

Shinyoung Park

✉ shinyoung.park.mail@gmail.com

🌐 syark-chem.me

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%.

PUBLICATIONS

- (1) Lee, K.; **Park, S.**; Park, M.; Kim, W. Y. MetalloGen: Automated 3D Conformer Generation for Diverse Coordination Complexes. In revision.
- (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](https://doi.org/10.1021/acs.jctc.4c01692) ([†]Equal contribution)

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 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

Test Scores: GRE: Verbal (170, 99%), Quantitative (170, 92%), Analytical Writing (4.5, 83%)

TOEFL: 116 (Reading: 30, Listening: 30, Speaking: 28, Writing: 28)