Pengfei Huo

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Appointments

2022-Present Associate Professor, Department of Chemistry, University of Rochester
2022-Present Associate Professor, Institute of Optics, Hajim School of Engineering, University of Rochester
2020-2022 Assistant Professor, Institute of Optics, Hajim School of Engineering, University of Rochester
2016-2022 Assistant Professor, Department of Chemistry, University of Rochester
2015-2016 Research Assistant Professor, Department of Chemistry, University of Rochester

Professional Preparation

California Institute of Technology	Theoretical Chemistry	Postdoc. 2012-2015
Boston University	Theoretical Chemistry	Ph.D. 2011
Boston University	Chemistry	M.A. 2009
Lanzhou University	Chemistry	B.S. 2007

Honors and Awards

- Hirschfelder Visiting Scholar, University of Wisconsin, Madison, 2023
- University Research Awards, University of Rochester, 2021
- ACS Petroleum Research Fund Outstanding Reviewer, 2021
- OpenEye Outstanding Junior Faculty Award in Computational Chemistry, ACS, 2020
- Cottrell Scholar, Research Corporation for Science Advancement, 2020
- J. Phys. Chem. Young Scientist, ACS, 2019
- National Science Foundation CAREER award, 2018
- National Science Foundation CHE Workshop Travel Award, 2017
- J. Phys. Chem. Lett top 5% reviewer, 2016
- PHYS Division Postdoctoral Research Awards (Young Investigator Award), 2014
- J. Chem. Phys top 20 reviewer, 2012
- Sugata Ray Memorial Award for International Students, Boston University, 2010
- National Science Foundation (NSF) travel fellowships, 2010

Current Support

1. National Science Foundation, CHE-2244683, "Quantum Dynamics Approaches to Simulate Polariton Photochemistry". PI, Total award amount: $490,637. Award period: 04/01/2023-01/31/2026.
2. Air Force Office of Scientific Research, FA9550-23-1-0438, "Ab-initio Quantum Electrodynamics Approaches to Investigate Polariton Chemistry in the Collective Coupling Regime". PI, Total award amount: $501,160 Award period: 08/01/2023-07/31/2026.
3. National Science Foundation, OAC-2311442, "Elements: An Integrated Software Platform for Simulating Polariton Photochemical and Photophysical Processes", Co-PI (PI: Yihan Shao) , Total award amount: $599,597 (sub-award to Huo: $287,458), Award period: 7/01/2023-06/30/2026.
4. National Science Foundation, CHE-2124398, "CCI Phase I: NSF Center for Quantum Electrodynamics for Selective Transformations". Co-PI (PI: Todd Krauss), Total award amount: $1,800,000 (level of support: 1.5 students/year). Award period: 09/01/2021-08/31/2024

5. Department of Energy, DE-SC0022171, "UNLOQ: Understanding coherence in Light-matter interfaces fOr Quantum science", Co-PI (PI: Todd Krauss), Total award amount: $2,205,694 (level of support: 2 students/year). Award period: 09/01/2021-08/31/2025 (no cost extension).

Previous Support

1. National Science Foundation, CHE-1845747, "CAREER: Quantum Dynamics of Photochemical Reactions in Solar Energy Conversions". PI, Total award amount: $649,968. Award period: 12/15/2018-11/30/2023
2. National Science Foundation, CHE-1836546, "QLC: EAGER: New Chemical Reactivity Enabled by Cavity Quantum Electrodynamics". PI, Total award amount: $295,095. Award period: 07/17/2018-06/30/2021
3. University Research Awards, U of Rochester, "Investigating Polariton Mediated Electron Transfer Reactions", PI (Co-PI: Todd Krauss and Nick Vamivakas), Total award amount: $57,500. Award period: 07/01/2021-07/30/2022
4. Research Corporation for Science Advancement, Cottrell Scholar Award, "Enabling New Chemical Reactivities Through Polariton Photochemistry". PI, Total award amount: $100,000. Award period: 07/01/2020-06/30/2023
5. National Science Foundation, CHE-1900125, "Collaborative Research: Investigating Photoinduced Charge Transfer Dynamics Across Molecule-Nanocrystal Interfaces". Co-PI, (PI: David McCamant) Total award amount: $416,000. Award period: 08/15/2019-07/31/2023.

