

# Xuezhi Bian

Graduate Student in Theoretical Chemistry

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## EDUCATION

08/2019 - Present	<b>Ph.D. Candidate in Theoretical Chemistry</b> Department of Chemistry, University of Pennsylvania Advisor: Prof. Joseph E. Subotnik	Philadelphia, PA
09/2015 - 06/2019	<b>B.S. in Chemistry, Hongyi Honor Degree</b> College of Chemistry and Molecular Science, Wuhan University Dissertation Advisor: Prof. Rui Yu	Wuhan, China
08/2017 - 08/2018	<b>Exchange Student</b> University of California, Berkeley	Berkeley, CA

## RESEARCH EXPERIENCE

6/2020 - Present	<b>Graduate Researcher at University of Pennsylvania</b> • Developing mixed-quantum classical algorithms for <i>ab initio</i> modeling of coupled spin-nuclear-electronic dynamics in molecular systems. • Studying the nuclear Berry Curvature effect in non-adiabatic molecular dynamics and its implications in the angular momentum transfer process under the Born-Oppenheimer framework. • Exploring spin-related chemical processes such as chiral-induced spin selectivity (CISS) through first-principle approaches.	Advisor: Prof. Joseph E. Subotnik
09/2018 - 06/2019	<b>Undergraduate Researcher at Wuhan University</b> • Design and realization of topological materials in classic electronic circuits systems.	Advisor: Prof. Rui Yu
10/2017 - 08/2018	<b>Undergraduate Researcher at UC Berkeley</b> • Optimization of range-separated hybrid functional in density functional theory.	Advisor: Prof. Eran Rabani

## AWARDS

• John G. Miller Graduate Fellowship	2023
• Penn Chemistry Graduate Committee's List	2019
• Wuhan University Outstanding Student Scholarship	2017
• Hongyi Scholarship of Wuhan University	2016, 2017
• Wuhan University Second Prize Scholarship	2016, 2017

## PUBLICATIONS

- [1] Z. Tao, **X. Bian**, Y. Wu, J. Rawlinson, R.G. Littlejohn, J.E. Subotnik "Total Angular Momentum Conservation in Ehrenfest Dynamics with a Truncated Basis of Adiabatic States" *arXiv* 2311.16995 (2023)
- [2] V. Athavale, **X. Bian**, Z. Tao, Y. Wu, T. Qiu, J. Rawlinson, R. G. Littlejohn, J. E. Subotnik "Surface hopping, electron translation factors, electron rotation factors, momentum conservation, and size consistency" *J. Chem. Phys.* 159, 114120 (2023)
- [3] **X. Bian**, Z. Tao, Y. Wu, J. Rawlinson, R.G. Littlejohn, J.E. Subotnik "Total Angular Momentum Conservation in Ab Initio Born-Oppenheimer Molecular Dynamics" *Phys. Rev. B* 108.L220304 (2023)
- [4] Z. Zhou, Y. Wu, **X. Bian**, J.E. Subotnik "Nonadiabatic Dynamics in a Continuous Circularly Polarized Laser Field with Floquet Phase-Space Surface Hopping" *J. Chem. Theor. Comp.* 19(3), 718-732 (2023)
- [5] **X. Bian**, Y. Wu, J.I. Rawlinson, R.G. Littlejohn, J.E. Subotnik "Modeling Spin-Dependent Nonadiabatic Dynamics with Electronic Degeneracy: A Phase-Space Surface-Hopping Method" *J. Phys. Chem. Lett.* 13(32), 7398-7404 (2022)
- [6] Y. Wu, **X. Bian**, J.I. Rawlinson, R.G. Littlejohn, J.E. Subotnik "A phase-space semiclassical approach for modeling nonadiabatic nuclear dynamics with electronic spin" *J. Chem. Phys.* 157, 011101 (2022) (Communication)
- [7] **X. Bian**, T. Qiu, J. Chen, and J. E. Subotnik "On the Meaning of Berry Force For Unrestricted Systems Treated With Mean-Field Electronic Structure" *J. Chem. Phys.* 156, 234107 (2022) (**Editor's Pick, JCP Editor's Choice 2022**)
- [8] **X. Bian**, Y. Wu, H.H. Teh, J.E. Subotnik "Incorporating Berry Force Effects into the Fewest Switches Surface-Hopping Algorithm: Intersystem Crossing and the Case of Electronic Degeneracy" *J. Chem. Theor. Comput.* 18(4), 2075-2090 (2022)
- [9] **X. Bian**, Y. Wu, H.H. Teh, Z. Zhou, H.T. Chen, J.E. Subotnik. "Modeling nonadiabatic dynamics with degenerate electronic states, intersystem crossing, and spin separation: A key goal for chemical physics" *J. Chem. Phys.* 154, 110901 (2021)
- [10] G. Miao, **X. Bian**, Z. Zhou, and J. E. Subotnik, "A "Backtracking" Correction for the Fewest Switches Surface Hopping Algorithm" *J. Chem. Phys.* 153, 111101 (2020) (Communication)

## CONFERENCES

Poster	59th Symposium on Theoretical Chemistry at Zurich	2023
Poster	Gordon Research Conference on Electron Spin Interactions with Chiral Molecules and Materials	2023
Poster	International Conference on Nuclear Quantum Effects in Chemistry	2023
Poster	American Conference on Theoretical Chemistry	2022

## TEACHING EXPERIENCE

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### Teaching assistant at Penn Chemistry:

Chem 101 General Chemistry I (Fall 2019)

Chem 102 General Chemistry II (Spring 2020)

## SKILLS

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**Languages:** Python, C/C++, MATLAB

**Technologies:** OpenMP, MPI, CUDA, PyTorch