Yuchen Wang

yuchenwang0607@gmail.com Personal Page Google Scholar

Professional Experience

Postdoctoral Associate — 2022 - current
The University of Chicago
PI: David A. Mazziotti

Education

Johns Hopkins University — 2017 - 2022
Advisor: David R. Yarkony — Ph.D. Chemistry

Johns Hopkins University — 2017 - 2020
M.A. Chemistry

University of Science and Technology of China — 2012 - 2016
B.S. Chemical Physics

Research Interests

- Quantum computing algorithms for quantum chemistry
- Machine learning for accelarating photochemistry and photobiology discovery
- Conical intersections and nonadiabatic dynamics
- Electronic structure theory with reduced density matrix
- Light-matter interaction

Publications

[19] **Y. Wang** and D. A. Mazziotti. "Optimizing chemistry ansatz with reinforcement learning". *arxiv* (2025).

[18] 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 (2025), 02LT02.

[17] **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 (2025), 1213.

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

[15] **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. Lett.* under review (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 (2024), 080202.

[13] **Y. Wang** and D. A. Mazziotti. "Quantum simulation of conical intersections". *Phys. Chem. Chem. Phys.* 26.15 (2024), 11491.

[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.* 15.7 (2024), 1846.

[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 (2024), 033020.

[10] **Y. Wang** and D. A. Mazziotti. "Electronic excited states from a variance-based contracted quantum eigensolver". *Phys. Rev. A* 108.2 (2023), 022814.

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

[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 (2022), 15060.

[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.* 155.15 (2021), 174115.

[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.* 154.9 (2021), 094121.

[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.* 16.11 (2020), 6776.

[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* 123.45 (2019), 9874.

[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* 123.25 (2019), 5231.

[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 (2019), 41.

[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.* 149.15 (2018), 154108.

Presentations and Talks

- Out of the shadow: molecular science with the quantum computing toolbox, faculty candidate seminar, presented at Indiana University Bloomington, 2025
- Quantum simulation of excited states and conical intersections from the contracted quantum eigensolver, poster presented at ACS fall meeting, Denver, Colorado, 2024
- Quantum chemistry with reduced density matrix tomography, contributed talk presented at Department of Statistics, The University of Chicago, 2024
- Excited state study based on quasi-diabatic potential energy matrices and contracted Schrödinger equation, contributed talk presented at Department of Chemistry, Nanjing University, 2023
- Machine learning potential energy and property matrices for nonadiabatic dynamics, poster presented at Gordon Research Conference on Molecular Interactions and Dynamics, Easton, Massachusetts, 2022, poster award winner
- On the quasi-diabatic representation of methylamine photodissociation, poster presented at 27th Dynamics of Molecular Collisions Conference, Big Sky, Montana, 2019

References

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

Teaching Experience

- Undergraduate level: Introductory Chemistry I&II · Organic Chemistry II · Applied Chemical Equilibrium and Reactivity with Lab
- Graduate level: Intermediate Quantum Chemistry