

# Shinyoung Park

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🌐 spark-chem.me

## EDUCATION

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

## RESEARCH EXPERIENCE

<b>Intelligent Chemistry Lab – KAIST Department of Chemistry</b> 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 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.<sup>†</sup>; Lee, J.<sup>†</sup>; **Park, S.<sup>†</sup>**; 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) (<sup>†</sup>Equal contribution)

## AWARDS AND HONORS

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<b>National Scholarship for Science and Engineering</b>   Ministry of Science and ICT, Korea	2023 – 2024
• National award for top academic performance in STEM fields; full tuition for two years.	

<b>Dean's List</b>   KAIST	<i>Spring 2020, Spring 2022, Fall 2022, Spring 2023, Fall 2023, Fall 2024</i>
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## ACADEMIC SERVICE

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

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**Programming and Other Languages:** Python, MATLAB, JavaScript,  $\text{\LaTeX}$ , 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)