Wenjie Dou

Contact
Assistant Professor of Chemistry
Assistant Professor of Physics (joint)
School of Science, Westlake University, Hangzhou, Zhejiang 310024, China
Email: douwenjie@westlake.edu.cn

Education

2013-2018 **Ph.D. in Theoretical Chemistry**
University of Pennsylvania, Philadelphia, PA, USA
Advisor: Prof. Joseph E. Subotnik
Thesis: Modeling Nonadiabatic Dynamics at Molecule-Metal Interfaces

2009-2013 **B.S. in Physics**
University of Science and Technology of China (USTC), Hefei, China
Thesis: Numerical Renormalization Group study of Kondo effects

Research Experience

Jan. 2021-present Assistant Professor*, Westlake University*
Aug. 2018-Dec. 2020 Postdoctoral Scholar*, University of California, Berkeley*

Honors and Awards

2026 ACS OpenEye/Cadence Outstanding Junior Faculty Award, *American Chemical Society*
2025 Tang Ao-Chin Youth Award in Theoretical Chemistry, *Chinese Chemical Society*
2022 Excellent Research Advisor at the COMP Virtual Asia-Pacific Graduate students symposium, *American Chemical Society*
2019 Finalist for Justin Jankunas Doctoral Dissertation Award, *American Physical Society*
2017 Dissertation Completion Fellowship*, University of Pennsylvania*
2016 John G. Miller Graduate Fellowship*, University of Pennsylvania*
2015 Douty Fund Fellowship*, University of Pennsylvania*
2012 Institute of Modern Physics Scholarship, *USTC*
2011 Outstanding Undergraduate Scholarship, *USTC*
2010 Outstanding Undergraduate Scholarship, *USTC*

Teaching Experience

2025 Quantum Chemistry*, Westlake University*
2024 Quantum Chemistry*, Westlake University*
2023 Quantum Chemistry*, Westlake University*
2022 Quantum Chemistry*, Westlake University*
2021 Quantum Chemistry*, Westlake University*
2014 General Chemistry lab II*, University of Pennsylvania*

Five representative Publications

1. W. Liu, Y. Su, Y. Wang*, **W. Dou***. "Memory Kernel Coupling Theory: Obtaining Time Correlation Function from Higher-order Moments" *Phys. Rev. Lett.* **135**, 148001 (2025).
2. Y. Wang, V. Mosallanejad, W. Liu, **W. Dou***. "Nonadiabatic dynamics near metal surfaces with periodic drivings: A generalized surface hopping in Floquet representation" *J. Chem. Theory Comput.* **20**, 644 (2024). (**Supplementary cover**)
3. V. Mosallanejad*, J. Chen, **W. Dou***. "Floquet-driven frictional effects" *Phys. Rev. B* **107**, 184314 (2023).
4. C. Zhao, Q. Ou, J. Lee*, **W. Dou***. "Stochastic resolution of identity to CC2 for large systems: excited state properties" *J. Chem. Theory Comput.* **20**, 5188 (2024).
5. W. Liu, R. Bi, C. Zhao, Y. Wang, **W. Dou***. "Absorption Spectra with Kernel Polynomial Neural Quantum States" *J. Phys. Chem. Lett.* **16**, 12216 (2025). (**Supplementary cover**)

Full Publications

Independent work

Preprint

1. A. Zhou, R. Bi, *et al*, **W. Dou***, L. Sun*. "Tunable spin-phonon polarons in a chiral molecular qubit framework" arXiv:2506.04885 (2025).
2. Y. Ma, **W. Dou***. "Orbital Surface Hopping with an Electron Thermostat Yields Accurate Dynamics and Detailed Balance" arXiv:2511.16939 (2025).
3. C. Zhao, **W. Dou***. "Noise-reduced stochastic resolution of identity to CC2 for large-scale calculations via tensor hypercontraction" arXiv:2509.21885 (2025).
4. Y. Su*, Y. Wang, **W. Dou**. "Nonperturbative Open Quantum Dynamics Bypass Influence Functional" arXiv: 2503.00297(2025).

