

# SONG EUN KIM, S.B.

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## RESEARCH INTERESTS

Developing machine learning models from first principles to explore physical systems, especially in materials science and physics.

## EDUCATION

**Massachusetts Institute of Technology (MIT) – Cambridge, MA**  
MEng, Computer Science and Engineering 09/2024 – 05/2025 (expected)

**Massachusetts Institute of Technology (MIT) – Cambridge, MA**  
SB, Computer Science and Engineering with Minor in Mathematics (4.9/5.0 GPA) 09/2021 – 05/2024

## RESEARCH EXPERIENCE AND EMPLOYMENT

**Undergraduate/Graduate Researcher**, Atomic Architects Group, MIT – Cambridge, MA 01/2022 – present

Supervised by Prof. Tess Smidt.

Currently in a collaboration with MIT-IBM Watson Lab to develop conditional generative models for pharmaceutical compounds.

Developed Symphony, a Euclidean symmetry ( $E(3)$ )-equivariant autoregressive ML model for 3D molecular structure generation, using the [e3nn-jax](#) Python library, and adapted it for transition metal complex prediction. Ongoing research to develop a similar equivariant autoregressive model for periodic structure generation.

Added spherical harmonic Fourier transforms to and from the sphere and a divide-and-conquer reduced tensor product algorithm to the e3nn-jax code base. Ported the latter algorithm into a parallelized version in Julia.

Helped develop an  $E(3)$ -equivariant ML model to characterize the magnetic properties of crystalline materials.

**Software Engineering Intern**, Google – Cambridge, MA 05/2024 – 08/2024

Prompt-engineered the Google Cloud Assistant (GCA) troubleshooting system's large language model to accurately respond to user troubleshooting queries given multiple pieces of information about the user's situation. Connected an API containing real-time Google Cloud service outages to the troubleshooting system for its LLM to use in its predictions.

**Software Engineering Intern**, Google | Gmail – Sunnyvale, CA 05/2023 – 08/2023

Increased Gmail security by implementing an antiabuse feature in JavaScript for client-side encrypted Gmail accounts, to block potentially harmful file types from being attached or downloaded.

**STEP Intern**, Google – Mountain View, CA 06/2022 – 09/2022

Improved Google search results by creating and tuning large language models for detecting badly formed queries, and developed syntactic filters in C++.

**Executive Data Team Intern**, Slalom – Seattle, WA 05/2021 – 01/2022

Prepared, trained, and tuned an XGBoost ML model in Python (sklearn) to predict company attritions. Analyzed internal financial, demographic, and customer/employee satisfaction data using Python, SQL, and Excel.

**Research Assistant**, Wake Forest University – *Winston-Salem, NC* 05/2020 – 08/2020

Studied with Prof. Jed Macosko. Created a Python simulation of vesicular stomatitis virus ribonucleoprotein motion within host cells, comparing different hypothesized modes of motion (e.g. pure Brownian, trap-to-trap).

**Research Assistant**, Purdue University – *West Lafayette, IN* 05/2018 – 03/2020

Studied structural biology and X-ray crystallography with Prof. Michael Rossmann and Dr. Andrei Fokine.

## PUBLICATIONS

**Symphony: Symmetry-Equivariant Point-Centered Spherical Harmonics for Molecule Generation**

A Daigavane, S Kim, M Geiger, and T Smidt; [12<sup>th</sup> International Conference on Learning Representations](#) (2024). Both a conference paper and a poster + video presentation.

**Machine Learning Magnetism Classifiers from Atomic Coordinates**

HA Merker, H Heiberger, L Nguyen, T Liu, Z Chen, N Andrejevic, NC Drucker, R Okabe, S Kim, Y Wang, T Smidt, and M Li; [iScience](#) (2022). (doi: 10.1016/j.isci.2022.105192)

## PRESENTATIONS

**MIT SuperUROP Fall Showcase** (poster presentation) – *Cambridge, MA* 12/2023

“Using E(3)-Equivariant Features for Autoregressive Transition Metal Complex Generation”

**Materials Research Society Fall Meeting** (invited oral presentation) – *Boston, MA* 12/2023

“Symphony: Symmetry-Equivariant Point-Centered Spherical Harmonics for Molecule Generation”

## LEADERSHIP AND MENTORING

**UROP (Undergraduate Research Opportunities Program) Mentor**, Atomic Architects Group, MIT – *Cambridge, MA* Starting 01/2025

Guiding an undergraduate student through the development of a web application for visualizing and interacting with generative models for molecules.

**Teaching Assistant**, 6.390 Introduction to Machine Learning, MIT – *Cambridge, MA* 09/2024 - present

Teaching a recitation section of ~75 (out of 400+ total) students, consisting of practice questions and reviews of content from lecture. Preparing content for each week’s classes, staffing office hours, grading midterm and final exams.

**Lab Assistant**, 6.390 Introduction to Machine Learning, MIT – *Cambridge, MA* 09/2023 – 12/2023

Supervised a class of ~400 students. Tested and calibrated content for the week’s in-class work, helped students during lab sections and office hours, checked their understanding of the material.

**ESPidier Co-Director**, MIT Educational Studies Program (ESP) – *Cambridge, MA* 09/2022 – 05/2023

The Educational Studies Program (ESP) is an MIT student group that runs several educational programs throughout the calendar year designed to instill a love of learning. Managed the development of a new Django website for ESP, including the framework needed to run middle-/high-school educational programs. Onboarded and supervised a new team of programmers, organized worksessions, created and maintained documentation for the website's code base.

**2022 Spring HSSP Co-Director**, MIT ESP – *Cambridge, MA* 12/2021 – 04/2022  
 Directed and organized Spring HSSP, a 5-week educational program for middle and high schoolers in the Boston area with 25 classes and 460 students.

## AWARDS AND HONORS

- **2025 Siebel Scholar**, Siebel Foundation (recognizing ~80 talented students at the world's leading graduate schools of business, computer science, bioengineering, and energy science) 2024
- Inducted into **Eta Kappa Nu** (IEEE-HKN), Beta Theta Chapter 2024
- **MIT SuperUROP Analog Devices Undergraduate Research and Innovation Scholar** 2023 – 2024
- **Jane Street INSIGHT Program Participant** (Software Engineering track) 2023
- **National Merit Scholar** 2021
- **Regeneron Science Talent Search Top 300** (the oldest and most prestigious science research competition for high school students in the US) 2021
- Two-time **National Center for Women & Information Technology (NCWIT) Aspirations in Computing National Honorable Mention** 2020, 2021
- **2020 Research Science Institute Research Scholar** (a prestigious summer program hosted by the Center for Excellence in Education where high school students conduct original scientific research under the guidance of experienced scientists) 2020
- Four-time **Le Grand Concours participant**; Platinum (2017), Gold (2018, 2019, 2020) national rating 2017 - 2020
- **USA Computing Olympiad, Gold Division** 2019 - 2020
- **U.S. National Chemistry Olympiad Honors** 2019
- **United States of America Junior Mathematical Olympiad (USAJMO) Qualifier** 2019
- Two-time **Math Prize for Girls at MIT Honorable Mention** 2018, 2019
- **Six-time American Invitational Mathematics Examination Qualifier** 2016 – 2021