

RUIHAO BI

School of Science, Westlake University, Zhejiang, P.R.China, 310024

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EDUCATION

School of Science, Westlake University (WLU)

Hangzhou, China

Graduate student (Wenjie, Dou Group)

Sept. 2022 – now

- Selected Coursework:

Quantum Chemistry (A), Chemical Kinetics & Reaction Dynamics (A), Spectroscopy and Group Theory (A),
Quantum Mechanics of Open Systems (A)

College of Chemistry, Xiamen University (XMU)

Xiamen, China

Research Assistant (Jun, Cheng Group)

Jul. 2021 – Jun. 2022

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

Nuclear Quantum Effects in the Dynamics of Electron Transfer near Metal Surfaces

Sept. 2022 – now

Advisor: Prof. Wenjie, Dou

Dou Group Website

- Developing electronic friction based methods for real time dynamics of electron transfers near metal surface, with special focuses on nuclear quantum effects, i.e., ZPE and tunneling.
- Prediction of tunneling rates for electron transfer near metal surfaces.

Study of stability of different surface hydroxyl terminations for $\text{SrFeO}_{3-\delta}$

Feb. 2022 – May. 2022

Advisor: Prof. Jun, Cheng

Cheng Group Website

- Ab initio. electronic structure calculations (DFT) of bulk and surfaces SrFeO_{3-x} . Study the formation energy of various defects.

MLP of TiO_2 Water Interface Model and its Application

Jul. 2021 – now

Advisor: Prof. Jun, Cheng

Cheng Group Website

- Trained DeePMD machine learning force field for TiO_2 -water interface geometries, with which we studied:
- $[1\bar{1}1]$ step-edge induced water molecule dissociations and double-row pattern;
- Adsorption water dissociation predicted by MD depends on the slab size, precisely, # of TiO_2 tri-layers.

Study Towards the Synthesis of Clonastatin B

Jun. 2019 – May 2021

Advisor: Prof. Yandong, Zhang

Zhang Group Website

- Trained organic lab skills for natural product synthesis.
- Study of a conformation driven facial-selective epoxidation reaction and a tertiary alcohol dehydration.

PROFESSIONAL SKILLS

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

Professional Softwares: DeePMD-kit, DPGEN, CP2K, VASP, LAMMPS, VMD, MDAnalysis

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.

LIST OF PUBLICATIONS

- ¹Y. Sun, C.-R. Wu, F. Wang, R.-H. Bi, Y.-B. Zhuang, S. Liu, M.-S. Chen, K. H.-L. Zhang, J.-W. Yan, B.-W. Mao, Z.-Q. Tian, and J. Cheng, “Step-induced double-row pattern of interfacial water on rutile TiO₂(110) at electrochemical conditions”, 10.26434/chemrxiv-2023-7wsqv (2023).
- ²Y.-B. Zhuang, R.-H. Bi, and J. Cheng, “Resolving the odd–even oscillation of water dissociation at rutile TiO₂(110)–water interface by machine learning accelerated molecular dynamics”, *The Journal of Chemical Physics* **157**, 10.1063/5.0126333 (2022).
- ³H. Cui, Y. Shen, Y. Chen, R. Wang, H. Wei, P. Fu, X. Lei, H. Wang, R. Bi, and Y. Zhang, “Two-stage syntheses of clonastatins a and b”, *Journal of the American Chemical Society* **144**, 8938–8944 (2022).