Published

5. W. Liu, R. Bi, C. Zhao, Y. Wang, **W. Dou***. "Absorption Spectra with Kernel Polynomial Neural Quantum States" *J. Phys. Chem. Lett.* **16**, 12216 (2025). (**Supplementary cover**)
6. C. Zhao, C. Li*, **W. Dou***. "Stochastic resolution of identity to CC2 for large systems: Excited-state gradients and derivative couplings" *J. Chem. Phys*. **163**, 234101 (2025).
7. Y. Wang, R. Bi, W. Liu, J. Han, **W. Dou***. "Mixed Quantum-Classical Approaches to Spin Current and Polarization Dynamics in Chiral Molecular Junctions" *J. Phys. Chem. Lett.* (accepted).
8. J. Han, Y. Wang, **W. Dou***. "Mixed Quantum–Classical Approaches to Electron Transmission through Chiral Molecules" *Chin. J. Chem. Phys*. (accepted).
9. Y. Liu, **W. Dou***. "From higher-order moments to time correlation functions in strongly correlated systems: A DMRG-based memory kernel coupling theory" *J. Chem. Phys.* **163**, 214102 (2025)
10. V. Mosallanejad*, **W. Dou***. "Two-mode Floquet quantum master approach for quantum transport through mesoscopic systems: Engineering of the fractional quantization" *Phys. Rev. B* **112**, 174308 (2025)
11. W. Liu, Y. Su, Y. Wang*, **W. Dou***. "Memory Kernel Coupling Theory: Obtaining Time Correlation Function from Higher-order Moments" *Phys. Rev. Lett.* **135**, 148001 (2025).

12. Y. Liu, **W. Dou***. "Electronic frictional effects near metal surfaces with strong correlations" *APL Comp. Phys.* **1**, 026103 (2025). (**Editor's Pick**)
13. C. Zhao, Q. Ou, C. Li*, **W. Dou***. "Stochastic resolution of identity to CC2 for large systems: Oscillator strength and ground state gradient". *J. Chem. Phys*. **163**, 024102 (2025).
14. V. Mosallanejad*, KL Chiu, **W. Dou***. "Space-averaged non-equilibrium Green's function approach for quantum transport in 3D" *J. Phys.: Condens. Matter* **37**, 265301 (2025).
15. R. Bi, W. Liu, **W. Dou***. "Universal Structure of Computing Moments for Exact Quantum Dynamics: Application to Arbitrary System-Bath Couplings" *J. Chem. Phys*. **162**, 224106 (2025).
16. V. Mosallanejad*, Y. Wang, J. Chen, **W. Dou***. "Floquet nonadiabatic dynamics in open quantum systems" *WIREs: Comput. Mol. Sci.* **15,** e70032 (2025).
17. W. Liu, J. Chen, **W. Dou***. "Enhancement of Chiral-Induced Spin Selectivity via Circularly Polarized Light" *J. Phys. Chem. C* **129**, 10181 (2025). (**Supplementary cover**)
18. Y. Wang, R. Bi, **W. Dou***. "Manipulating nonadiabatic dynamics by plasmonic nanocavity" *J. Phys. Chem. Lett.* **16,** 4139 (2025).
19. Y. Ma, R. Bi, **W. Dou***. "Orbital Surface Hopping from Orbital Quantum-Classical Liouville Equation for Nonadiabatic Dynamics of Many-electron Systems" *J. Chem. Theory Comput.* **21**, 3847 (2025). (**Supplementary cover**)
20. J. Chen, J. Lee*, **W. Dou***. "How to correct Ehrenfest nonadiabatic dynamics in open quantum systems: Ehrenfest plus random force dynamics" *J. Chem. Phys*. **162**, 044104 (2025).
21. Y. Wang, **W. Dou***. "Interband and intraband transitions, as well as charge mobility in driven two-band model with electron phonon coupling" *J. Chem. Phys.* **161**, 204104 (2024).
22. C. Zhao, J. Lee*, **W. Dou***. "Stochastic resolution of identity to CC2 for large systems: ground-states and triplet states properties". *J. Phys. Chem. A* **128**, 9302 (2024). (**Supplementary cover**)
23. W. Liu, J. Chen, **W. Dou***. "Polaritons under Extensive Disordered Molecular Rotation in Optical Cavities" *J. Phys. Chem. C* **128**, 12544 (2024). (**Supplementary cover**)
24. C. Zhao, Q. Ou, J. Lee*, **W. Dou***. "Stochastic resolution of identity to CC2 for large systems: excited state properties" *J. Chem. Theory Comput.* **20**, 5188 (2024).
25. R. Bi, Y. Su, Y. Wang, L. Sun, **W. Dou***. "Spin-lattice relaxation with non-linear couplings: Comparison between Fermi's golden rule and extended dissipaton equation of motion" *J. Chem. Phys.* **161**, 024105 (2024).
26. G. Meng, J. Gardner, **W. Dou**, R. J. Maurer*, B. Jiang*. "First-principles Nonadiabatic Dynamics of Molecules at Metal Surfaces with Vibrationally Coupled Electron Transfer" *Phys. Rev. Lett.* **133**, 036203 (2024).
27. J. Chen, W. Liu, V. Mosallanejad*, **W. Dou***. "Floquet Nonadiabatic Nuclear Dynamics with Photoinduced Lorentz-Like Force in Quantum Transport" *J. Phys. Chem. C* **128**, 11219 (2024).
28. J. Chen, Y. Wang, **W. Dou***. "Floquet nonadiabatic mixed quantum–classical dynamics in periodically driven solid systems" *J. Chem. Phys.* **160,** 214101 (2024).
29. Y. Wang, **W. Dou***. "Electron transfer at molecule-metal interfaces under Floquet engineering: Rate constant and Floquet Marcus theory" *ACS Phys. Chem Au.* **4**, 160 (2024). (**Supplementary cover**)
30. Y. Wang, V. Mosallanejad, W. Liu, **W. Dou***. "Nonadiabatic dynamics near metal surfaces with periodic drivings: A generalized surface hopping in Floquet representation" *J. Chem. Theory Comput.* **20**, 644 (2024). (**Supplementary cover**)