Publications

(∗ indicates the corresponding author)

42. B. M. Weight, D. Weix, Z. Tonzetich, T.D. Krauss, and **P. Huo**∗, "Cavity Quantum Electrodynamics Enables para- and ortho- Bromination of Nitrobenzene", preprint: 10.26434/chemrxiv-2023-l0lwk (**2024**).
41. M. A. D. Taylor, B. M. Weight, and **P. Huo**∗, "Reciprocal Asymptotically Decoupled Hamiltonian for Cavity Quantum Electrodynamics", Phys. Rev. B, *submitted* preprint: arXiv:2311.08531v1 (**2024**).
40. W. Ying, M. A.D. Taylor, and **P. Huo**∗, "Resonance Theory of Vibrational Polariton Chemistry at the Normal Incidence" (**invited Article**), Nanophotonics, preprint:10.26434/chemrxiv-2023-3chzx (**2024**).
39. W. Ying, D. Hu, and **P. Huo**∗, "Resonance Enhancement of Vibrational Polariton Chemistry Obtained from the Mixed Quantum Classical Dynamics Simulations", J. Phys. Chem. Lett. 14, 11208-11216 (**2023**)
38. M. E. Mondal, E. Koessler, J. Provazza, A. Vamivakas, S. Cundiff, T. D. Krauss, and **P. Huo**∗, "Quantum Dynamics Simulations of the 2D Spectroscopy for Exciton Polaritons", J. Chem. Phys. 159, 094102 (**2023**)
37. W. Ying, **P. Huo**∗, Resonance Theory and Quantum Dynamics Simulations of Vibrational Polariton Chemistry, J. Chem. Phys. 159, 084104 (**2023**).
35. A. Mandal, M. A. D. Taylor, B. M. Weight, E. R. Koessler, X. Li, and **P. Huo**∗, "Theoretical Advances in Polariton Chemistry and Molecular Cavity Quantum Electrodynamics" (**invited Review** for the Polariton Chemistry Theme Issue, selected for a supplementary journal cover), Chem. Rev. 123, 16, 9786-9879 (**2023**).
34. D. L. Bossion, W. Ying, S.N. Chowdhury, and **P. Huo**∗, "Erratum: "Non-adiabatic mapping dynamics in the phase space of the $SU(N)$ Lie group" [J. Chem. Phys. 157, 084105 (2022)]", J. Chem. Phys. 159, 029901 (**2023**).

33. A. Mandal, M. A. D. Taylor, and **P. Huo***, "Theory for Cavity Modified Ground-State Reactivities via Electron-Photon Interactions", (**invited Article** in *Early-Career and Emerging Researchers in Physical Chemistry*, selected for a journal cover), J. Phys. Chem. A. 127, 6830-6841 (**2023**).
32. B. M. Weight, T.D. Krauss, and **P. Huo***, "Investigating Molecular Exciton Polaritons Using Ab Initio Cavity Quantum Electrodynamics", J. Phys. Chem. Lett. 14, 5901-5913 (**2023**).
31. D. Hu and **P. Huo***, "Ab Initio Molecular Cavity Quantum Electrodynamics Simulations Using Machine Learning Models" J. Chem. Theory Comput. 8, 2353-2368 (**2023**).
30. D. L. Bossion, S.N. Chowdhury, and **P. Huo*** "Non-adiabatic Ring Polymer Molecular dynamics in the Phase Space of the $SU(N)$ Lie Group", J. Chem. Phys. 158, 044123 (**2023**).
29. D. Hu, A. Mandal, B. M. Weight, and **P. Huo***, "Quasi-Diabatic Propagation Scheme for Simulating Polariton Chemistry", J. Chem. Phys. 157, 194109 (**2022**).
28. W. Zhou, D. Hu, A. Mandal and **P. Huo***, "Nuclear Gradient expressions for Molecular Cavity Quantum Electrodynamics Simulations using Mixed Quantum-Classical Methods", J. Chem. Phys. 157, 104118 (**2022**).
27. D. L. 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. 157, 084105 (**2022**).
26. E. R. Koessler, A. Mandal, and **P. Huo***, "Incorporating Lindblad decay dynamics into mixed quantum-classical simulations", J. Chem. Phys. 157, 064101 (**2022**).
25. M. A. D. Taylor, A. Mandal, and **P. Huo***, "Resolving ambiguities of the mode truncation in cavity quantum electrodynamics", Optics Lett. 47, 1446 (**2022**).
24. A. Mandal, X. Li, and **P. Huo***, "Theory of Vibrational Polariton Chemistry in the Collective Coupling Regime", (Invited article for the J. Chem. Phys."Emerging Investigator" Special Issue) J. Chem. Phys. 156, 014101 (**2022**).
23. B. M. Weight, A. Mandal, and **P. Huo***, "Ab-initio Symmetric Quasi-Classical Approach to Investigate Molecular Tully Models", J. Chem. Phys. 155, 084106 (**2021**).
22. M. H. Farag, A. Mandal and **P. Huo***, "Polariton Induced Conical Intersection and Berry Phase", Phys. Chem. Chem. Phys. 23, 16868-16879 (**2021**).
21. X. Li, A. Mandal, and **P. Huo***, "Theory of Mode-Selective Chemistry through Polaritonic Vibrational Strong Coupling", J. Phys. Chem. Lett. 12, 6974-6982 (**2021**).
20. X. Li and **P. Huo***, "Investigating Tunneling Controlled Chemical Reactions Through ab-initio Ring Polymer Molecular Dynamics", (selected for a supplementary journal cover), J. Phys. Chem. Lett. 12, 6714-6721(**2021**).
19. L. Qiu, A. Mandal, O. Morshed, M. T. Meidenbauer, W. Girten, **P. Huo***, A. N. Vamivakas* and T. D. Krauss*, "Molecular Polaritons Generated from Strong Coupling between CdSe Nanoplatelets and a Dielectric Optical Cavity" (selected for a supplementary journal cover), J. Phys. Chem. Lett. 12, 5030 (**2021**).
18. D. Bossion, S. Chowdhury and **P. Huo***, "Non-Adiabatic Ring Polymer Molecular Dynamics with Spin Mapping Variables", J. Chem. Phys. J. Chem. Phys. 154, 124124 (**2021**).
17. S. Chowdhury and **P. Huo***, "Non-adiabatic Matsubara Dynamics and Non-adiabatic Ring Polymer Molecular Dynamics". (Invited article for the J. Chem. Phys. "Emerging Investigator" Special Issue) J. Chem. Phys. 154, 124124 (**2021**).
16. X. Li, A. Mandal* and **P. Huo***, "Cavity Frequency-Dependent Theory for Vibrational Polariton Chemistry", (selected for Editors' Highlights) Nat. Comm.12, 1315 (**2021**).
15. S. Chowdhury, A. Mandal, and **P. Huo***, "Ring-Polymer Quantization of Photon Field in Polariton Chemistry", J. Chem. Phys. 154, 044109 (Invited article for the J. Chem. Phys. "Polariton Chemistry" Special Issue) (**2021**).
14. S. S. Yamijala and **P. Huo***, "Direct Non-adiabatic Simulations of the Photoinduced Charge Transfer Dynamics", J. Phys. Chem. A, 125, 628-635 (Invited article for the "Josef Michl Festschrift") (**2021**).

