

# Seongsu Kim

M.S. Candidate

Department of Artificial Intelligence

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

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## EDUCATION

- 3/2023 - 8.2025 **M.S., Pohang University of Science and Technology (POSTECH), Korea**  
*Artificial Intelligence for Scientific Research*  
Topic 1. *Machine Learning for Solid States Physics and Quantum Chemistry*  
Topic 2. *Generative Model for Material and Molecular Science*  
Advisor: Prof. Sungsoo Ahn, and Prof. 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

## PUBLICATIONS & CONFERENCES

High-order Equivariant Flow Matching for Density Functional Theory Hamiltonian Prediction  
[Seongsu Kim](#), Nayoung Kim, Dongwoo Kim, and Sungsoo Ahn  
*Preprint, 2025*

Flexible MOF Generation with Torsion-Aware Flow Matching  
Nayoung Kim, [Seongsu Kim](#), and Sungsoo Ahn  
*Preprint, 2025*

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, [arXiv:2410.17270 \(2024\)](#). *  
*NeurIPS AIDrugX Workshop, 2024*

Gaussian Plane-Wave Neural Operator for Electron Density Estimation  
[Seongsu Kim](#) and Sungsoo Ahn  
*International Conference on Machine Learning (ICML), 2024, [arXiv:2402.04278 \(2024\)](#).  [project github](#) *

## EXPERIENCE

- 9/2021 - 2/2023 **Computational Many-body Physics Laboratory, Korea** Research Intern
  - 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 Laboratory, Korea** Research Intern
  - 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
  - Gwangju Institute of Science and Technology (Advisor: Prof. Keunyoung Kim)
  - Investigated the correspondence of deep learning and the Ads/CFT

## PROJECTS

- 9/2023 - 11/2023 **Multiple Canonicalizations for Model Agnostic Equivariance** POSTECH  
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	<b>Government-Sponsored Presidential Science Scholarship</b> Received scholarship 2 times	Scholarship
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## REVIEWER OF

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2025	International Conference on Learning Representations ( <b>ICLR</b> , Notable reviewer)
2024	International Conference on Machine Learning ( <b>ICML</b> )
2023	Association for the Advancement of Artificial Intelligence ( <b>AAAI</b> )

## WORK EXPERIENCE

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

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

## SKILLS

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Languages	<b>Python (Proficient)</b> , 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