RUIHAO BI

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EDUCATION

College of Chemistry, Xiamen University (XMU) Xiamen, China

Research Assistant (Jun, Cheng Group) 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

Study of thermodynamic stability of different surface hydroxyl terminations for $SrFeO_{3-\delta}$ Feb. 2022 – now

Advisor: Prof. Jun, Cheng Cheng Group Website

- Performed PBE+U calculations of different bulk phases of $SrFeO_{3-\delta}$. According to optimized cell parameter and band gap selected U_{eff} for further calculation.

MLP of TiO_2 Water Interface Model and its Application Jul. 2021 – now

Advisor: Prof. Jun, Cheng Cheng Group Website

- Trained machine learning potential (MLP) for TiO_2 110 - water interface system;
- Performed ns-scale MLP accelerated MD simulation of stepped TiO_2 interface. Analysing the MD trajectory helped us explain a double row pattern discovered in our EC-STM experiment;
- Researched the well known size-effect in TiO_2 simulations. Studied the size-effect on surface water dissociation by performing DPMD for interface models ranging from 3 to 17 Ti – O tri-layers.

Study Towards the Synthesis of Clionastatin B Jun. 2019 – May 2021

Advisor: Prof. Yandong, Zhang Zhang Group Website

- Trained organic lab skills for natural product synthesis.
- Studied a conformation driven facial-selective epoxydation reaction.
- Researched dehydration reactions for a tertiary alcohol.

PROFESSIONAL SKILLS

Programming skills: shell, Python, C++, Cython

- Scripting with python and shell for simple workflows, plotting, and small-scale computing.
- Experience in accelerating larger computation in python using multiprocessing, and C-library functions.

Computation Packages & Practical softwares:

- Familiar with DeePMD-kit and DPGEN suite for machine-learning potential training.
- Familiar with CP2K electronic structure calculation.
- LAMMPS, VMD, MDAnalysis, ASE, and etc.

SELECTED AWARDS

- Wang Laoji Scholarship, XMU (2/96) Apr. 2021.
- Successful Participant of Mathematical Contest in Modelling May 2020.
- Elite Undergraduate Program of Chemistry Scholarship, XMU (15/168). 2018–2021, 4 times
- Scholarship of Academic Excellence, XMU. (10/168) Mar. 2018.