Xuezhi Bian

Graduate Student in Theoretical Chemistry

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EDUCATION

08/2019 - Present **Ph.D. Candidate in Theoretical Chemistry** **Philadelphia, PA**
Department of Chemistry, University of Pennsylvania
Advisor: Prof. Joseph E. Subotnik

09/2015 - 06/2019 **B.S. in Chemistry, Hongyi Honor Degree** **Wuhan, China**
College of Chemistry and Molecular Science, Wuhan University
Dissertation Advisor: Prof. Rui Yu

08/2017 - 08/2018 **Exchange Student** **Berkeley, CA**
Universisty of California, Berkeley

RESEARCH EXPERIENCE

6/2020 – Present **Graduate Researcher at University of Pennsylvania** **Advisor: Prof. Joseph E. Subotnik**

- Developing mixed-quantum classical algorithms for *ab initio* 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.

09/2018 – 06/2019 **Undergraduate Researcher at Wuhan Univeristy** **Advisor: Prof. Rui Yu**

- Design and realization of topological materials in classic electronic circuits systems.

10/2017 – 08/2018 **Undergraduate Researcher at UC Berkeley** **Advisor: Prof. Eran Rabani**

- Optimization of range-separated hybrid functional in density functional theory.

AWARDS

- John G. Miller Graduate Fellowship in Physical Chemistry 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] 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)

[2] **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" *arXiv* 2303.13787 (2023)

[3] 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)

[4] **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)

[5] 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)

[6] **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**)

[7] **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)

[8] **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)

[9] 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

Teaching assistant:
Chem 101 General Chemistry I (Fall 2019)
Chem 102 General Chemistry II (Spring 2020)

SKILLS

Languages: Python, C/C++, MATLAB

Technologies: OpenMP, MPI, CUDA, PyTorch