KAIST-MILA Prefrontal AI Research Center	Invited Talk
15/7/2024	<b>Gaussian Plane-wave Neural Operator for Electron Density Estimation</b> KAIST-POSTECH joint AI Workshop	Presentation

## HONORS & AWARDS

---

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

## REVIEWER

---

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

## WORK EXPERIENCE

---

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

## LANGUAGES

---

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

## SKILLS

---

Backgrounds	Computational physics, Quantum mechanics, Statistical physics
Languages	<b>Python (Proficient)</b> , 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