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**
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*
Adivisor: 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

MOFFlow: Flow Matching for Structure Prediction of Metal-Organic Frameworks
Nayoung Kim, <u>Seongsu Kim</u>, Minsu Kim, Jinkyu Park and Sungsoo Ahn
Neural Information Processing Systems (NeurIPS) AIDrugX Workshop, **2024**, arXiv:2410.17270 (2024).

Gaussian Plane-Wave Neural Operator for Electron Density Estimation
<u>Seongsu Kim</u> 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**   **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

9/2024 - present
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

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

2025   International Conference on Learning Representations (**ICLR**)

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

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