Wenxiang Ying

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EDUCATION & APPOINTMENTS

University of Pennsylvania — Postdoctoral Researcher, 2025 - present
- *Advisor: Prof. Abraham Nitzan*

University of Rochester — M.S. and Ph.D. in Chemistry, 2025
- *Advisor: Prof. Pengfei Huo*
- *Thesis: Theory and Quantum Dynamics Investigations of Polariton Chemistry, Photo-Physics, and Transport*

University of Science and Technology of China (USTC) — B.S. in Chemical Physics, 2020

SELECTED PROFESSIONAL EXPERIENCE

Max-Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany — 10.26.2025 - 10.31.2025
- *Unravelling the Mysteries of Vibrational Strong Coupling (UnMySt) Theory Workshop / Hackathon*
- *Organizers: Dominik Sidler, Angel Rubio*

Flatiron Institute, New York, NY, United States — 09.29.2025 - 10.03.2025
- *Ab Initio Quantum Electrodynamics for Quantum Materials Engineering School*
- *Organizers: Simone Latini, Johannes Flick, Michael Ruggenthaler, Angel Rubio*

Arizona State University, Phoenix, AZ, United States — 09.09.2025 - 09.28.2025
- *Host: Prof. Maxim Sukharev*

Institute of Software, Chinese Academy of Science, Beijing, China — 06.15.2023 - 07.14.2023
- *Host: Prof. Shenggang Ying, Prof. Mingsheng Ying*

USTC, Hefei, Anhui, China — 09.01.2020 - 07.15.2021
- *Host: Prof. Xiao Zheng, Prof. YiJing Yan*

Boston University, Boston, MA, United States — 07.05.2019 - 08.31.2019
- *Host: Prof. David F. Coker*

CURRENT RESEARCH INTEREST AND SPECIALITY

- **Quantum Dynamics Methods**. Hierarchical equations of motion; approximated quantum master equations; tensor network approaches; the mixed-quantum-classical approaches; ring-polymer molecular dynamics.
- **Cavity Quantum Electrodynamics**. Exciton polariton photo physics and transport, vibration polariton chemistry, collective strong light-matter interaction, cavity spectroscopy.
- **Finite-Difference Time-Domain (FDTD) Simulations**. Nanoparticle metasurfaces.
- **Ab Initio Approaches**. Excited state electronic structure methods (CASSCF, CASPT2, MRCI, EOM-CC, TDDFT), *ab initio* nonadiabatic molecular dynamics for photo excited systems.

SKILLS

- **Languages**: English (*fluent*), Chinese Mandarin (*native*)
- **Programming**: Python, C, C++, Fortran, Shell Scripting
- **Softwares**: Gaussian, Molpro, PySCF, Avogadro, Quantum Espresso

PUBLICATIONS

(∗ denotes the corresponding authors, # denotes authors contributed equally)

Preprints

[18]. **W. Ying***, and A. Nitzan*, "Electron transfer in confined electromagnetic fields: a unified Fermi's golden rule rate theory, and extension to lossy cavities", arXiv:2511.04017;

[17]. Y. Lai*, **W. Ying**, T. D. Krauss, and P. Huo*, "Analytic Rate Theory of Polariton Relaxation that Explains Long Polariton Lifetime", **ChemRxiv** 2025;

Journal Articles

[16]. **W. Ying**, M. Elious Mondal, Eric R. Koessler, S. M. Vega, and P. Huo*, "Collective Effects in Polariton Chemistry, Photophysics, and Transport", **Annu. Rev. Phys. Chem.** 2026, 77 (accepted);

[15]. **W. Ying**#, B. X.-K. Chng#, M. Delor, and P. Huo*, "Microscopic Theory of Polariton Group Velocity Renormalization", **Nat. Commun.** 2025, 16 (1), 6950;

[14]. S. M. Vega#, **W. Ying**#, and P. Huo*, "Theoretical Insights into the Resonant Suppression Effect in Vibrational Polariton Chemistry", **J. Am. Chem. Soc.** 2025, 147 (23), 19727–19737; **(highlighted by University of Rochester News Center)**

