

Shinyoung Park

+82 10-7105-8024
shinyoung.park.mail@gmail.com
sypark-chem.me

EDUCATION

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

RESEARCH EXPERIENCE

Intelligent Chemistry Lab – KAIST Department of Chemistry Undergraduate Researcher with Prof. Woo Youn Kim	Daejeon, Korea Dec 2022 – Present
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- 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.
 - Co-authored publication in *J. Chem. Theory Comput.*
- 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.
 - Co-authored manuscript currently in revision for *J. Chem. Inf. Model.*
- Extended capabilities of **ACE-REACTION**, a graph-theoretic reaction network exploration method.
 - Designed 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 allocation to reduce TS search computing costs by 20–30%.

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**, DOI: [10.1021/acs.jcim.5c02074](https://doi.org/10.1021/acs.jcim.5c02074) [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](https://doi.org/10.1021/acs.jctc.4c01692) ([†]Equal contribution) [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 2022, Fall 2022, Spring 2023, Fall 2023, Fall 2024

ACADEMIC SERVICE

KAIST Department of Chemistry Student Council
Head of the Internationalization Team
Member of the Design Team and the Academic Affairs Team

Daejeon, Korea
Aug 2023 – Feb 2024
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, L^AT_EX, 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)