13. A. Mandal*, **S. M. Vega**† and **P. Huo***, "Polarized Fock States and the Dynamical Casimir Effect in Molecular Cavity Quantum Electrodynamics", (selected for a supplementary journal cover) J. Phys. Chem. Lett. 11, 9215 (**2020**).
12. M. A. D. Taylor†, A. Mandal, W. Zhou and **P. Huo***,"Resolution of Gauge Ambiguities in Molecular Cavity Quantum Electrodynamics", Phys. Rev. Lett. 125, 123602 (**2020**).
11. A. Mandal*, T. D. Krauss* and **P. Huo***, "Polariton Mediated Electron Transfer via Cavity Quantum Electrodynamics" J. Phys. Chem. B. 124, 6321-6340 (**2020**).
10. W. Zhou, A. Mandal and **P. Huo***, "Quasi-Diabatic Scheme for Non-adiabatic On-the-fly Simulation", J. Phys. Chem. Lett. 10, 7062 (**2019**).
9. A. Mandal and **P. Huo***, "Investigating New Reactivities Enabled by Polariton Photochemistry", (Highlighted as the most highly cited articles in 2019 and 2020, selected as part of the Polaritons in Physical Chemistry virtual issue) J. Phys. Chem. Lett. 10, 5519-5529 (**2019**).
8. S. Chowdhury and **P. Huo***, "State Dependent Ring Polymer Molecular Dynamics for Investigating Excited Nonadiabatic Dynamics", J. Chem. Phys. 150, 244102 (Invited article for the "Dynamics of Open Quantum Systems" Special Issue). (**2019**).
7. A. Mandal, J. S. Sandoval, F. A. Shakib* and **P. Huo***, "Quasi Diabatic Propagation Scheme for Direct Simulation of Proton-Coupled Electron Transfer Reaction", J. Phys. Chem. A 123, 2470, (Invited article for the "Young Scientists" Special Issue) (**2019**).
6. J. S. Sandoval, A. Mandal and **P. Huo***, "Symmetric Quasi Classical Dynamics with Quasi Diabatic Propagation Scheme", J. Chem. Phys. 149, 044115 (**2018**).
5. A. Mandal, F. A. Shakib* and **P. Huo***, "Investigating Photoinduced Proton Coupled Electron Transfer Reaction using Quasi Diabatic Dynamics Propagation", J. Chem. Phys. 148, 244102 (**2018**).
4. A. Mandal, S. S. Yamijala, and **P. Huo***, "Quasi-Diabatic Representation for Non-Adiabatic Quantum Dynamics Propagation", J. Chem. Theory Comput. 14, 1828 (**2018**).
3. S. Chowdhury and **P. Huo***, "Coherent State Mapping Ring-Polymer Molecular Dynamics for Non-Adiabatic Quantum Propagations", J. Chem. Phys. 147, 214109 (**2017**).
2. F. A. Shakib* and **P. Huo***, "Ring Polymer Surface-Hopping: Incorporating Nuclear Quantum Effects Into Non-Adiabatic Molecular Dynamics Simulations", J. Phys. Chem. Lett. 8, 3073 (**2017**).
1. M. Castellanos† and **P. Huo***, "Enhancing Singlet-Fission Dynamics by Suppressing Destructive Interference between Charge-Transfer Pathways", J. Phys. Chem. Lett. 8, 2480 (**2017**).

