

Chan Young Joe

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PROFILE

Researcher specializing in computational chemistry, molecular dynamics, and AI-driven chemical modeling, with growing expertise in environmental risk assessment and bioaccumulation modeling. Strong foundations in quantum chemistry, statistical data analysis, and large language model applications in chemistry. Currently applies computational and data-science methods to environmental health research in industry while continuing academic collaborations.

CURRENT POSITION

Researcher, Data Science Team Jan. 2026 – Present
Research Institute of Environmental Health and Safety, EH R&C Co. Incheon, Korea

- Develops a flux-based dynamic energy budget–toxicokinetic (DEB-TK) model of fish bioaccumulation
- Tests regulatory bioaccumulation screening against EU Biocidal Products Regulation assessments
- Builds mechanistic uptake models for PFAS in fish gut and paddy rice
- KEITI project on safety management of household chemical products (collaborative research since Apr. 2025)

EDUCATION

University of Seoul Seoul, Korea
M.S. in Applied Chemistry (Computational Chemistry), advisor Prof. Rakwoo Chang Sep. 2024 – Feb. 2026

- Thesis: *Application of Artificial Intelligence for Solving Chemical Problems*
- GPA 4.46/4.5

University of Seoul Seoul, Korea
B.S. in Applied Chemistry; B.E. in Artificial Intelligence (double major) Mar. 2021 – Aug. 2024

- Cum laude; 1st in the Department of Applied Chemistry; 2nd-highest cumulative GPA in the College of Natural Sciences among August 2024 graduates
- Early graduation; GPA 4.37/4.5 (cumulative 4.28)

National Institute for Lifelong Education (NILE), Korea University Seoul, Korea
B.S. in Mathematics Jan. 2025 – Dec. 2026 (expected)

Yangseo High School
High school diploma Mar. 2018 – Feb. 2021

ADDITIONAL TRAINING

Korea Environmental Conservation Institute (KECI)
Chemical Substance Safety Management Cooperation Course Sep. 2024 – Feb. 2026

- Track: Hazardous Substance Testing; funded by the Ministry of Climate, Energy and Environment, Republic of Korea; Certificate of Completion (Feb. 2026)

RESEARCH EXPERIENCE

Researcher, Computational Molecular Modeling Laboratory Jun. 2021 – Feb. 2026
University of Seoul (Prof. Rakwoo Chang) Seoul, Korea

- Large language models (in-context learning, fine-tuning) for molecular property prediction
- Molecular dynamics of membranes and enzymes; hybrid multigrained sampling

Visiting Researcher, Department of Bioengineering Jun. 2024 – Aug. 2024
Lehigh University (Prof. Wonpil Im) Bethlehem, PA, USA

- Short-term research stay supported by Prof. Rakwoo Chang (University of Seoul)

Research Intern Jul. 2023 – Feb. 2024
Molcube Corporation (CEO Wonpil Im)

- Molecular dynamics simulation system development, bug reporting, and troubleshooting

RESEARCH PROJECTS

Bioaccumulation and human-exposure prediction of hazardous substances considering the natural environment and food chain (with EH R&C)	<i>Apr. 2025 – Present</i>
LoRA-based LLM flash-point prediction model for chemical safety (with Prof. Jaeyoung Sung, Chung-Ang University)	<i>Nov. 2024 – Present</i>
Hybrid sampling molecular dynamics method for systems with complex energy landscapes	<i>Jun. 2024 – Present</i>
Quantum algorithms for chemical simulation (with Prof. Doyeol Ahn, University of Seoul)	<i>Apr. 2024 – Aug. 2024</i>
CO and O ₂ desolvation pathway analysis of the Ch-CODH enzyme by molecular dynamics (with Prof. Yonghwan Kim, UNIST)	<i>Mar. 2023 – Mar. 2024</i>
AI-chemistry convergence research: LLM fine-tuning and in-context learning for chemical property prediction; MD-based phospholipid bilayer property prediction (with Prof. Kyungwoo Song, Yonsei University)	<i>Mar. 2022 – Present</i>
Molecular dynamics simulation of chlorosulfolipid-based cell membranes	<i>Jun. 2021 – Dec. 2021</i>

PUBLICATIONS

Peer-reviewed

Lee, J.-H.*; **Joe, C. Y.** A flux-based bioaccumulation model for growing organisms: integrating advective-diffusive uptake at exchange organs into dynamic energy budget theory. *Environ. Toxicol. Chem.* **2026**, vgag253, DOI: 10.1093/etjnl/vgag253.

