Yuchen Wang

yuchenwang@uchicago.edu | Personal Page | Google Scholar

Professional Experience

The University of Chicago *Chicago, IL*
Postdoctoral Associate, PI: David A. Mazziotti *2022 – current*

Education

Johns Hopkins University *Baltimore, MD*
Ph.D. Chemistry, Advisor: David R. Yarkony† *2017 – 2022*

University of Science and Technology of China *Hefei, Anhui*
B.S. Chemical Physics, Rank 2% *2012 – 2016*

Research Interests

- Quantum computing algorithms for quantum chemistry
- Machine learning for photochemistry
- Electronic structure theory with reduced density matrix
- Light-matter interactions and conical intersections

Preprints and Submitted Manuscripts

[] R. Dutta, C. Cianci, A. V. Soudackov, **Y. Wang**, C. Xu, D. A. Mazziotti, L. F. Santos, and V. S. Batista. "Qumode-Based Variational Quantum Eigensolver for Molecular Excited States". *Submitted to J. Chem. Theory Comput.*

[] **Y. Wang**. "On the nonparametric diabatization of coupled electronic states". *Submitted to J. Phys. Chem.*

Peer-reviewed Publications (19)

[19] **Y. Wang**, I. Avdic, and D. A. Mazziotti. "Shadow ansatz for the many-fermion wave function in scalable molecular simulations on quantum computing devices". *Phys. Rev. A*, 112, 022432 (2025).

[18] **Y. Wang** and D. A. Mazziotti. "Quantum many-body simulations from a reinforcement-learned exponential Ansatz". *Phys. Rev. A* 112, 022403 (2025).

[17] S. Warren, **Y. Wang**, C. L. Benavides-Riveros, and D. A. Mazziotti. "Quantum algorithm for polaritonic chemistry based on an exact ansatz". *Quantum Sci. Technol.* 10, 02LT02 (2025).

[16] **Y. Wang**, C. Cianci, I. Avdic, R. Dutta, S. Warren, B. Allen, N. P. Vu, L. F. Santos, V. S. Batista, and D. A. Mazziotti. "Characterizing conical intersections of cytosine on quantum computers". *J. Chem. Theory. Comput.* 21, 1213 (2025).

[15] C. Avanessian, **Y. Wang**, and D. R. Yarkony. "Floquet-engineered photodissociation simulated using coupled potential energy and dipole matrices". *J. Phys. Chem. Lett.* 15, 9905 (2024).

[14] S. Warren, **Y. Wang**, C. L. Benavides-Riveros, and D. A. Mazziotti. "Exact ansatz of fermion-boson systems for a quantum device". *Phys. Rev. Lett.* 133, 080202 (2024).

[13] **Y. Wang** and D. A. Mazziotti. "Quantum simulation of conical intersections". *Phys. Chem. Chem. Phys.* 26, 11491 (2024).

[12] J. Zhou, Y. Shu, **Y. Wang**, J. Leszczynski, and O. V. Prezhdo. "Dissociation time, quantum yield and dynamic reaction pathways in the thermolysis of Trans-3,4-dimethyl-1,2-dioxetane". *J. Phys. Chem. Lett.* 15, 1846 (2024).

[11] C. L. Benavides-Riveros, **Y. Wang**, S. Warren, and D. A. Mazziotti. "Quantum simulation of excited states from parallel contracted quantum eigensolvers". *New J. Phys.* 26, 033020 (2024).

[10] **Y. Wang** and D. A. Mazziotti. "Electronic excited states from a variance-based contracted quantum eigensolver". *Phys. Rev. A* 108, 022814 (2023).

[9] **Y. Wang**, L. M. Sager-Smith, and D. A. Mazziotti. "Quantum simulation of bosons with the contracted quantum eigensolver". *New J. Phys.* 25, 103005 (2023).