31. V. Mosallanejad*, Y. Wang, **W. Dou***. "Floquet non-equilibrium Green's function and Floquet quantum master equation for electronic transport: The role of electron-electron interactions and spin current with circular light" *J. Chem. Phys.* **160**, 164102 (2024).
32. R. Bi, **W. Dou***. "Electronic friction near metal surface: Incorporating nuclear quantum effect with ring polymer molecular dynamics" *J. Chem. Phys.* **160**, 074110 (2024).
33. W. Liu, Z.H. Chen, Y. Su, Y. Wang, **W. Dou***. "Predicting rate kernels via dynamic mode decomposition" *J. Chem. Phys.* **159**, 144110 (2023).
34. J. Bätge*, Y. Wang, A. Levy, **W. Dou***, M. Thoss*. "Periodically driven open quantum systems with vibronic interaction: Resonance effects and vibrationally mediated decoupling" *Phys. Rev. B* **108**, 195412 (2023).
35. Y. Wang, **W. Dou***. "Nonadiabatic dynamics near metal surfaces under Floquet engineering: Floquet electronic friction vs Floquet surface hopping" *J. Chem. Phys.* **159**, 094103 (2023).
36. V. Mosallanejad, H. Li, G. Cao, K. Chiu, **W. Dou**, G. Guo*. "The cell-centered Finite-Volume self-consistent approach for heterostructures: 1D electron gas at the Si–SiO2 interface" *J. Phys.: Condens. Matter* **35**, 475301 (2023).
37. Y. Wang, **W. Dou***. "Nonadiabatic dynamics near metal surface with periodic drivings: A Floquet surface hopping algorithm" *J. Chem. Phys.* **158**, 224109 (2023).
38. V. Mosallanejad*, J. Chen, **W. Dou***. "Floquet-driven frictional effects" *Phys. Rev. B* **107**, 184314 (2023).
39. J. P. Philbin*, Y. Wang*, P. Narang*, **W. Dou***. "Chemical reactions in imperfect cavities: enhancement, suppression, and resonance" *J. Phys. Chem. C* **126**, 14908 (2022).
40. R. Yang, Z. He, S. Lin, **W. Dou**, Z. Wang, H. Wang, J. Liu*. "Tunable Tribovoltaic Effect via Metal–Insulator Transition" *Nano Lett.* **22**, 9084 (2022).
41. K. Tong, **W. Dou***. "Numerical study of non-adiabatic quantum thermodynamics of the driven resonant level model: Non-equilibrium entropy production and higher order corrections" *J. Phys.: Condens. Matter* **34**, 495703 (2022).
42. J. Bätge, A. Levy, **W. Dou***, M. Thoss*. "Nonadiabatically driven open quantum systems under out-of-equilibrium conditions: Effect of electron-phonon interaction" *Phys. Rev. B* **106**, 075419 (2022).
43. G. Liu, J. Liu*, **W. Dou***. "Nonadiabatic quantum dynamics of tribovoltaic effects at sliding metal-semiconductor interfaces" *Nano energy* **96**, 107034 (2022).
44. J.P. Philbin*, A. Levy*, P. Narang*, **W. Dou***. "Asymmetric Spin Transport in Colloidal Quantum Dot Junctions" *J. Phys. Chem. C* **125**, 26661 (2021).
45. R. Yang, R. Xu, **W. Dou**, M. Benner, Q. Zhang, J. Liu*. "Semiconductor-based dynamic heterojunctions as an emerging strategy for high direct-current mechanical energy harvesting" *Nano Energy* **83**, 105849 (2021).
46. A. Levy*, **W. Dou***. "Modeling Energy Transfer in Quantum Thermal Machines" *Physics* **13**, 129 (2020).