[13]. D. Hu*, B. X.-K. Chng, **W. Ying**, and P. Huo*, "Trajectory-based Non-adiabatic Simulations of the Polariton Relaxation Dynamics", **J. Chem. Phys.** 2025, 162 (12), 124113;

[12]. B. X.-K. Chng, M. E. Mondal, **W. Ying**, and P. Huo*, "Quantum Dynamics Simulations of Exciton Polariton Transport", **Nano Lett.** 2025, 25 (4): 1617-1622;

[11]. B. X.-K. Chng, **W. Ying**, Y. Lai, A.N. Vamivakas, S.T. Cundiff, T.D. Krauss*, and P. Huo*, "Mechanism of Polariton Decoherence in the Collective Light-Matter Couplings Regime", **J. Phys. Chem. Lett.** 2024, 15 (47): 11773–11783;

[10]. **W. Ying***, Y. Su, Z.-H. Chen, Y. Wang*, and P. Huo*, "Spin Relaxation Dynamics with a Continuous Spin Environment: the Dissipaton Equation of Motion Approach", **J. Chem. Phys.** 2024, 161 (14), 144112;

[9]. Y. Lai*, **W. Ying**, and P. Huo*, "Rate Theory and Quantum Master Equation for Polariton Relaxation Dynamics", **J. Chem. Phys.** 2024, 161 (10), 104109;

[8]. **W. Ying***, M. E. Mondal, and P. Huo*, "Theory and Quantum Dynamics Simulations of Exciton-Polariton Motional Narrowing", **J. Chem. Phys.** 2024, 161 (6), 064105;

[7]. **W. Ying**, and P. Huo*, "Resonance Theory of Vibrational Strong Coupling Enhanced Polariton Chemistry and The Role of Photonic Mode Lifetime", **Commun. Mater.** 2024, 5 (1): 110;

[6]. **W. Ying**, M. A.D. Taylor, and P. Huo*, "Resonance Theory of Vibrational Polariton Chemistry at the Normal Incidence", **Nanophotonics** 2024, 13 (14): 2601-2615;

[5]. D. Hu, **W. Ying***, and P. Huo*, "Resonance Enhancement of Vibrational Polariton Chemistry Obtained from the Mixed Quantum-Classical Dynamics Simulations", **J. Phys. Chem. Lett.** 2023, 14 (49): 11208–11216;

[4]. **W. Ying***, and P. Huo*, "Resonance Theory and Quantum Dynamics Simulations of Vibrational Polariton Chemistry", **J. Chem. Phys.** 2023, 159 (8): 084104;

[3]. D. Bossion*, **W. Ying**, S.N. Chowdhury, and P. Huo*, "Non-adiabatic Mapping Dynamics in the Phase Space of $SU(N)$ Lie Group", **J. Chem. Phys.** 2022, 157 (8): 084105;

[2]. S. Chen, B.B. Gong, J. Gu, Y. Lin, B. Yang, Q.Q. Gu, R. Jin, Q. Liu, **W. Ying**, X.X. Shi, W.L. Xu, L.H. Cai, Y. Li, Z.H. Sun, S.Q. Wei, W.H. Zhang, and J.L. Lu, "Dehydrogenation of Ammonia Borane by Platinum–Nickel Dimers: Regulation of the Heteroatom Interspace Boosts Bifunctional Synergetic Catalysis," **Angew. Chem. Int. Ed.** 2022, 61 (41), e202211919;

[1]. S. Chen, L. Huang, Z.H. Sun, L.N. Cao, **W. Ying**, X.X. Shi, W. Liu, J. Gu, X.S. Zheng, J.F. Zhu, Y. Lin, S.Q. Wei, and J.L. Lu, "Synthesis of Quasi-Bilayer Subnano Metal-Oxide Interfacial Cluster Catalysts for Advanced Catalysis," **Small** 2020, 16 (52): 2005571;