Joe, C. Y.; Song, K.*; Chang, R.* Evaluating in-context learning in large language models for molecular property regression. *J. Comput. Chem.* **2026**, 47, e70308, DOI: 10.1002/jcc.70308.

In Preparation

Joe, C. Y.* Which steps do self-driving laboratories automate? A cross-field database of published closed-loop platforms.

Joe, C. Y.* Silent but deadly? Physics says seldom, memory says mostly.

CONFERENCE PRESENTATIONS

Sim, H.; **Joe, C. Y.***; Chang, R.* Modeling membrane permeability, biotransformation rate and assimilation efficiency constants of complex organic chemicals using machine learning. Presented at the 137th General Meeting of the Korean Chemical Society, Apr. 2026; poster PHYS.P-479.

Joe, C. Y.; Lee, J.-H.* Integrated DEB-TK model for fish bioaccumulation assessment of neutral organic chemicals: theoretical formulation and empirical validation. Presented at the 2026 Spring General Meeting of the Korean Society of Environmental Health, Jeju, Korea, May 2026; poster P-EaRA-40. Best Poster Award.

Joe, C. Y.; Song, K.*; Chang, R.* Evaluating in-context learning in large language models for molecular property regression. Presented at Pacificchem 2025, Honolulu, HI, Dec. 15–20, 2025; poster PHY006.

Joe, C. Y.; Sim, H.; Chang, R.* Modeling membrane permeability and biotransformation rate constants of complex organic chemicals using machine learning and retrieval-augmented LLMs. Presented at the 136th General Meeting of the Korean Chemical Society, Changwon, Korea, Oct. 2025; poster PHYS.P-149.

Joe, C. Y.; Chang, R.* Exploring in-context learning in large language models for molecular property prediction and chemical screening. Presented at the 2025 Fall Meeting of the Korean Society of Environmental Toxicology & Chemistry, 2025; poster.

Joe, C. Y.; Chang, R.* Advancing chemical property prediction using in-context learning and representation enhancements in large language models. Presented at the 135th General Meeting of the Korean Chemical Society, Suwon, Korea, Apr. 2025; poster PHYS.P-9.

Joe, C. Y.; Hong, J.; Chang, R.* Hybrid molecular dynamics simulations using a multigraining approach. Presented at the 134th General Meeting of the Korean Chemical Society, 2024; poster PHYS.P-81.

Joe, C. Y.; Chang, R.* Predicting chemical compound solubility and toxicity using GPT models: a comparative analysis. Presented at the 2024 Fall Meeting of the Korean Society of Environmental Toxicology & Chemistry, Oct. 2024; poster. Best Poster Award.

Joe, C. Y.; Chang, R.* Predicting chemical compound solubility with GPT models: a comparative analysis. Presented at the 133rd General Meeting of the Korean Chemical Society, 2024; poster.

Joe, C. Y.; Hong, J.; Nam, Y.; Jung, M.; Chang, R.* Exploring physical and biological phenomena through computational molecular modeling. Presented at the KICHe C1 Gas Refinery Symposium, 2023; poster.

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INTELLECTUAL PROPERTY

Database of biotransformation rate constants, membrane permeability, and assimilation efficiency for machine-learning model development 2025

Database producer’s right, Korea Copyright Commission, Reg. No. D-2025-000238 (registered Dec. 29, 2025); right holder: University of Seoul Industry–Academic Cooperation Foundation; built with Hyeonsu Sim in the bioaccumulation and human-exposure prediction project (with EH R&C)

HONORS AND AWARDS

Best Poster Award, 2026 Spring General Meeting of the Korean Society of Environmental Health	2026
Outstanding Paper Award, President of the University of Seoul (<i>J. Comput. Chem.</i> paper)	2026
Best Poster Award, System Chemistry Global Leading Research Center Winter Symposium	2025
Best Poster Award, Fall Meeting of the Korean Society of Environmental Toxicology & Chemistry	2024
President’s Award, graduation with honors (cum laude), University of Seoul	2024
Academic Excellence Award, every semester, University of Seoul	2021 – 2024
Encouragement Award (3rd), UOS Chemical Safety Management Graduate Program	2023
Excellence Presentation Award, University President Prize (1st), UOS Chemical Safety Management Graduate Program	2022