Previous work

47. H.H. Teh, **W. Dou**, J.E. Subotnik. "Spin Polarization through A Molecular Junction Based on Nuclear Berry Curvature Effects" *Phys. Rev. B* **106**, 184302 (2022).

48. **W. Dou**, J. Lee, J. Zhu, L. Mejía, D.R. Reichman, R. Baer, E. Rabani. "Time-Dependent Second-Order Green's Function Theory for Neutral Excitations" *J. Chem. Theory Comput.* **18**, 5221 (2022).
49. J. Chen, **W. Dou**, J.E. Subotnik. "Active Spaces and Non-Orthogonal Configuration Interaction Approaches for Investigating Molecules on Metal Surfaces" *J. Chem. Theory Comput.* **18**, 7321 (2022).
50. H.H. Teh, **W. Dou**, J.E. Subotnik. "Antisymmetric Berry Frictional Force at Equilibrium in the Presence of Spin-Orbit Coupling" *Phys. Rev. B* **104**, L201409 (2021).
51. J. Chen, Z. Jin, **W. Dou**, J.E. Subotnik. "Electronic Structure for Multielectronic Molecules near a Metal Surface" *J. Phys. Chem. C* **125**, 2884 (2021).
52. **W. Dou**, M. Chen, T.Y. Takeshita, R. Baer, D. Neuhauser, E. Rabani. "Range-Separated Stochastic Resolution of Identity: Formulation and Application to Second Order Green's Function Theory" *J. Chem. Phys.* **153**, 074113 (2020).
53. A. J. Coffman, **W. Dou**, S. Hammes-Schiffer, J.E. Subotnik. "Modeling voltammetry curves for proton coupled electron transfer: The importance of nuclear quantum effects" *J. Chem. Phys.* **152**, 234108 (2020).
54. **W. Dou**, J. Bätge, A. Levy, M. Thoss. "Universal approach to quantum thermodynamics in the strong coupling regime" *Phys. Rev. B* **101**, 184304 (2020).
55. Z. Jin, **W. Dou**, J.E. Subotnik. "Configuration interaction approaches for solving quantum impurity models" *J. Chem. Phys.* **152**, 064105 (2020).
56. **W. Dou**, J.E. Subotnik. "Non-Adiabatic Molecular Dynamics at Metal surfaces" *J. Phys. Chem. A* **124**, 751(2020).
57. **W. Dou**, T.Y. Takeshita, M. Chen, R. Baer, D. Neuhauser, E. Rabani. "Stochastic Resolution of Identity for Real-Time Second-Order Green's Function: Ionization Potential and Quasi-particle Spectrum" *J. Chem. Theory Comput.* **15**, 6703 (2019).
58. T.Y. Takeshita, **W. Dou**, D.G.A. Smith, W.A. de Jong, R. Baer, D. Neuhauser, E. Rabani. "Stochastic resolution of identity second-order Matsubara Green's function theory" *J. Chem. Phys.* **151**, 044114 (2019).
59. A. Levy, **W. Dou**, E. Rabani, D.T. Limmer. "A complete quasiclassical map for the dynamics of interacting fermions" *J. Chem. Phys.* **150**, 234112 (2019).
60. J.E. Subotnik, G. Miao, N. Bellonzi, H.H. Teh, **W. Dou**. "A demonstration of consistency between the quantum classical Liouville equation and Berry's phase and curvature for the case of complex Hamiltonians" *J. Chem. Phys.* **151**, 074113 (2019).
61. **W. Dou**, J. E. Subotnik. "Perspective: How to understand electronic friction" *J. Chem. Phys.* **148**, 230901 (2018).
62. **W. Dou**, M.A. Ochoa, A. Nitzan, J. E. Subotnik. "Universal approach to quantum thermodynamics in the strong coupling regime" *Phys. Rev. B* **98**, 134306 (2018).
63. **W. Dou**, J. E. Subotnik. "Universality of electronic friction. II. Equivalence of the quantum-classical Liouville equation approach with von Oppen's nonequilibrium Green's function methods out of equilibrium" *Phys. Rev. B* **97**, 064303 (2018).
64. **W. Dou**, C. Schinabeck, M. Thoss, J. E. Subotnik. "A broadened classical master equation approach for treating electron-nuclear coupling in non-equilibrium transport" *J. Chem. Phys.* **148**, 102317 (2018).