[8] **Y. Wang**, H. Guo, and D. R. Yarkony. "Nonadiabatic dynamics of NH_3 A state photodissociation into the NH($a^1\Delta, X^3\Sigma^-$) + H_2 channel: Semi-classical simulations with full geometry-dependent spin-orbit and derivative couplings". *Phys. Chem. Chem. Phys.* 24, 15060 (2022).

[7] **Y. Wang** and D. R. Yarkony. "Conical intersection seams in spin-orbit coupled systems with an even number of electrons: A numerical study based on neural network fit surfaces". *J. Chem. Phys.* 155, 174115 (2021).

[6] **Y. Wang**, Y. Guan, H. Guo, and D. R. Yarkony. "Enabling complete multichannel nonadiabatic dynamics: A global representation of the two-channel coupled, $1,2^1$A and 1^3A states of NH_3 using neural networks". *J. Chem. Phys.* 154, 094121 (2021).

[5] S. Han, **Y. Wang**, Y. Guan, D. R. Yarkony, and H. Guo. "Impact of diabolical singular points on nonadiabatic dynamics and a remedy: Photodissociation of ammonia in the first band". *J. Chem. Theory Comput.* 16, 6776 (2020).

[4] **Y. Wang**, Y. Guan, and D. R. Yarkony. "On the impact of singularities in the two-state adiabatic to diabatic state transformation: A global treatment". *J. Phys. Chem. A* 123, 9874 (2019).

[3] **Y. Wang**, C. Xie, H. Guo, and D. R. Yarkony. "A quasi-diabatic representation of the $1,2^1$A states of methylamine". *J. Phys. Chem. A* 123, 5231 (2019).

[2] D. R. Yarkony, C. Xie, X. Zhu, **Y. Wang**, C. L. Malbon, and H. Guo. "Diabatic and adiabatic representations: Electronic structure caveats". *Comput. Theor. Chem.* 1152, 41 (2019).

[1] **Y. Wang** and D. R. Yarkony. "Determining whether diabolical singularities limit the accuracy of molecular property based diabatic representations: The $1,2^1$A states of methylamine". *J. Chem. Phys.* 149, 154108 (2018).

Presentations and Talks (7)

Out of the shadow: molecular science with the quantum computing toolbox
Faculty Candidate Seminar, Indiana University, Bloomington, IN, 2025

Quantum simulation of conical intersections from the contracted quantum eigensolver
Poster Presentation, ACS Fall Meeting, Denver, CO, 2024

Quantum chemistry from reduced density matrix tomography
Invited Talk, Department of Statistics, The University of Chicago, Chicago, IL, 2024

Excited state theory: from electronic structure to quantum dynamics
Invited Talk, Department of Chemistry, Nanjing University, Nanjing, China, 2023

Light-induced conical intersections revealed by machine learning dipole surfaces
Poster Presentation, 28th Dynamics of Molecular Collisions Conference, Snowbird, UT, 2023

Machine learning potential energy and property matrices for nonadiabatic dynamics
*Poster Presentation, Gordon Research Conference on Molecular Interactions and Dynamics, Easton, MA, 2022 (**Poster Award Winner**)*

On the quasi-diabatic representation of methylamine photodissociation
Poster Presentation, 27th Dynamics of Molecular Collisions Conference, Big Sky, MT, 2019

Teaching Experience

- **Undergraduate level:**
  - Introductory Chemistry I & II (AS.030.101, AS.030.102)
  - Introductory Chemistry I & II Laboratory (AS.030.105, AS.030.106)
  - Organic Chemistry II (AS.030.206)
  - Applied Chemical Equilibrium and Reactivity with Lab (AS.030.103, honor class)
  - Average TA rating from students: 4.2/5
- **Graduate level:** Intermediate Quantum Chemistry (for non-theory track)

References

- Prof. David A. Mazziotti, The University of Chicago, damazz@uchicago.edu
- Prof. David R. Yarkony†, Johns Hopkins University, yarkony@jhu.edu
- Prof. Victor Batista, Yale University, batista@yale.edu
- Prof. Hua Guo, University of New Mexico, hguo@unm.edu