Rui-Hao Bi

Curriculum Vitae, dated July 22, 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 drasticly 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

- 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)