65. G. Miao, **W. Dou**, J. E. Subotnik. "Vibrational Relaxation at a Metal Surface: Electronic Friction Versus Classical Master Equations" *J. Chem. Phys.* **147**, 224105 (2017).
66. **W. Dou**, J. E. Subotnik. "Universality of electronic friction: The equivalence of the Head-Gordon--Tully model and von-Oppen's NEGF approach at equilibrium" *Phys. Rev. B* **96**, 104305 (2017).
67. **W. Dou**, G. Miao, J. E. Subotnik. "Born-Oppenheimer Dynamics, Electronic Friction, and the Inclusion of Electron-Electron Interactions" *Phys. Rev. Lett.* **119***,* 046001 (2017).
68. **W. Dou**, J. E. Subotnik. "A generalized surface hopping algorithm to model non-adiabatic dynamics near metal surfaces: The case of multiple electronic orbitals" *J. Chem. Theory Comput.* **13***,* 2430 (2017).
69. **W. Dou**, J. E. Subotnik. "Electronic friction near metal surfaces: A case where molecule-metal couplings depend on nuclear coordinates" *J. Chem. Phys.* **146***,* 092304 (2017).
70. **W. Dou**, J. E. Subotnik. "A many-body states picture of electronic friction: The case of multiple orbitals and multiple electronic states" *J. Chem. Phys.* **145**, 054102 (2016).
71. W. Ouyang, **W. Dou**, A. Jain, J. E. Subotnik. "Dynamics of Barrier Crossings for the Generalized Anderson–Holstein Model: Beyond Electronic Friction and Conventional Surface Hopping" *J. Chem. Theory Comput.* **12**, 4178 (2016).
72. **W. Dou**, A. Nitzan, J. E. Subotnik. "Molecular electronic states near metal surfaces at equilibrium using potential of mean force and numerical renormalization group methods: Hysteresis revisited" *J. Chem. Phys.* **144**, 074109 (2016).
73. **W. Dou**, J. E. Subotnik. "A broadened classical master equation approach for nonadiabatic dynamics at metal surfaces: Beyond the weak molecule-metal coupling limit" *J. Chem. Phys.* **144**, 024116 (2016).
74. **W. Dou**, A. Nitzan, J. E. Subotnik. "Frictional effects near a metal surface" *J. Chem. Phys.* **143**, 054103 (2015).
75. **W. Dou**, A. Nitzan, J. E. Subotnik. "Surface hopping with a manifold of electronic states. III. Transients, broadening, and the Marcus picture" *J. Chem. Phys.* **142**, 234106 (2015).
76. **W. Dou**, A. Nitzan, J. E. Subotnik. "Surface hopping with a manifold of electronic states. II. Application to the many-body Anderson-Holstein model" *J. Chem. Phys.* **142**, 084110 (2015).
77. W. Ouyang, **W. Dou**, J. E. Subotnik. "Surface hopping with a manifold of electronic states. I. Incorporating surface-leaking to capture lifetimes" *J. Chem. Phys.* **142**, 084109 (2015).

Grants

1. Natural Science Foundation of China (NSFC), General Program, "Theoretical study on chemical molecular dynamics in an optical cavity." PI, 560,000 RMB, 1/1/2023-12/31/2016
2. Natural Science Foundation of China (NSFC), Excellent Youth (Early Career) Program, "Excited-state dynamics and electronic structure theory in complex systems." PI, 1,000,000 RMB, 1/1/2023-12/31/2025
3. Natural Science Foundation of China (NSFC), China-Israel Binational Program, "Quantum transport in chiral induced spin selectivity: electronic structure and dynamical studies." PI, 2,000,000 RMB, 1/1/2024-12/31/2026
4. Zhejiang Natural Science Foundation, Key Research and Development Program, "Theoretical studies of chiral induced spin selectivity." PI, 1,000,000 RMB, 1/1/2024-12/31/2026

5. Dean's Special Research Projects, Major Project, “Theoretical studies of spin-phonon interactions in molecular qubits.” PI, 1,500,000 RMB, 1/1/2026-12/31/2028

