Shinyoung Park

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Education

Korea Advanced Institute of Science and Technology (KAIST) — Daejeon, Korea
B.S. in Chemistry — *Expected Feb 2026*

- 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 a wide range of interpolation transition state (TS) search methods.
  - Devised a novel stereochemical manipulation technique to obtain low-energy TS structures.
  - Validated AutoCG with Gaussian and ORCA across three benchmark sets, comprising 32 reactions.
  - Drafted and revised the manuscript published in *J. Chem. Theory Comput.* titled Facilitating Transition State Search with Minimal Conformational Sampling Using Reaction Graph.
- Developed MetalloGen, an automated tool for generating 3D conformers of organometallic complexes with challenging polydentate and polyhapto ligands.
  - Proposed solutions for polyhapto ligand embedding and conformer refinement.
  - Benchmarked MetalloGen with CREST and Gaussian on 80 organometallic complexes from diverse transition metal reactions and real-world catalytic mechanisms.
  - Drafted the majority of the manuscript, currently submitted.
- Extended capabilities of ACE-Reaction, a graph-theoretic reaction network exploration method, as part of the Undergraduate Research Program.
  - Proposed and implemented an atom mapping scheme for unbalanced reactions using mixed-integer linear programming with SciPy.
  - Developed an autoregressive message passing neural network with PyTorch Geometric for sampling reactions within a defined activation barrier.
  - Optimized HPC resource allocation of ACE-Reaction; reduced TS search computing cost by 20–30%.

Awards and Honors

KFAS Overseas PhD Scholarship (Trainee) | Korea Foundation for Advanced Studies — *2026 – 2030*

- Highly selective scholarship supporting doctoral study at top global universities.

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 2022, Fall 2022, Spring 2023, Fall 2023, Fall 2024*

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
English Proficiency: GRE: Verbal (170, 99%), Quantitative (170, 92%), Analytical Writing (4.5, 83%)
TOEFL: 116 (Reading: 30, Listening: 30, Speaking: 28, Writing: 30)

Publications

(1) 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)

(2) Lee, K.; *Park, S.*; Park, M.; Kim, W. Y. MetalloGen: Automated 3D Conformer Generation for Diverse Coordination Complexes. Submitted.