Selected Publications

- A. Mandal, M. A. D. Taylor, B. M. Weight, E. R. Koessler, X. Li, and **P. Huo***, "Theoretical Advances in Polariton Chemistry and Molecular Cavity Quantum Electrodynamics", Chem. Rev. 123, 16, 9786-9879 (**2023**).
- W. Ying, **P. Huo***, Resonance Theory and Quantum Dynamics Simulations of Vibrational Polariton Chemistry, J. Chem. Phys. 159, 084104 (**2023**).
- D. L. Bossion, S.N. Chowdhury, and **P. Huo*** "Non-adiabatic Ring Polymer Molecular dynamics in the Phase Space of the $SU(N)$ Lie Group", J. Chem. Phys. 158, 044123 (**2023**).
- M. A. D. Taylor, A. Mandal, W. Zhou and **P. Huo***,"Resolution of Gauge Ambiguities in Molecular Cavity Quantum Electrodynamics", Phys. Rev. Lett. 125, 123602 (**2020**).
- S. Chowdhury and **P. Huo***, "Non-adiabatic Matsubara Dynamics and Non-adiabatic Ring Polymer Molecular Dynamics". J. Chem. Phys. 154, 124124 (**2021**).
- X. Li, A. Mandal* and **P. Huo***, "Cavity Frequency-Dependent Theory for Vibrational Polariton Chemistry", Nat. Comm.12, 1315 (**2021**).
- A. Mandal*, S. M. Vega, and **P. Huo***, "Polarized Fock States and the Dynamical Casimir Effect in Molecular Cavity Quantum Electrodynamics", J. Phys. Chem. Lett. 11, 9215 (**2020**).

- W. Zhou, A. Mandal and **P. Huo***, "Quasi-Diabatic Scheme for Non-adiabatic On-the-fly Simulation", J. Phys. Chem. Lett. 10, 7062 (**2019**).
- A. Mandal and **P. Huo***, "Investigating New Reactivities Enabled by Polariton Photochemistry", J. Phys. Chem. Lett. 10, 5519-5529 (**2019**).

Previous Publications

12. **P. Huo**, C. Uyeda, J. D. Goodpaster, J. C. Peters, and T. F. Miller*, "Breaking the Correlation between Energy Costs and Kinetic Barriers in Hydrogen Evolution via a Cobalt Pyridine-Diimine-Dioxime Catalyst", ACS Catal. 6, 6114 (**2016**).
11. M. Lee, **P. Huo*** and D.F. Coker*, "Semi-classical Path Integral Dynamics: Photosynthetic Energy Transfer with Realistic Environment Interactions", Ann. Rev. Phys. Chem. 67, 27 (**2016**).
10. **P. Huo** and T. F. Miller*, "Electronic Coherence and the Kinetics of Inter-complex Energy Transfer in Light-harvesting Systems", Phys. Chem. Chem. Phys. 17, 30914 (**2015**).
9. **P. Huo***, T. F. Miller* and D.F. Coker*, "Communication: Predictive Partial Linearized Path Integral Simulation of Condensed Phase Electron Transfer Dynamics", J. Chem. Phys. 139, 151103 (**2013**).
8. **P. Huo** and D.F. Coker*, "Consistent schemes for non-adiabatic dynamics derived from partial linearized density matrix propagation", (Special Issue on Non-adiabatic dynamics inspired by John Tully) J. Chem. Phys. 137, 22A535 (**2012**).
7. **P. Huo** and D.F. Coker*, "Semi-classical path integral non-adiabatic dynamics: a partial linearized classical mapping Hamiltonian approach", (William H. Miller Festschrift) Mol. Phys. 110, 1035 (**2012**).
6. **P. Huo** and D.F. Coker*, "Influence of environment-induced correlated fluctuations in electronic coupling on coherent excitation energy transfer dynamics in model photosynthetic systems, J. Chem. Phys. 136, 115102 (**2012**).
5. **P. Huo** and D.F. Coker*, "Communication: Partial linearized density matrix dynamics for dissipative, non-adiabatic quantum evolution", J. Chem. Phys. 135, 201101 (**2011**).
4. J. Moix, J. Wu, **P. Huo**, D.F. Coker* and J.Cao*, "Efficient energy transfer in light-harvesting systems, III: The influence of the eighth bacteriochlorophyll on the dynamics and efficiency in FMO, J. Phys. Chem. Lett. 2, 3045 (**2011**).
3. **P. Huo** and D.F. Coker*, "Theoretical Study of Coherent Exciton Transfer in Cryptophyte Phycocyanin 645 at Physiological Temperature, J. Phys. Chem. Lett. 2, 825 (**2011**).
2. **P. Huo** and D.F. Coker*, "Iterative linearized density matrix propagation for modeling coherent excitation energy transfer in photosynthetic light harvesting, J. Chem. Phys. 133, 184108 (**2010**).
1. **P. Huo**, S. Bonella, L. Chen and D. F. Coker*, "Linearized approximations for condensed phase non-adiabatic dynamics: Multi-layered baths and Brownian dynamics implementation (Eli Pollak Festschrift), Chem. Phys. 370, 87 (**2010**).