Invited Talks

1. *CECAM meeting*, “Exact quantum dynamics from memory kernel coupling theory” Shanghai, July. 2026 (upcoming)
2. *Boston theoretical chemistry seminar,* “Excited-state electronic structure theory and non-adiabatic dynamics in complex systems”, BU, MIT and Harvard, April. 2026 (upcoming)
3. *Physical chemistry seminar,* “Excited-state electronic structure theory and non-adiabatic dynamics in complex systems”, University of Rochester, Mar. 2026 (upcoming)
4. *Joint quantum seminar,* “Excited-state electronic structure theory and non-adiabatic dynamics in complex systems”, Emory University, Mar. 2026 (upcoming)
5. *Physical chemistry seminar,* “Excited-state electronic structure theory and non-adiabatic dynamics in complex systems”, Purdue University, Mar. 2026 (upcoming)
6. *Physical chemistry seminar,* “Excited-state electronic structure theory and non-adiabatic dynamics in complex systems”, Yale University, Mar. 2026 (upcoming)
7. *Theoretical chemistry seminar,* “Excited-state electronic structure theory and non-adiabatic dynamics in complex systems”, University of Wisconsin Madison, Mar. 2026 (upcoming)
8. *ACS meeting*, “Tunable Spin-Polaron in a Chiral Metal Complex Framework” Atlanta, Mar. 2026 (upcoming)
9. *Ultrafast spectroscopy workshop*, “Memory kernel coupling theory for spin-phonon interactions” Hong Kong University of Science and Technology, Dec. 2025
10. *Tang Ao-Chin memorial and theoretical chemistry workshop*, “Memory kernel coupling theory for spin-phonon interactions” Changchun, Nov. 2025
11. *Excited State Quantum Chemistry Workshop*, “Stochastic resolution of identity for excited state energy and nonadiabatic couplings” Qingdao, Oct. 2025
12. *The 3rd World Materials Conference*, “Memory kernel coupling theory for spin-lattice effects in molecular qubits” Guilin, Oct. 2025
13. *Virtual International Seminar on Theoretical Advancements (VISTA)*, “Exact quantum dynamics for spin-lattice effects in molecular qubits” Online, Sep. 2025
14. *19th National Conference on Chemical Dynamics*, “Memory kernel coupling theory: Exact quantum dynamics for open quantum systems” Chunan, Sep. 2025
15. *AI4Science colloquium at ByteDance*, “Scalable Neural Quantum State based Kernel Polynomial Method for Optical Properties from the First Principle” Online, August 2025
16. *Theoretical Chemistry Committee Meeting*, “Exact quantum dynamics and electronic structure theory” Yinchuan, August 2025
17. *Quantum Transport in Nanoscale Molecular Systems workshop*, “Quantum transport and spintronics with light-matter interactions” Kirchberg in Tirol, Austria, July 2025
18. *Chinese Chemistry Society Meeting on Surface Science,* “Exact quantum dynamics from memory kernel coupling theory”, Chengdu, May 2025
19. *Princeton Center Theoretical Science workshop*, “Spin-lattice relaxation with nonlinear couplings”, Princeton University, April 2025
20. *Electronic structure theory workshop,* “Stochastic resolution of identity to CC2 for large systems: Oscillator strength and energy gradient”, Huanan Normal University, Guangzhou, April 2025

