Rui-Hao Bi

Curriculum Vitae, dated May 21, 2025

+(86) 18605025530 ◇ Hangzhou, Zhejiang, China

biruihao@westlake.edu.cn ◇ https://github.com/ruihao99

Education

Westlake University (WLU) Hangzhou, China

Ph.D. Candidate in Chemistry Aug 2022 – Jun 2027 (expected)

- Completed all required coursework and successfully defended thesis proposal (Dec. 2024).
- Research focuses on open quantum systems, nuclear quantum effects, nonadiabatic surface dynamics, and chemical reaction rate theory.

Xiamen University (XMU) Xiamen, China

B.S. in Chemistry Sep 2017 – Jun 2021

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

Publication List

Nonadiabatic dynamics and Nuclear Quantum Effects

1. Y. Wang, **R. Bi**, and W. Dou, "Manipulating nonadiabatic dynamics by plasmonic nanocavity", J. Phys. Chem. Lett. **16**, 4139–4147 (2025) [pdf]
2. Y.-T. Ma, **R.-H. Bi**, and W. Dou, "Orbital surface hopping from the orbital quantum-classical liouville equation for nonadiabatic dynamics of many-electron systems", J. Chem. Theory Comput. **21**, 3847–3856 (2025) [pdf]
3. **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]
4. **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 for accessing nonadiabatic effects at quantum temperatures.

- Investigated the temperature dependence of spin-lattice relaxation time in the strong spin-phonon coupling regime.
- Developed and implemented the Orbital Surface Hopping (OSH) method; benchmarked against FCI-FSSH and IESH.
- (Ongoing) Developing a Floquet-based surface hopping method for nonadiabatic dynamics driven by shaped laser pulses.
- (Ongoing) Constructing exact quantum correlation functions from memory kernels reconstructed via higher-order moments.

Xiamen University (XMU) Xiamen, China
Research Assistant to Prof. Jun Cheng Jun 2021 – Jun 2022

- Trained machine learning potentials for the TiO_2-water interface using Density Functional Theory (DFT) data.
- Simulated step-edge-enhanced water dissociation on rutile TiO_2.
- Reproduced step-edge-induced water double-row patterns on rutile TiO_2 observed via Scanning Tunneling Microscopy (STM).
- Performed molecular dynamics simulations with a 3000-atom slab model to obtain a converged water dissociation degree on rutile TiO_2.

Xiamen University (XMU) Xiamen, China
Research Assistant to Prof. Yandong Zhang Jun 2019 – May 2021

- Trained in synthetic organic techniques, including Schlenk line operation, column chromatography, and NMR spectroscopy.
- Investigated the elimination reaction of a hydroxyl group adjacent to a 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, Julia, Linux, CP2K, DeepMD-kit, LAMMPS
Language: Mandarin Chinese (native), English (proficient, TOEFL iBT: 103, dated Nov. 2021)