

강민기 Mingi Kang

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RESEARCH INTEREST

My research has focused on predicting molecular properties and reactivity using *ab initio* calculations. Currently, I am particularly interested in two areas: accelerating chemical discovery through Machine Learning Potentials and understanding large-scale systems via MLP-based MD simulations at *ab initio* accuracy.

SKILLS

1. Programming Languages
 - **Python** (Advanced), Julia (Intermediate), Basic Bash
2. Scientific Skills
 - Computational Chemistry: **ASE**, **PySCF**, **Psi4**, GAMESS-US, etc.
 - Machine Learning: **PyTorch**, scikit-learn
 - Visualization Tools: **VMD**, **matplotlib**, seaborn, etc.
3. Code Development
 - Collaboration & Issue Tracking: **Git**
 - Python **packaging** & deployment
 - Basic Docker & Familiarity with **Linux** (ubuntu)
 - Cloud Service: Google Cloud Platform (**GCP**), AWS
4. Large Data Processing
 - File Formats: **HDF5**, SQL (MariaDB)
 - Data Collection: Web Crawling, APIs

RESEARCH EXPERIENCE

Project Semester (Grant \$1000)

July 2024 – December 2024

Lab of Ultrafast Spectroscopy • Advisor: Jae Yoon Shin

- Collected and preprocessed of organic molecule dataset (10K) using the PubChem API
- Performed large-scale (50K) QM calculations and built a normal mode perturbed molecular dataset
- Fine-tuned of Universal Machine Learning Potentials (MLP) to improve accuracy in the transition state TS region
- Studied of MLP-based MD simulations and simulated Carbon polymerizations and acetylene annulation reactions
- Developed an ASE-compatible distortion interaction analysis calculation python package for applying MLP models

X-Corps Program

November 2019 – April 2020

Biomedical Nano-engineering Lab • Advisor: Gyudo Lee

- Studied a paper-based colorimetric biosensor for measuring ethanol concentration and their color quantifications
- Synthesized polyaniline (PANI) NPs and immobilized ADH on PANI-coated paper
- Proposed a method for pH prediction using an RGB color picker and studied the correction of lighting brightness effect

KUS Living Lab Program

December 2019 – February 2020

Immune Control Lab • Advisor: Hyun Sik Jun

- Established a database of medicinal properties of indigenous plant in Sejong
- Investigated natural drug candidates for anti-cancer and anti-inflammatory effects

PROJECTS

Personal Projects (*Computational Chemistry*)

- ASE Calculators: Developed various ASE Calculators for interfacing with PySCF, XequilNet, and MLatom
- OverlayMol: Interactive Molecular Overlay plot and reaction trajectory viewer using Plotly
- aimDIAS: MLP (AIMNet2) based Activation Strain Analysis package
- CompChem Archive: A collection of minor projects and studies in computational chemistry

Image to Music Recommendation Service (*Deep Learning*) | [Github](#) |
2024 Like Lion Data Analysis School DATATON

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
- Studied a CNN-based sentiment classification model
- Designed the service architecture, developed, and deployed the website using Streamlit

Deepfake Voice Detection (*Deep Learning*) | [Github](#) |
2024 Like Lion Data Analysis School • Mentor: Dongbin Na

Sep 2024- May 2015

- Investigated technical trends in synthetic TTS and studied relevant literature on deepfake detection
- Proposed a strategy for generating deepfake voice data
- Preprocessed audio data by adjusting sampling rates and converting file formats to wav
- Transformed auto data into Mel spectrogram for modeling

PRESENTATIONS

1. Theoretical approach to molecular structural theory | [Presentation](#) |
Informal Seminar Organized by COCO, undergraduate academic club

May 2023

2. Measurement of Partial Molar Volume | [Presentation](#) |
Physical Chemistry Lab Course Seminar

March 2023

3. Introduction to UV-Vis Spectroscopy | [Presentation](#) |
Analytical Chemistry Lab Course Seminar

November 2020

3. Brief Introduction of Aldol Condensation Reaction | [Presentation](#) |
Organic Chemistry Lab Course Seminar

June 2020

EDUCATION

Korea University, Sejong Campus

March 2019 – Present

B.S. Advanced Materials Chemistry | GPA (Cumulative, Major): (3.99, 4.11) / 4.5

MILITARY SERVICE

The Republic of Korea's Army (Sergeant)

April 2021 – October 2022

18-Month Mandatory Military Service

ADDITIONAL ACTIVITIES

TECHIT Data Analysis School

February 2024 – July 2024

Certificated in 6-Month Data Science & Artificial Intelligence Boot Camp