

MINGI KANG

kangmg@korea.ac.kr | github.com/kangmg

Last updated: August 13, 2025

RESEARCH INTEREST

My research interests focus on understanding chemical phenomena at the microscopic level through computational chemistry methodologies and accelerating these investigations using AI. Based on this fundamental understanding, I aim to explore and design novel materials and catalysts.

SKILLS

Computational Chemistry

- Ab initio calculation: Psi4, PySCF, GAMESS-US, Gaussian, ORCA, CP2K etc.
- Molecular Dynamics: OpenMM, ASE
- Modeling & Simulation: scikit-learn, pytorch, Training ML potentials

Scientific Skills

- Job scripting & submission in HPC server (PBS, SGE) via SSH
- Dataset construction & handling (HDF5, SQL)
- Data visualization

Development Skills

- Workflow automation
- Python packaging & deployment
- Git, Cloud service, API

RESEARCH EXPERIENCE

Bachelor's Thesis

Lab of Ultrafast Spectroscopy, Korea University (Sejong)

March 2025 - Present

Prof. Jae Yoon Shin

- Investigated kinetic behavior of ionic liquids in porous filters (Polyethersulfone and Anodisc)
- Performed molecular dynamics calculations using force fields and fine-tuned ML potentials
- Built simulation systems and analyzed dynamic trajectories to determine diffusion coefficients

CURT Research Program

Laboratory of Inorganic Chemistry, Korea University (Sejong)

July 2025 - Present

Prof. Ho-Jin Son

- Studied reaction mechanisms of homogeneous transition metal catalysts using DFT and MLP methods
- Computed Gibbs energy profiles through various levels of DFT
- Developed automated job submission scripts and established workflows for Gibbs energy profile calculation

Winter Internship

The Meta Lab, KENTECH

January 2025 - February 2025

Prof. Geun Ho Gu

- Fine-tuned universal MLP models for heterogeneous catalyst systems
- Reproduced surface adsorption energies using MLP and compared results with DFT

Project Semester

Lab of Ultrafast Spectroscopy, Korea University (Sejong)

July 2024 - December 2024

Prof. Jae Yoon Shin

- Collected and preprocessed organic molecule dataset (10K samples) using the PubChem API
- Performed large-scale ab initio calculations (50K) and built normal mode perturbed molecular dataset
- Fine-tuned ANI Machine Learning Potentials (MLP) to improve accuracy in transition state regions
- Conducted MLP-based molecular dynamics simulations of carbon polymerizations and acetylene annulation reactions
- Developed Python package for MLP-based distortion interaction analysis calculations

X-Corps Research Program

Biomedical Nano-engineering Lab, Korea University (Sejong)

November 2019 - April 2020

Prof. Gyudo Lee

- Developed paper-based colorimetric biosensor for ethanol concentration measurement and color quantification
- Synthesized polyaniline (PANI) nanoparticles and immobilized ADH on PANI-coated paper
- Proposed RGB color picker method for pH prediction and studied lighting brightness effect corrections

EDUCATION

Korea University (Sejong) | GPA: 4.12 / 4.5
B.S. in Advanced Material Chemistry

March 2019 - Present

PROJECTS

ASE Community Code Development

- Implemented ASE calculator interfaces for g-xTB, PySCF, MLatom, and XequiNet
- Developed optimizer wrappers for asemd and geomeTRIC to enhance integration of ASE-centered workflows

Distortion Interaction Analysis

- Implemented ASE interfaces for distortion interaction analysis calculations
- Enabled flexible computations and streamlined computational workflows

randatoms

- Developed a molecular filtering package using pickle-based metadata caching
- Used indexed HDF5 storage to enable fast random access and optimize I/O performance for large-scale molecular datasets

Molecular Visualizer

- Developing molecular visualization tools including ASE-native viewer aseview and OverlayMol
- Supports visualization of molecular normal modes, overlay diagrams, and animations with publication-ready quality

Image to Music Recommendation Service

June 2024

- Proposed the project topic and managed its scheduling, planning, and overall design
- Collected various types of data using APIs and web crawling, and performed data preprocessing
- Designed the service architecture, developed, and deployed the website using Streamlit

Deepfake Voice Detection

Sep 2024 - May 2025

- Proposed a strategy for generating deepfake voice data
- Preprocessed audio data by adjusting sampling rates and converting file formats to wav
- Transformed audio data into Mel spectrogram for modeling

SCHOLARSHIPS

Chi-Woo Lee Scholarship

- Korea University, 2025, KRW 5,000,000

Academic Excellence Scholarship

- Korea University, 2025, KRW 2,350,000

AWARDS & HONORS

Excellent Research Report Award

- S-CURT Research Program, Korea University, 2025

RESEARCH GRANTS

Project Semester Research Grant

- Korea University, 2024, KRW 1,500,000

ADDITIONAL ACTIVITY

Data Science Bootcamp

February 2023 - July 2023

- Completed a 6-month intensive course on data science and machine learning

MILITARY SERVICE

Country's Army (Sergeant)

July 2022 - January 2024

- Completed mandatory military service.