


Seongsu Kim

Ph.D. Candidate
Department of Artificial Intelligence

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EDUCATION

- 3/2023 - present **Ph.D., Pohang University of Science and Technology (POSTECH), Korea**
Topic 1. *Geometrical Deep Learning for Solid States Physics and Quantum Chemistry*
Topic 2. *Generative Model for Material and Molecular Science*
Artificial Intelligence for Scientific Research
Advisor: Prof. Sungsoo Ahn
- 3/2016 - 2/2023 **B.Sc., Gwangju Institute of Science and Technology (GIST), Korea**
Majored in *physics*
Minored in *mathematics, computer science*
- 7/2017 - 8/2017 **University of California, Berkeley**
Summer session study abroad program

PUBLICATIONS & CONFERENCES

Nayoung Kim, Seongsu Kim, Minsu Kim, Jinkyu Park and Sungsoo Ahn., MOFFlow: Flow Matching for Structure Prediction of Metal-Organic Frameworks. *Neural Information Processing Systems (NeurIPS) AIDrugX Workshop, 2024*

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

EXPERIENCE

- 9/2021 - 2/2023 **Computational Many-body Physics Laboratory** 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** 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** 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 with reduced sensitivity to data deformation

TEACHING AND MENTORING

- 9/2023 - 12/2023 **Teaching Assistant for *Introduction to AI***
 - (Prof. Sungsoo Ahn, POSTECH)
 - Prepared supplementary materials and assignments with Python.
 - Formulated and graded problems for midterm and final exams
- 7/2019 - 8/2019 **Volunteer for IT and Cultural Education Abroad (Chisinau, Moldova)**
 - GIST-NIA, World Friend International IT and culture volunteer program
 - Served as a team leader and educational volunteer for IT and cultural exchange
 - Taught Python, Arduino, and drone classes in English to the Moldovan students.
 - Received the award for Excellence of the Voluntary mission
- 9/2019-12/2019 **Teaching Assitant for *Multivariable Calculus and Application***
 - (Prof. Chiwok Hwang, GIST)
 - Evaluated and graded weekly assignments
 - Graded midterm and final exams
 - Lectured supplementary sessions once a week

- 5/2017 - 9/2017 **Astronomical Observational Mentoring**
- *Creativity Cultivation Project of GIST*
 - Built a small observatory in a suburban area
 - Taught astronomical observations to elementary school students

EXTRACURRICULAR

- 3/2019 - 12/2019 **Entrepreneur Club**
- *(Received 2,000\$ sponsorship from GIST)*
 - Served as the club president and the back-end developer of application
 - Hosted weekly meetings and study groups
 - Developed a game based on the college life
 - Developed flee market application and school community application

HONORS & AWARDS

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|-----------------|--|--------------------|
| 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

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| 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**
Mandatory military service

LANGUAGES

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

SKILLS

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| 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 |