강민기 Mingi Kang

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

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 | June 2024
2024 Like Lion Data Analysis School DATATON

- 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 | Sep 2024- May 2015
2024 Like Lion Data Analysis School • Mentor: Dongbin Na

- 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 | May 2023
Informal Seminar Organized by COCO, undergraduate academic club

2. Measurement of Partial Molar Volume | Presentation | March 2023
Physical Chemistry Lab Course Seminar

3. Introduction to UV-Vis Spectroscopy | Presentation | November 2020
Analytical Chemistry Lab Course Seminar

3. Brief Introduction of Aldol Condensation Reaction | Presentation | June 2020
Organic Chemistry Lab Course Seminar

EDUCATION

Korea University, Sejong Campus March 2019 – Present
B.S. Advanced Materials Chemistry | GPA (Cumulative, Major): (3.99, 4.11) / 4.5

TECHIT Data Analysis School February 2024 – July 2024
Certificated in 6-Month Data Science & Artificial Intelligence Boot Camp

MILITARY SERVICE

The Republic of Korea's Army (Sergeant) April 2021 – October 2022
18-Month Mandatory Military Service