Invited Presentations and Symposia

75. June 16, 2024, American Conference on Theoretical Chemistry, Chapel Hill, NC
74. March 17th-21st, 2024 ACS New Orleans, LA
73. February 25, 2024, The 63rd Sanibel Symposium, St. Augustine Beach, FL
72. December 1st, 2023, CUNY workshop: New Frontiers of quantum chemistry/dynamics theories and simulation methods, Graduate Center, CUNY, New York, NY
71. November 2nd, 2023, Department of Chemistry, NYU Shanghai (Virtual)
70. October 26th, 2023, Department of Chemistry, University of Notre Dame, Notre Dame, IN
69. October 16th, 2023, Department of Chemistry, University of Southern California, Los Angeles, CA
68. September 15th, 2023, Department of Chemistry, University of Missouri-Columbia, Columbia, MO

67. June 2023, The Strong Coupling of Organic Molecules (SCOM) 2023, San Diego, CA
66. June 2023, Telluride workshop on "Polariton Chemistry and Molecular Cavity Quantum Electrodynamics", Telluride, CO
65. April 19th, 2023, Center for Photochemical Sciences, Bowling Green State University, OH
64. March 2023, ACS meeting, Indianapolis, Peter G. Wolynes 70th Birthday Symposium, Indianapolis, ID
63. March 2023, ACS meeting, Indianapolis, the symposium on multi-dimensional spectroscopy, Indianapolis, ID
61. March 21st, 2023, Department of Chemistry and Theoretical Chemistry Institute, University of Wisconsin, Madison, WI
60. February 17th, 2023, Department of Chemistry, Dalhousie University, Nova Scotia, Canada
59. July 2022, Telluride workshop on "Condensed Phase Dynamics", Telluride, CO
58. June 2022, CECAM workshop on"Local vs Collective Interactions in Polaritonic Chemistry", Bordeaux, France
57. May 12, 2022, Department of Chemistry, University of Texas, Austin, Texas
56. May 3, 2022, Department of Chemistry, Rutgers University, New Brunswick, New Jersey
55. April 27, 2022, Laboratory for Laser Energetics, University of Rochester, Rochester, NY
54. March 30, 2022, Department of Chemistry, Princeton University, Princeton, New Jersey
53. Mar 20-24, 2022, Symposium on "Molecular Polaritons", 2022 ACS meeting, San Diego, CA
52. January 19, 2022, Department of Chemistry, University of Warwick, United Kingdom (Virtual)
51. October 22, 2021, Department of Chemistry, University of South Carolina, Columbia, South Carolina
50. October 6, 2021, Theory Seminar Series on "Theory and Simulation of Electronic and Optical Processes in Molecules and Materials" (virtual)
49. September 29, 2021, Pitzer Center Theory Seminar, Department of Chemistry, University of California, Berkeley (virtual)
48. Sep 23, 2021, Department of Chemistry, University of Pennsylvania, Philadelphia, PA (virtual)
47. Sep 13-17, 2021, VI International Conference on Metamaterials and Nanophotonics (virtual)
46. July 2021, Telluride workshop on "Nonequilibrium Phenomena, Nonadiabatic Dynamics and Spectroscopy" , Telluride, CO
45. June 2021, Telluride Workshop on "Quantum Effects in Condensed-Phase Systems", Telluride, CO
44. Jun 08, 2021, Department of Chemistry, University of California, San Diego (virtual)
43. May 18, 2021, Department of Chemistry, Columbia University (virtual)
42. May 14, 2021, Department of Chemistry, Virginia Polytechnic Institute and State University (virtual)
41. May 04, 2021, Department of Chemistry, University of California, Irvine (virtual)
40. May 03, Department of Chemistry, Boston University (virtual)
39. Apr 27, 2021, Division of Chemistry and Chemical Engineering, California Institute of Technology (virtual)
38. Apr 22, 2021, Department of Chemistry and Biochemistry, Cornell University (virtual)
37. Apr 14, 2021 "Bill Hase Memory Symposium", 2021 ACS (virtual)
36. Apr 13, 2021, Department of Chemistry, University of Toronto (virtual)
35. Apr 08, 2021, "Don Kouri Memory Symposium", 2021 ACS (virtual)
34. Apr 08, 2021, Department of Chemistry, University of Michigan (virtual)
33. Apr 06, 2021, Department of Chemistry, Duke University (virtual)

