JAEHYUNG LEE

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EDUCATION

Johns Hopkins University, Baltimore, MD
Ph.D. in Materials Science Engineering January 2025 – Present

Columbia University, New York, NY
M.S. in Chemical Engineering Graduation: December 2024

Pennsylvania State University, State College, PA
B.S. in Chemical Engineering Graduation: May 2023

WORK EXPERIENCE

EnerSys, Reading, PA Jan 2022 – Jun 2022
Advanced Quality Engineer Intern

- Worked as an engineering intern performing failure mode effective analyses of Li-ion and lead-acid battery cells.
- Resolved a total of 204 production part deviation cases and gave monthly updates to project manager and C-suite.
- Partnered with diverse teams to generate a production line Li-ion battery control plan for a next-generation product.

United States Forces Korea, Camp Humphreys, South Korea Jun 2018 – Feb 2020
KATUSA (E-5 Sergeant)

- Served 21 months of mandatory military service as a KATUSA (Korean Augmentation to the United States Army).
- Acted as a personal interpreter for a U.S. Army captain during joint Republic of Korea and U.S. Army operations.

RESEARCH EXPERIENCE

Johns Hopkins University, Baltimore, MD Jan 2025 – Present
Doctoral Student

- Developing materials discovery workflows integrating DFT data with machine learning for energy applications.
- Building and applying neural network models to predict properties such as energies, forces, and electronic behavior.
- Designed agentic AI platforms that combine LLMs with scientific APIs to enable automated design workflows.
- Optimized large-scale DFT and ML workloads on HPC systems, including VASP and GPU-accelerated inference.
- Curating and maintaining materials datasets for training, benchmarking, and validating machine learning models.

Columbia University, New York, NY Jan 2024 – Dec 2024
Graduate Research Assistant

- Pursued atomistic scale research in Urban Lab, using computational tools to model and analyze materials behavior.
- Trained ML interatomic potentials of lithium nickel oxide and titanium oxide to perform efficient calculations.
- Awarded the Société de Chimie Industrielle Scholarship to conduct research and present at the poster session.

Pennsylvania State University, State College, PA Aug 2020 – May 2023
Undergraduate Research Assistant

- Performed research of analyzing catalytic sites in metal oxides based on DFT results in Janik and Alexopoulos Labs.
- Mentored newly joined undergraduate students on how to utilize computational methods and machine learning tools.

TEACHING EXPERIENCE

Johns Hopkins University, Baltimore, MD Jan 2025 – Present

- Teaching Assistant, EN.510.312 Physical Chemistry of Materials I: Thermodynamics Spring 2026
- Teaching Assistant, EN.520.677 Applied Quantum Computing Fall 2026

EXTRACURRICULAR ACTIVITIES

Columbia University Department of Chemical Engineering, New York, NY Apr 2024 – Dec 2024
MS Ambassador

- Represented the department as an ambassador by communicating with admitted students and sharing program insight.
- Assisted the development of the MS handbook and participated as a panelist at the department master's colloquium.

American Institute of Chemical Engineers PSU Chapter, State College, PA Aug 2020 – May 2023
Vice President

- Hosted monthly mentorship sessions and academic discussions among chemical engineering undergraduate students.
- Accompanied professors to represent Penn State University in the 2021 and 2022 AIChE National Conferences.

Engineers Without Borders PSU Chapter, State College, PA Aug 2020 – May 2023
Development Committee Chair

- Led a subgroup in the club to design and facilitate the construction of a water supply facility in Namutamba, Uganda.
- Managed corporate networking and organized fundraising outreach events as chair of the development committee.

PUBLICATIONS

1. **J. Lee**, *et al*. **AGAPI-Agents: An Open-Access Agentic AI Platform for Accelerated Materials Design on AtomGPT.org**. *J. Phys. Chem. Lett*., under review. Preprint: arXiv:2512.11935.
2. **J. Lee**, *et al*. **Lessons Learned from the 2025 Agentic AI for Science Hackathon**. *Mach. Learn.: Sci. Technol.*, under review. Preprint: ChemRxiv:15001345.
3. F. Abel, **J. Lee**, *et al*. **RamanGPT: Bidirectional Mapping Between Crystal Structures and Raman Spectra with Graph Neural Networks and Generative Transformers**. *npj Comput. Mater*., under review. Preprint: arXiv:2606.03764.
4. B. Slautin, K. Barakati, U. Pratiush, C. Lowe, C. Bodinger, B. Cossairt, M. Ahmadi, A. Houton, T. Bazhirov, **J. Lee**, *et al*. **From Photons to Electrons: Accelerated Materials Discovery via Random Libraries and Automated Scanning Transmission Electron Microscopy**. *Microsc. Today*, under review. Preprint: arXiv:2603.20858.
5. G. Han, T. Li, X. Xu, **J. Lee**, *et al*. **The search for high-entropy fuel-cell catalysts using disorder descriptors**. *Nano Futures* **9**(4), 045001 (2025). https://doi.org/10.1088/2399-1984/ae19b0.

SELECTED PRESENTATIONS

1. "SlakoNet DB: A Cross-Domain Tight-Binding Database of Electronic Structure," Workshop on Recent Developments in Electronic Structure (ESW), Madison, WI, June 2026.
2. "BatteryMat: A Machine Learning Accelerated DFT Framework for Screening Battery Cathode Materials," Materials Research Society (MRS) Spring Meeting & Exhibit, Honolulu, HI, April 2026.
3. "AGAPI: An Agentic AI Platform for Quantum Materials Design," NIST Quantum Matters in Materials Science (QMMS) Workshop, Gaithersburg, MD, February 2026.
4. "Analysis of Cathode Materials for Lithium-Ion Batteries Using Machine Learning Potentials," Société de Chimie Industrielle Biennial International Palladium Medal Ceremony, New York, NY, May 2024.