Ruihao Bi

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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 efficient python code for computing dissociation degree of adsorbed water;
- Discovered that Ti_{5c} adsorbed waters distribute closer towards one of the rows of $O_b r$.

Synthetic Study Towards Clionastatin B

Jun. 2019 – May 2021

Advisor: Prof. Yandong, Zhang

Zhang Group Website

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

Profession Skills

Programming Language: shell, Python

- Familiar with shell and python scripting;
- Developing statistical analysis on MD trajectories (MDAnalysis, ase).

Calculation Packages: DeePMD-kit series, CP2K, LAMMPS, VMD

• Familiar with DeePMD MLP training and dataset 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). 2017–2021, 4 times