21. *Computational physical science workshop,* "Excited-state electronic structure and nonadiabatic dynamics with light-matter interactions", Fudan University, Shanghai, Mar. 2025
22. *Theoretical chemistry Frontier,* "Quantum dynamics in complex systems", Hong Kong Chinese University, Shenzhen, Jan. 2025
23. *Excited-state dynamics workshop,* "Excited-state electronic structure and nonadiabatic dynamics", Beijing Normal University, Beijing, Dec. 2024
24. *Chemical theory and mechanism meeting,* "Memory kernel for time correlation function in complex quantum systems", Fudan, Shanghai, Dec. 2024
25. *Computational Physics Frontier,* "Nonadiabatic dynamics with strong light-matter interactions", USTC, Hefei, Nov. 2024
26. *Statmech meeting,* "Nonadiabatic dynamics with nuclear quantum effects near metal surfaces", NYU shanghai, Nov. 2024
27. *11th Triennial Congress of the International Society for Theoretical Chemical Physics (ISTCP)*, "Floquet non-adiabatic dynamics for strong light-matter interactions near metal surfaces", Qingdao, Oct. 2024
28. *Qchem workshop at 11th Triennial Congress of the International Society for Theoretical Chemical Physics*, "Stochastic CC2 for large systems: ground state and excited state properties", Qingdao, Oct. 2024
29. *Domcke Symposium: Dynamics, Spectroscopy, Machine Learning,* "Memory kernel for time correlation function in complex quantum systems", Hangzhou, Oct. 2024
30. *Chemical physics frontier*, "Memory kernel for time correlation function in complex quantum systems", Hefei, Aug. 2024
31. *National conference for theoretical and computational chemistry*, "Floquet nonadiabatic dynamics for strong light-matter interactions", Changchun, July 2024
32. *NYU Shanghai*, "Excited-state electronic structure theory and non-adiabatic dynamics in complex systems", May 2024
33. *University of Science and Technology of China*, "Nonadiabatic Dynamics with Strong Light-Matter Interactions: Floquet Frictional Effects, Lorentz-Like Forces, and Spin Manipulation", Suzhou, Mar. 2024
34. *Shenzhen Bay Lab*, "Nonadiabatic dynamics and electronic structure theory for strong light-matter interactions", Shenzhen, Dec. 2023
35. *Electronic structure theory and dynamics workshop*, "Stochastic CC2 theory for large systems: ground state and excited state properties", Beijing, Dec. 2023
36. *Chinese Physical Society Statmech meeting*, "Quantum thermodynamics in the strong coupling regimes", Kunming, July. 2023
37. *Beijing Normal University,* "Chiral induced spin selectivity: theory and challenges", Beijing, Aug. 2023
38. *Chinese Chemistry Society Meeting,* "Nonadiabatic dynamics of strong light-matter interactions", Qingdao, June 2023
39. *Electronic structure theory workshop*, "Stochastic CC2 theory for large systems: ground state and excited state properties", Changchun, April 2023
40. *University of Science and Technology of China*, "Nonadiabatic dynamics and electronic structure theory for strong light-matter interactions", Hefei, April 2023

41. *Beijing Normal University,* "Nonadiabatic dynamics of strong light-matter interactions", Beijing, Dec. 2022
42. *Statmech meeting*, "Nonadiabatic dynamics of strong light-matter interactions", *Xiamen,* Nov. 2022
43. *University of Massachusetts Amherst*, "Strong light-matter interactions at metal surfaces and inside an optical cavity", online, March 2022
44. *Zhejiang University*, "Strong light-matter interactions at metal surfaces and inside an optical cavity", Hangzhou, June 2022
45. *Zhejiang Normal University*, "Quantum thermodynamics in the strong coupling regimes", November 2021
46. *Spectroscopy workshop,* "Excited states nonadiabatic dynamics and electronic structure", Hangzhou, October 2021
47. *Huazhong University of Science and Technology* "Excited states nonadiabatic dynamics and electronic structure", Wuhan, July 2021
48. *Strong correlation and topology Workshop,* "Many-body nonadiabatic dynamics and electronic structure theory as applied to chemisorption and photochemistry", Wuhan, July 2021
49. *Hangzhou Dianzi University*, "Excited states nonadiabatic dynamics and electronic structure: Theory and Applications to electrochemistry, photochemistry, and nanomaterials", Hangzhou, July 2021
50. *Tsinghua University*, "Excited states nonadiabatic dynamics and electronic structure: Theory and Applications to electrochemistry, photochemistry, and nanomaterials", Beijing, March 2021
51. *Zhejiang University,* "Many-body nonadiabatic dynamics and electronic structure theory as applied to chemisorption and photochemistry", Hangzhou, March 2021
52. *C2SEPEM at UC Berkeley*, "Time-dependent second-order Green's function for excited-state electronic structure", Berkeley*,* March 2021
53. *Westlake University*, "Many-body nonadiabatic dynamics and electronic structure theory as applied to chemisorption and photochemistry", Hangzhou, March 2021
54. *Fifth Edition of Catalysis and Chemical Engineering*, "Nonadiabatic electron transfer near metal surfaces", San Francisco, February 2021
55. *Physical Chemistry Seminar at Penn state* "Many-body nonadiabatic dynamics and electronic structure theory as applied to chemisorption and photochemistry", College Park*,* December 2019
56. *C2SEPEM Scientific Advisory Board Meeting*, "Stochastic Resolution of Identity to Imaginary and Real-Time Second-Order Green's Function: Ground-State and Quasi-Particle Properties", Berkeley*,* November 2019
57. *American Chemical Society (ACS) Meeting*, "Beyond Born-Oppenheimer dynamics at metal surfaces", Orlando, March 2019
58. *American Physical Society (APS) Meeting*, "Nonadiabatic dynamics at metal surfaces: Surface hopping and electronic friction", Boston, March 2019
59. *Theoretical Chemistry Seminar at UC Berkeley* "Nonadiabatic dynamics at metal surfaces: Surface hopping and electronic friction", Berkeley, September 2018
60. *Electronic Structure and Penn conference in theoretical chemistry,* "Nonadiabatic dynamics at molecule-metal interfaces", Philadelphia, June 2018

