# Rui-Hao Bi

Curriculum Vitae, dated October 19, 2024

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## EDUCATION

**Westlake University (WLU)**  Hangzhou, China
*Ph.D. in Chemistry*  Aug 2022 – Jun 2027 (expected)

- Finished all required courses and passed thesis proposal defense.
- Research interests: nuclear quantum effects, metal surface nonadiabatic dynamics and chemical rate theory.

**Xiamen University (XMU)**  Xiamen, China
*B.S. in Chemistry*  Sep 2017 – Jun 2021

- GPA 3.79/4.00 (Rank: 3/97); selected to Elite Undergraduate Program (Top 15%).
- Relevant coursework: Calculus, Physics, Physical Chemistry, Chemical Kinetics and Dynamics. (All top 5%)

## PUBLICATION LIST

### Nonadiabatic dynamics and Nuclear Quantum Effects

1. **R.-H. Bi**, Y. Su, Y. Wang, L. Sun, and W. Dou, "Spin-lattice relaxation with non-linear couplings: Comparison between Fermi's golden rule and extended dissipaton equation of motion", J. Chem. Phys. **161**, 024105 (2024) [pdf]

2. **R.-H. Bi** and W. Dou, "Electronic friction near metal surface: Incorporating nuclear quantum effect with ring polymer molecular dynamics", J. Chem. Phys. **160**, 074110 (2024) [pdf]

### Machine Learning Accelerated Molecular Dynamics for Electrochemical Interfaces

1. Y. 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 $TiO_2$(110) under electrochemical conditions", Chem. Sci., Edge Article (2024) [code]

2. Y.-B. Zhuang, **R.-H. Bi**, and J. Cheng, "Resolving the odd-even oscillation of water dissociation at rutile $TiO_2$(110)-water interface by machine learning accelerated molecular dynamics", J. Chem. Phys. **157**, 164701 (2022) [code]

### Synthetic Organic Chemistry

1. H. Cui, Y. Shen, Y. Chen, R. Wang, H. Wei, P. Fu, X. Lei, H. Wang, **R.-H. Bi**, and Y. Zhang, "Two-Stage Syntheses of Clionastatins A and B", J. Am. Chem. Soc. **144**, 8938–8944 (2022)

## RESEARCH EXPERIENCE

**Westlake University (WLU)**  Hangzhou, China
*Research Assistant to Prof. Wenjie Dou*  Aug 2022 – Jun 2027 (expected)

- Developed a ring polymer molecular dynamics (RPMD) extension to the electronic friction model.
- Studied the temprature scaling of the spin-lattice relaxation time in the strong spin-phonon coupling regime.
- (on-going) Studying the full configuration interaction (FCI) solution of the Newns-Anderson model, is there any many-body effects missing from the standard Indpendent Electron Surface Hopping (IESH) method?
- (on-going) Developing Floquet-based surface hopping method for nonadiabatic dynamics under the driving of an shaped laser pulse. How good is Floquet-based method when the laser is not exactly periodic?
- (on-going) Proposing a generalized Langevin dynamics model to explain how the collective coupling of molecules to the photocavity can drastically affect the chemical reaction rates.

**Xiamen University (XMU)** Xiamen, China

*Research Assistant to Prof. Jun Cheng* Jun 2021 – Jun 2022

- Trained machine learning model for $TiO_2$-water interface with Density Functional Theory (DFT) data.
- Simulation of step-edge enhanced water dissociation on rutile $TiO_2$.
- Simulation of step-edge induced water double row patterns on rutile $TiO_2$ observed in Scanning Tunneling Microscopy (STM).
- Converged the water dissociation degree on rutile $TiO_2$ with a 3000-atom rutile slab.

**Xiamen University (XMU)** Xiamen, China

*Research Assistant to Prof. Yandong Zhang* Jun 2019 – May 2021

- Trained in synthetic organic chemistry, including Schlenk line operation, column chromatography, and NMR.
- Studied the elimination reaction of a hydroxyl group adjacent to the neopentyl position on a cyclohexane ring.

## TEACHING AND INTERNSHIPS

**Westlake University** Hangzhou, China

*Teaching assistant* Sep 2023 – Jan 2024

- Tutoring duty for the Undergraduate "Computer and Programming" course (instructor: Prof. Yue Zhang).

## SELECTED AWARDS AND HONORS

- Best Poster Award, 11th Triennial Congress of the International Society for Theoretical Chemical Physics (ISTCP, 9 / *ca.* 280), Oct. 2024.
- National Scholarship, WLU (3 / School of Science), Oct. 2024.
- Wang Laoji Scholarship, XMU (2/96) Apr. 2021.
- Successful Participant of Mathematical Contest in Modelling (MCM)[©] May 2020.
- Elite Undergraduate Program of Chemistry Scholarship, XMU (15/168) 2018–2021, 4 times.
- Scholarship of Academic Excellence, XMU (10/168) Mar. 2018.

## COMPUTER AND LANGUAGE SKILLS

**Programming & Software:** C/C++, Fortran, Python, Linux, CP2K, DeepMD-kit, LAMMPS

**Language:** Mandarin Chinese (native), English (proficient, TOEFL iBT: 103, dated Nov. 2021)