Shinyoung Park

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Education

Korea Advanced Institute of Science and Technology (KAIST) — Daejeon, Korea
B.S. in Chemistry — *Feb 2026 (Expected)*
- **Cumulative GPA: 4.27/4.30**

Research Experience

Intelligent Chemistry Lab – KAIST Department of Chemistry — Daejeon, Korea
Undergraduate Researcher with Prof. Woo Youn Kim — *Dec 2022 – Present*

- **Developed the AutoCG package for generating input reactant/product conformations for interpolation transition state (TS) search methods.**
  - Devised strategies to obtain low-energy TS structures and validated AutoCG on 32 benchmark reactions.
  - Published article in *J. Chem. Theory Comput.* as co-first author.
- **Developed MetalloGen, an automated tool for generating 3D conformers of organometallic complexes with challenging polydentate and polyhapto ligands.**
  - Proposed ligand embedding/refinement strategies and benchmarked MetalloGen on 80 complexes.
  - Published article in *J. Chem. Inf. Model.* as second author.
- **Extended capabilities of ACE-Reaction, a graph-theoretic reaction network exploration method.**
  - Devised and implemented an atom mapping scheme for unbalanced reactions using mixed-integer linear programming with SciPy.
  - Developed a message passing neural network with PyTorch Geometric to sample low-barrier reactions.

Publications

(1) Lee, K.; **Park, S.**; Park, M.; Kim, W. Y. **MetalloGen: Automated 3D Conformer Generation for Diverse Coordination Complexes.** *J. Chem. Inf. Model.* **2025**, *65* (21), 11878–11891. DOI: 10.1021/acs.jcim.5c02074 [Article PDF] [GitHub]

(2) Lee, K.[†]; Lee, J.[†]; **Park, S.**[†]; Kim, W. Y. **Facilitating Transition State Search with Minimal Conformational Sampling Using Reaction Graph.** *J. Chem. Theory Comput.* **2025**, *21* (5), 2487–2500. DOI: 10.1021/acs.jctc.4c01692 ([†]Equal contribution) [Article PDF] [GitHub]

Awards and Honors

National Scholarship for Science and Engineering | **Ministry of Science and ICT, Korea** — *2023 – 2024*
- National award for top academic performance in STEM fields; full tuition for two years.

Dean's List | **KAIST** — *Spring 2020, Spring/Fall 2022, Spring/Fall 2023, Fall 2024*
- Awarded to top six students per department each semester.

Academic Service

KAIST Department of Chemistry Student Council Daejeon, Korea
Head of the Internationalization Team *Aug 2023 – Feb 2024*
Member of the Design Team and the Academic Affairs Team *Mar 2022 – Aug 2023*

- Founded the Internationalization Team to support international students and compiled A Guide to the Department of Chemistry, a comprehensive English-language resource featuring essential information, curated links, and practical guidance.
- Supported international students by translating Korean announcements and documents into English and providing Korean-English interpretation at departmental events.
- Designed promotional materials, including pamphlets highlighting Department of Chemistry labs and their research for prospective undergraduate and graduate students.
- Coordinated the 2022 KAIST Chemie Camp, where high school students nationwide were invited to explore and experience cutting-edge chemistry research and education at KAIST.

Technical Skills

Programming and Other Languages: Python, MATLAB, JavaScript, LaTeX, Markdown
Libraries: NumPy, SciPy, Matplotlib, Pandas, RDKit, PyTorch, PyTorch Geometric, scikit-learn
Developer Tools: Git, Bash, SSH, SLURM, Vim/Neovim, VS Code, JupyterLab, GitHub, GitHub Pages
Chemistry Tools: Gaussian, ORCA, MOPAC, xTB, CREST, ChemDraw, Avogadro, PyMOL, Mnova
Graphic Design Tools: Adobe Photoshop, Adobe Illustrator
Test Scores: GRE: Verbal (170, 99%), Quantitative (170, 92%), Analytical Writing (4.5, 83%)
TOEFL: 116 (Reading: 30, Listening: 30, Speaking: 28, Writing: 28)