32. Mar 30, 2021, Department of Chemistry, Massachusetts Institute of Technology (virtual)
31. Mar 19, 2021, CUNY workshop on "Quantum Dynamics of Excitons and Exciton-Light Interactions", The Graduate Center at CUNY, New York, NY (virtual)
30. Mar 08, 2021, Department of Chemistry, Northwestern University (virtual)
29. Mar 02, 2021, Department of Chemistry, New York University (virtual)
28. Feb 10, 2021, Department of Chemistry, University of Illinois Urbana-Champaign (virtual)
27. September 2020, Polariton Chemistry Webinar (virtual)
26. August 2020, Pitzer Center Theory Seminar, Department of Chemistry, University of California, Berkeley (virtual)
25. August 2020, Symposium on "OpenEye Outstanding Junior Faculty Award in Computational Chemistry", ACS 2020 (virtual)
24. July 2020, Telluride Workshop on "Quantum Frontiers in Molecular Science" (virtual)
23. December 2019, Los Alamos National Laboratory, Los Alamos, NM
22. October 2019, Symposium on "Recent Advances in Electron and Proton Transfer Theories', The Graduate Center at CUNY, New York, NY
21. October 2019, Department of Chemistry, Colgate University, Hamilton, NY
20. July 2019, Telluride Workshop on "Quantum Effects in Condensed-Phase Systems", Telluride, CO
19. July 2019, Telluride workshop on "Nonequilibrium Phenomena, Nonadiabatic Dynamics and Spectroscopy" , Telluride, CO
18. June 2019, 102nd Canadian Chemistry Conference and Exhibition, Quebec City, Canada
17. May 2019, Great Boston Area Theoretical Chemistry Lecture, Boston, MA
16. April 2019, Symposium on" Non-adiabatic dynamics in dense manifolds of states", ACS 257th National Meeting, Orlando, FL
15. July 2018, CECAM workshop on "Non-adiabatic quantum dynamics: From Theory to Experiments", Lausanne, Switzerland
14. June 2018, Telluride workshop on "Quantum Frontiers in Molecular Science Workshop", Telluride, CO
13. June 2018, NSF MolSSI Workshop on Modular Software Infrastructure for Excited State Dynamics, Buffalo, NY
12. June 2017, "Enhancing singlet-fission dynamics by suppressing destructive interference between charge-transfer pathways", Singlet Fission Workshop, Lyons, CO
11. June 2017, 45th Middle Atlantic Regional Meeting (MARM 2017), Hershey, PA
10. July 2016, Telluride workshop on "Charge and Energy Transfer in Photoreactions and Photodynamics", Telluride, CO
9. March 2016, Department of Chemistry, Boston University, Boston, MA
8. Jan 2015, Department of Chemistry, Michigan State University, East Lansing, MI
7. Dec 2014, Department of Chemistry, University of Rochester, Rochester, NY
6. Dec 2014, Department of Chemistry, California State University, Northridge, CA
5. Nov 2014, Department of Chemistry, Virginia Polytechnic Institute and State University, Blacksburg, VA
4. Oct 2014, Department of Chemistry, University of Houston, Houston, TX
3. Oct 2014, "New theoretical approaches to simulate exciton transfer, charge separation, and proton reduction", Notre Dame Radiation Laboratory, Notre Dame, IN
2. Aug 2014, "Intra-molecular proton transfer and hydrogen generation in cobalt catalyst", invited talk, 284th ACS meeting, San Francisco, CA

1. Aug 2013, "Predictive approach to calculate the rate constant in condense phase reactions", "Summer School on Mathematical and Computational Methods in Quantum Dynamics" Madison, WI