SCHOLARSHIPS

AI SeoulTech Graduate Scholarship	Fall 2025
Seoul Mayor Scholarship	Spring 2022, Spring 2024
Dean’s Scholarship	Fall 2023
Samsung Donor Scholarship	Spring 2023, Fall 2023
Student Leader Scholarship	Spring 2022, Fall 2022
Industry-University Cooperation Foundation Scholarship	Fall 2021, Spring 2022, Fall 2022, Spring 2025, Fall 2025
Academic Excellence Scholarship	Fall 2021, Fall 2022, Spring 2023
Hyungseol Scholarship, every semester	Fall 2021 – Spring 2024
University Innovation Support Program Scholarship	Spring 2021, Fall 2021, Fall 2022, Fall 2023, Spring 2024
Research Scholarship	Spring 2022, Fall 2022
Seoul Hope Scholarship, Seoul Scholarship Foundation	Spring 2022

OPEN-SOURCE SOFTWARE

PFAS–rice uptake model | *Python, HYDRUS-1D, Streamlit* github.com/ccy5123/pfas-rice-model

- Mechanistic four-compartment (root–stem–leaf–grain) uptake model for anionic PFAS in paddy rice, covering 12 calibrated PFCA/PFSA congeners
- Coupled to HYDRUS-1D soil transport; parameterisable from chemical structure; interactive web application

sci-adk | *Python, Claude Code* github.com/ccy5123/sci-adk

- Verification kit for agent-assisted research: AI agents propose, and a deterministic engine judges each claim against decision rules frozen before the experiment
- Append-only evidence record with headless re-verification by third parties and tamper-evident provenance

MAFIS | *Python, Ollama* github.com/ccy5123/MAFIS

- Local-first multi-agent AI research assistant for long-term value investing: a six-agent crew (Economist, Analyst, Valuer, Skeptic, Defender, Steward) writes fully cited equity research reports from local LLMs and Python-computed financial facts
- Supports US and Korean equities; 475 unit tests

KorJpnIme | C++, Python, Windows TSF

- Windows TSF input method for typing Japanese on a Korean 2-beolsik keyboard, with full compound-vowel and final-consonant handling
- Mozc OSS dictionary (about 1.29M entries) with Viterbi-based top-K kanji segmentation

TEACHING EXPERIENCE

University of Seoul, Department of Applied Chemistry

Teaching Assistant, <i>Chemistry and Computer</i>	Fall 2025
Teaching Assistant, <i>Chemistry and Experiment I</i> (2 sections) and <i>Physical Chemistry I</i>	Spring 2025
Teaching Assistant, <i>Chemistry and Experiment II</i> and <i>Chemistry and Computer</i>	Fall 2024
Teaching Assistant, <i>Physical Chemistry I</i>	Spring 2023
Tutor, <i>General Chemistry</i>	Fall 2024, Spring 2025

LEADERSHIP AND ACTIVITIES

Co-Founder and Vice President, Korean Traditional Archery Club, University of Seoul	Mar. 2022 – Aug. 2024
Founding President, Student Government, Department of Applied Chemistry, University of Seoul	Jan. 2022 – Dec. 2022

TECHNICAL SKILLS

Computational chemistry and MD: CHARMM, NAMD, GROMACS, OpenMM

Programming: Python, Fortran, C++, UNIX/HPC (SLURM)

Machine learning: PyTorch, TensorFlow, scikit-learn, Hugging Face; LLM fine-tuning (LoRA) and in-context learning; local LLM deployment (Ollama); retrieval-augmented generation (RAG)

AI-augmented engineering: agentic systems and harnesses around LLMs (context engineering, tool orchestration, evaluation and audit loops, reproducibility scaffolding); routine development with AI coding agents (Claude Code) under structured review and test-driven workflows

Statistical data analysis: exploratory data analysis, regression modeling, performance evaluation

Languages: Korean (native), English (working proficiency), Japanese (working knowledge)

CERTIFICATES AND LICENSES

Amateur Radio Operator License, 1st Class

Unmanned Power Flight Vehicle Operator Certificate, 4th Class

Hunting License, 1st Class (shotgun and airgun)

Driver's Licenses: 1st Class Large; 1st Class Ordinary (manual); 2nd Class Small (motorcycle over 125 cc); 1st Class Special (large trailer, wrecker)