Contributed Talks

1. *Pacifichem meeting*, “Memory kernel coupling theory: exact quantum dynamics for complex systems”, Hawaii, Dec. 2025 (upcoming)
2. *Workshop on ab initio theory from molecules to materials*, “Stochastic approach to CC2 theory for very large systems”, Beijing, July 2025
3. *ACS meeting*, “Non-adiabatic dynamics of light-matter interactions: Floquet engineering and plasmonic cavity”, New Orleans, Mar. 2024
4. *Chinese Chemistry Society Meeting*, “Nonadiabatic dynamics at metal surfaces: surface hopping vs electronic friction”, Zhuhai, April 2021

Mentoring and Students

Current members

Chongxiao Zhao (fifth year PhD student)
Yunhao Liu (fourth year PhD student)
Wei Liu (fourth year PhD student)
Ruihao Bi (fourth year PhD student)
Jiayue Han (third year PhD student)
Yufei Bu (second year graduate student)
Ruixin Sun (first year graduate student)
Mingyu Xia (first year graduate student)
Vahid Mosallanejad (Research assistant professor/Postdoc)
Yongtao Ma (Research assistant professor/Postdoc)

Student awards and grants

Wei Liu (National scholarship)
Chongxiao Zhao (Student award at the ACS COMP Virtual Asia-Pacific Graduate students symposium)
Vahid Mosallanejad (Wenzhou Fund, 200,000RMB, Zhejiang Province)
Yu Wang (NSFC, 250,000RMB, Youth program)
Ruihao Bi (National scholarship; Best poster award at *ISTCP-2024*)

Past members

Dr. Yu Wang (Postdoc, now associate professor at Hebei University of Technology)
Dr. Jingqi Chen (PhD student, now at Tongkuai Optics Co.)
Yangzhou Xia (undergraduate research student, now PhD student at UC Berkeley)
Kaiyi Tong (undergraduate research student, now PhD student at UNC, Chapel Hill)
Guangming Liu (graduate student, now PhD student at University of Notre Dame)
Jiaqi Han (graduate student, now PhD student at Westlake University)
Kaiwen Yang (undergraduate research student, now PhD student at Rice)
Chunyu Yang (undergraduate research student, now PhD student at Duke)
Yang Xu (undergraduate research student, now PhD student at Shenzhen Bay Lab)
Chengcheng Yu (undergraduate research student, now PhD student at USTC)
Yiran Cai (undergraduate research student, now undergraduate at UCL)

Service

School service

- Faculty searching committee (2021-2024)
- Graduate study committee (2024-)
- Colloquium committee (2021-)
- Curriculum committee (2021-2024)
- HPC advisory board at Westlake (2021-)
- Design college entrance exam for Westlake University (2025)

External service

- Journal Service
  1. Early Career Advisory Board for *Chemical Reviews*
  2. Reviewer for Scientific journals: *PRL, JCP, JCTC, PRB, PRA, PRE, PRR, PRX quantum, Nano Letter, Nature Comm., JPCL, JPCA, JPCC*
- Grant and proposal Review
  1. *Ad hoc* Review for NSFC grants: General program, Youth program
  2. Panel review for NSFC: Excellent youth program, Key research and development program (panel review, mid-term, and final), Major program
  3. *Ad hoc* Review for Chinese Academy of Science: Representative annual achievements of the research institutes in CAS
  4. Panel review for Chinese Academy of Science: Strategy priority research program (category B and category C)
  5. *Ad hoc* Review for Ministry of Education: Institutes applying for granting chemistry doctoral degrees
- ACS member (COMP and PHYS division member) and *Chinese Chemical Society* (CCS) member
  1. Early career member, theoretical chemistry committee, *Chinese Chemical Society*
  2. Organizer and Chair, ACS COMP Virtual Asia-Pacific Graduate students symposium (Fall 2022, Fall 2023, Spring 2024)
  3. Organizer, Electronic structure theory symposium, *Chinese Chemistry Society Meeting* 2026