Other Oral Presentations and Posters

25. August 2023, "Ab-initio Quantum Electrodynamics Approaches to Investigate Polariton Photochemistry", Poster, Quantum Control of Light and Matter Gordon Research Conference, New Port, RI
24. March 2023, "Resolution of Gauge Ambiguities in Molecular Cavity Quantum Electrodynamics", 2023 Spring APS, Las Vegas, NV
23. August 2022, "Theory of vibrational Strong coupling in polariton chemistry", Poster, Electron Donor-Acceptor Gordon Research Conference, New Port, RI
22. August 2019, "Investigating New Reactivities Enabled by Polariton Photochemistry", Poster, Quantum Control Gordon Research Conference, New Port, RI
21. August 2018, "Quasi-diabatic representation for nonadiabatic dynamics propagation", ACS 256th National Meeting, Boston, MA
20. August 2018, "Enhancing singlet-fission dynamics by suppressing destructive interference between charge-transfer pathways", ACS 256th National Meeting, Boston, MA
19. August 2018, "Investigating photoinduced proton-coupled electron transfer reaction using quasi diabatic propagation", ACS 256th National Meeting, Boston, MA
18. August 2018, "New theoretical approaches for investigating new photochemical reactivities", Poster, Donor-acceptor Gordon Conference, New Port, RI
17. June 2018, "Investigating Photoinduced Proton Coupled Electron Transfer Reaction using Quasi Diabatic Dynamics Propagation", Poster, 3rd International Conference on Proton Coupled Electron Transfer, Blowing Rock, NC (*Best Poster award*)
16. March 2018, "Quasi Diabatic Representation for Nonadiabatic Quantum Dynamics Propagation", APS March Meeting, Los Angeles, CA
15. March 2018, "Charge transfer and singlet fission quantum dynamics in organic photovoltaic", APS March Meeting, Los Angeles, CA
14. April 2017, "Understanding the quantum dynamics of photosynthetic energy transfer with realistic environment interactions", ACS 253rd National Meeting, San Francisco, CA
13. April 2017, "Charge transfer and singlet fission quantum dynamics in organic photovoltaic", ACS 253rd National Meeting, San Francisco, CA
12. April 2017, "New theoretical approaches to simulate photoinduced proton-coupled electron transfer reactions", ACS 253rd National Meeting, San Francisco, CA
11. August 2016, "Semi-classical Path-Integral Dynamics for understanding energy transfer and charge separation processes in light-harvesting systems", ACS 252nd National Meeting, Philadelphia, PA
10. August 2016, "Quantum Embedding Method to simulate proton reduction reactions in transition-metal catalysts", ACS 252nd National Meeting, Philadelphia, PA
9. July 2016, "New theoretical approaches to simulate exciton transfer, charge separation, and proton reduction", Poster, Donor-acceptor Gordon Conference, New Port, RI
8. March 2016, "Electronic coherence and the kinetics of energy transfer in light-harvesting systems", APS meeting, Baltimore, MD
7. Jan 2014, "Intra-molecular proton transfer and hydrogen generation in cobalt catalyst", poster, Mini Stat Mech Meeting, Berkley, CA
6. Apr 2012, "Consistent schemes for non-adiabatic dynamics derived from partial linearized density matrix propagation", poster, 243th ACS meeting, San Diego, CA
5. Jan 2012, "Theoretical study of coherent energy transfer in photosynthetic systems by Partial Linearized path integral approach", poster, Mini Stat Mech Meeting, Berkley, CA

4. Jan 2012, "Semi-classical path integral non-adiabatic dynamics: a partial linearized classical mapping Hamiltonian approach", poster, Quantum Molecular Dynamics: A Conference in Honor of William H. Miller, Berkley, CA
3. Aug 2011, "Partial linearized density matrix dynamics for dissipative, non-adiabatic quantum evolution", poster, ACTC meeting, Telluride, CO
2. Aug 2010, "Theoretical study of coherent energy transfer in photosynthetic systems", poster, 240th ACS meeting, Boston, MA (*Best Poster award in Physical Chemistry*)
1. May 2010, "Iterative Linearized Density Matrix Propagation Scheme, a new approach to study Coherent ExcitonTransfer in Photosynthetic systems", poster, CECAM meeting, Dublin, Ireland.

Mentees

- Postdoc Scholars: Dr. **Yifan Lai** (2022-present), Dr. **Duncan Bossion** (2019-2022, now Assistant Professor at the University of Rouen, France), Dr. **Deping Hu** (2021-2022, now Assistant Professor at the Beijing Normal University, Zhuhai, China), Dr. **Marwa Farag** (2019-2021, now Quantum Algorithm Scientist at Ford), Dr. **Farnaz Shakib**, (2016- 2018, now Assistant Professor at the New Jersey Institute of Technology), Dr. **Sharma Yamijala** (2016-2018, now Assistant Professor at the Indian Institute of Technology, Madras), Dr. **Wanghuai Zhou** (2018-2020, now Assistant Professor at Hubei University of Automotive Technology, China)
- Graduate Students: **Sutirtha Chowdhury** (2015-2021, now Scientist at Intel), **Xinyang Li** (2015-2021, now postdoc at Los Alamos National Lab), **Arkajit Mandal** (2016-2021, now postdoc at Columbia University), **Juan Sebastian Sandoval** (2016-2018, now graduate student at U of Rochester), **Wenxiang Ying** (2020-present), **Eric Koessler** (2020-present), **Mike Taylor** (2020-present), **Braden Weight** (2020-present), **Elious Mondal** (2021-present), **Benjamin Chng** (2021-present), **Sebastian Montillo** (2022-present), **Santanu Poddar** (2022-present)
- Undergraduate Students: **John Alejandro Montilla** (2023-present), **Jialong Wang** (2022-present), **Mateo Londono Castellanos** (2022, now Graduate Student at SUNY Stony Brook), **Rudin Kraja** (2022, now Graduate Student at CUNY), **Aamod Atre** (2021, now Graduate Student at the Technical University of Munich), **Matt DeLorenzo** (2020-2021), **Michael A. D. Taylor** (2019-2020, now Graduate Student at the University of Rochester), **Sebastian. M. Vega** (2019, now Graduate Student at the University of Rochester), **Shreif Abdallah** (2019, now Software Engineer at Coinbase), **Rachel Clune** (2017-2018, now Graduate Student at UC Berkeley), **Claire Dickerson** (2017-2018, now Graduate Student at UCLA), **Zak Marshall-Carter** (2017-2018, now Graduate Student at Fordham University Law School), **Alessandro Rognoni** (2017, now Graduate Student at the University of Milan), **Matthew Aquilina** (2017, now Graduate Student at the University of Cambridge), **Yoshimi Araki** (2017, now Engineer at Honda Aircraft Company) , **Maria Castellanos** (2016, now Graduate Student at MIT), **Matthew Carbone** (2015-2016, now Postdoc Scholar at Brookhaven National Laboratory)

