Mingi KANG

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

Scientific Skills

- HPC server & scheduling e.g. PBS, SGE
- Dataset handling (HDF5, SQL)
- Data visualization

Development Skills

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

Research Experience

Bachelor's Thesis *March 2025 - Present*
Lab of Ultrafast Spectroscopy, Korea University (Sejong) *Prof. Jae Yoon Shin*

- Investigated dynamic 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 *July 2025 - Present*
Laboratory of Inorganic Chemistry, Korea University (Sejong) *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 *January 2025 - February 2025*
The Meta Lab, KENTECH *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 *July 2024 - December 2024*
Lab of Ultrafast Spectroscopy, Korea University (Sejong) *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

Education

Korea University (Sejong) | *GPA: 4.12 / 4.5* *March 2019 - Present*
B.S. in Advanced Material Chemistry

Projects

Distortion Interaction Analysis

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

Molecule Aligner

- Developed a Python package for merging, interpolating, and aligning molecular trajectories
- Enabled construction of smooth, multi-step reaction pathways from mixed molecular inputs

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

ASE Community Code Development

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

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 2024 - July 2024*

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

Military Service

Country's Army (Sergeant) *April 2021 - October 2022*

- Completed mandatory military service.