

RUIHAO BI

Department of Chemistry, Xiamen University, Fujian, P.R.China, 361005

Telephone: +86 18605025530 | Email: biruihao@stu.xmu.edu.cn | Github: Detailed CV

EDUCATION

College of Chemistry, Xiamen University (XMU)

Xiamen, China

Research Assistant

Jul. 2021 – now

Bachelor of Chemistry

Sept. 2017 — Jun. 2021

- 1st Year: College of Materials, 2nd–4th Year: College of Chemistry.
- Overall GPA: 3.79/4.00, Major GPA: 3.85/4.00, Rank: 3/96.
- English skill: TOEFL iBT: 103 (R30, L29, S21, W23), tested in Nov. 2021.

Selected Coursework:

- Calculus I (100/100, top 1%), Calculus II (95/100, top 2%), Physics I (93/100, top 1%), Physical Chemistry II (95/100, top 3%), Chemical Kinetics & Reaction Dynamics (95/100, top 1%)

ACADEMIC EXPERIENCE

MLP of TiO₂ Water Interface Model and its Application

Jul. 2021 – now

Advisor: Prof. Jun, Cheng

Cheng Group Website

- Trained machine learning potential (MLP) for terraced TiO₂ 110 - water interface system;
- Developed various efficient python scripts for computing statistical properties from MD trajectories, for instance, dissociation degree of adsorbed water;
- Discovered waters adsorbed above Ti_{5c} distribute closer towards one of two rows of O_{br}.

Study Towards the Synthesis of Clionastatin B

Jun. 2019 – May 2021

Advisor: Prof. Yandong, Zhang

Zhang Group Website

- An optimized procedures for a facial-selective enone epoxidation. (yield 80%, d.r. 5:1);
- Attempts to dehydrate a neopentyl alcohol (sterically hindered and susceptible to rearrangement).

PROFESSIONAL SKILLS

Programming Language: shell, Python

- Familiar with shell and python scripting;
- Statistical analysis of MD trajectories (MDAnalysis, ase).

Calculation Packages: DeePMD-kit series, CP2K, LAMMPS

- Familiar with DeePMD-kit MLP training and DPGEN data set generation.

SELECTED AWARDS

- The Wang Laoji Scholarship, XMU (2/96) Apr. 2021.
- Successful Participant of Mathematical Contest in Modelling May 2020.
- The Elite Undergraduate Program of Chemistry Scholarship, XMU (15/168).
2018–2021, 4 times