Teaching

- Physical Chemistry II (undergraduate level): Basic principles of Statistical Mechanics, Partition functions and Boltzmann Statistics, Non-interacting quantum molecular systems, Thermodynamics Laws, Work and Heat, Free energies, phase equilibria, solutions, chemical equilibrium, and chemical kinetics.
- Quantum Mechanics (graduate level): Basic Principle of Quantum Mechanic, Superposition, Simple problems in one-dimension, The postulates of quantum mechanics, General formalism of Quantum Mechanics, Dirac Notation, Representation theory, The time-dependent Schrdinger equation and Heisenberg Equation of Motion, Schrodinger picture, Heisenberg Picture, and Interaction Picture, The Heisenberg Uncertainty Relations, Harmonic Oscillator (Raising and Lowering operator approach), Quantum Angular Momentum, The Hydrogen atom, Variational Principle, Time-independent and time-dependent perturbation theory

- Computational Chemistry (graduate level): Review of Classical Mechanics (Hamiltonian formalism, Poisson bracket, symplectic map) and Statistical Mechanics, numerical integrator (velocity Verlet), molecular dynamics simulation techniques, Monte-Carlo approach, free energy methods, basic quantum mechanics, Born-Oppenheimer approximation, variational principle, many-electron wavefunction, Hartree-Fock (HF) theory, correlated Wave Function methods, Perturbation theory, Density-Functional Theory (DFT), methods for excited states, non-adiabatic quantum dynamics.
- Statistical Mechanics (Graduate level): Review of Classical Mechanics (Hamiltonian formalism, Liouville's theorem), Ensemble theory, Non-interacting quantum systems, Bose-Einstein and Fermi-Dirac statistics, phase transitions and critical phenomena, Non-equilibrium statistical mechanics, the Green-Kubo focoupling molecular vibrations with a quantized radiation field inside an optical cavityrmalism

Additional Synergistic Activities

1. **University Activities**: **Chair**, Dept. of Chemistry Graduate Recruiting Committee (2022-present); Dept. of Chemistry Graduate Recruiting Committee (2015-present); Dept. of Chemistry Graduate Study Committee (2016-present); Dept. of Chemistry Faculty Recruiting Committee (2022-present); Affiliated faculty member of the *Institute of Optics*; Affiliated faculty member of *Materials Science Graduate Program*; Affiliated faculty member of the *Condensed-matter program* in the Department of Physics, Affiliated faculty member of the *Center for Energy and Environment*;
2. **Review Panels**: National Science Foundation *ad-hoc* reviewer and review panel, Department of Energy *ad-hoc* reviewer, DOE Center for Integrated Nanotechnologies *ad-hoc* reviewer, Air Force Office of Scientific Research (AFOSR) *ad-hoc* reviewer, ACS Petroleum Research Fund (PRF) *ad-hoc* reviewer, CECAM (Centre Européen de Calcul Atomique et Moléculaire) *ad-hoc* reviewer, Canada Foundation for Innovation review panel, Israel Science Foundation (ISF) *ad-hoc* reviewer, The Cyprus Institute for high performance computing *ad-hoc* reviewer
3. **Review Journal Articles**: The Journal of Physical Chemistry letters top 5% reviewer (2016), The Journal of Chemical Physics (2012 top 20 reviewers), Journal of the American Chemical Society, Accounts of Chemical Research, Nature Chemistry, Nature Communications, Chemical Science, Proceedings of the National Academy of Sciences USA, Phys. Rev. Lett., Reviews of Modern Physics, Physical Chemistry Chemical Physics, The Journal of Physical Chemistry A, B, C, ACS Nano, Inorganic Chemistry, Applied Physics Letters, Computer Physics Communications, Optics Letters
4. **Diversity, Equity, and Inclusion Activities**: Organizer of the "Journey to the Molecular World" summer school through a collaboration with Kearns Center at the University of Rochester. Representative on behalf of the Department of Chemistry at UR for the "Equity in Graduate Education Consortium"
5. **Organizing Meetings**: Lead organizer of the Telluride Workshop on "Polariton Chemistry and Molecular Cavity Quantum Electrodynamics"; Co-Organizer of the PHYS program "Charge Transfer and Energy Conversion at Interfaces and Defects" the spring ACS National Meeting, Indianapolis, IN (2023); Organizer of the Quantum Dynamics program of the ACS Northeast Regional Meeting (2022); Co-Organizer of the COMP program of the ACS Mid-Atlantic Regional Meeting (2022); Co-organizer for a special symposium on Theoretical Chemistry and Quantum Dynamics in honor of Prof. David Coker's 60th birthday (2018)