SELECTED HONORS AND AWARDS

Chemical Computing Group Excellence Award for Graduate Students, ACS COMP Division 2025
Finalist of ACS Physical Chemistry Graduate Awards in Theoretical Chemistry, ACS PHYS Division 2024
Moses Passer Memorial Fellowship, University of Rochester 2024
Esther M. Conwell Graduate Fellowship, University of Rochester 2023
Excellent Teaching Assistant Award, USTC 2020, 2021

TEACHING, MENTORSHIP, AND SERVICE

Teaching

- **University of Rochester**: Teaching Assistant for CHM 469 & 470 Computational Chemistry I & II (Spring 2023, Spring 2024), CHM 132 General Chemistry Lab (Spring 2023), CHM 252/442 Physical Chemistry II (Spring 2022), CHM 251/441 Physical Chemistry I (Fall 2021).
- **USTC**: Teaching Assistant for 003158(.03/.05/e.01/.01) Quantum Physics (Fall 2019, Spring 2020, Fall 2020, Spring 2021).

Mentorship

- **Graduate Students**: Benjamin X.-K. Chng, Sebastian M. Vega, Santanu Poddar, Rahul Chourasiya.
- **Undergraduate Students**: Mateo L. Castellanos (currently PhD student at Stony Brook University).

Service

- **Contributing Reviews to Scientific Journals**: *Science*, *The Journal of Physical Chemistry Letters*, *The Journal of Chemical Physics*.

INVITED TALKS AT UNIVERSITIES, INSTITUTIONS & LABORATORIES

10. 10/26/2025, Max-Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany.
9. 09/04/2025, UnMySt Virtual Seminar, European Research Council (ERC) Synergy Project.
8. 06/28/2025, Bejing Normal University, Zhuhai, Guangdong, China.
7. 06/27/2025, South China Normal University, Guangzhou, Guangdong, China.
6. 06/24/2025, Westlake University, Hangzhou, Zhejiang, China.
5. 06/23/2025, USTC, Hefei, Anhui, China.
4. 02/17/2025, Virtual Talk at Professor Abraham Nitzan's Group, University of Pennsylvania.
3. 10/22/2024, Virtual Talk at Professor Joonho Lee's Group, Harvard University.
2. 09/25/2024, ACS PHYS Graduate Award Virtual Symposium.
1. 07/26/2023, Hefei National Research Center for Physical Sciences at the Microscale & USTC, Hefei, Anhui, China.

CONTRIBUTIONS TO INTERNATIONAL CONFERENCES

7. W. Ying, and P. Huo, "Quantum Dynamics Simulations of Polariton Chemistry, Photo Physics, and Transport", poster, at ACS Fall Meeting, Washington, DC, United States, August 17-21, 2025.
6. W. Ying, and P. Huo, "Quantum Dynamics Simulations of Polariton Chemistry, Photo Physics, and Transport", poster, at Penn Conference on Theoretical Chemistry (PCTC), Philadelphia, PA, United States, May 2-4, 2025.
5. W. Ying, M. E. Mondal, and P. Huo, "Theory and Quantum Dynamics Simulations of Exciton-Polariton Motional Narrowing", poster, at ACS Spring Meeting, San Diego, CA, United States, March 23-27, 2025.
4. W. Ying, M. E. Mondal, and P. Huo, "Theory and Quantum Dynamics Simulations of Exciton-Polariton Motional Narrowing", oral and poster, at APS March Meeting, Anaheim, CA, United States, March 16–21, 2025.

3. W. Ying, M. E. Mondal, and P. Huo, “Theory and Quantum Dynamics Simulations of Exciton-Polariton Motional Narrowing”, poster, at American Conference on Theoretical Chemistry (ACTC), Chapel Hill, NC, United States, June 17-20, 2024.

2. W. Ying and P. Huo, “Resonance Theory of Vibrational Polariton Chemistry”, oral and poster, at APS March Meeting, Minneapolis, MN, United States, March 3-8, 2024.

1. W. Ying and P. Huo, “Chemical Reactivity Under Vibrational Strong Coupling”, poster, at Quantum Control of Light and Matter Gordon Research Conference, Newport, RI, United States, August 6-11, 2023.