Pengfei Huo

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Appointments

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

- 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
- Best Poster - 3rd International Conference on Proton Coupled Electron Transfer, 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.

Independent Publications

(∗ indicates the corresponding author, † indicates the undergraduate coauthor)

19. M. H. Farag, A. Mandal and **P. Huo**∗, "Polariton Induced Conical Intersection and Berry Phase", Preprint. DOI:10.26434/chemrxiv.14128298.v1 (**2021**).
18. 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", Preprint. DOI:10.26434/chemrxiv.13972910.v1 (**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*) accepted, Preprint. DOI:10.26434/chemrxiv.13501668.v1 (**2021**).
16. X. Li, A. Mandal∗ and **P. Huo**∗, "Cavity Frequency-Dependent Theory for Vibrational Polariton Chemistry", Nat. Comm. Nature Commun. 12, 1315 (*Selected for Editors' Highlights*) (**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", 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", 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**).

Current and Pending 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. 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
3. 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
4. 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: 08/15/2019-07/31/2022
5. Department of Energy Early Career Award (**pending**), "New Quantum Dynamics Approaches for Polariton Photochemistry", PI, Total award amount: $750,000 (estimated)

Invited Presentations and Symposia

- **2021.** University of Pennsylvania (02/04), University of Illinois Urbana-Champaign (02/10), New York University (03/02), Northwestern University (03/08), Duke University (04/06), University of Michigan (04/08), University of Toronto (04/08), Cornell University (04/22), Caltech (04/27), UC San Diego (04/30), Boston University (05/03), UC Irvine (05/04).
- **2020.** Polariton Chemistry Webinar (September), Pitzer Center Theory Seminar, University of California, Berkeley (August), ACS 2020 virtual National Meeting (OpenEye Outstanding Junior Faculty Award in Computational Chemistry) (August), Quantum Frontiers in Molecular Science Telluride Workshop (July)
- **2019.** Los Alamos National Laboratory (December), Recent Advances in Electron and Proton Transfer Theories workshop, The Graduate Center at CUNY (October), Colgate University (October), Quantum Control Gordon Research Conference (August), Quantum Effects in Condensed-Phase Systems Workshop in Telluride (July), Nonequilibrium Phenomena, Nonadiabatic Dynamics and Spectroscopy Workshop in Telluride (June), 102nd Canadian Chemistry Conference and Exhibition (June), Great Boston Area Theoretical Chemistry Lecture, Boston (May), ACS 257th National Meeting, Orlando, FL (April),
- **2018.** ACS 256th National Meeting, Boston, MA (August), Donor-acceptor gordon Conference (August), CECAM Non-adiabatic quantum dynamics: From Theory to Experiments Workshop, Lausanne, Switzerland (June), 3rd International Conference on Proton Coupled Electron Transfer (June), NSF MolSSI Workshop on Modular Software Infrastructure for Excited State Dynamics, Buffalo, NY (June), APS March Meeting, Los Angeles, CA (March),
- **2017.** Singlet Fission Workshop, Lyons, CO (June), 45th Middle Atlantic Regional Meeting (MARM 2017), Hershey, PA (June), ACS 253rd National Meeting, San Francisco, CA (April).
- **2016.** ACS 252nd National Meeting, Philadelphia, PA (August), Donor-acceptor gordon Conference, New Port, RI (August), Telluride Theoretical chemistry workshop, Telluride, CO (July), APS 2016 meeting, Baltimore, MD (Match), Boston University (March).

Mentees

- Postdoc Scholars: Dr. **Duncan Bossion** (2019-present), Dr. **Marwa Farag** (2019-present), Dr. **Farnaz Shakib**, (2016- 2018) (Assistant Professor at the New Jersey Institute of Technology), Dr. **Sharma Yamijala** (2016-2018) (Assistant Professor at the Indian Institute of Technology, Madras), Dr. **Wanghuai Zhou** (2018-2020), Assistant Professor at Hubei University of Automotive Technology, China
- Graduate Students: **Sutirtha Chowdhury** (2015-present), **Xinyang Li** (2015-present) **Arkajit Mandal** (2016-present), **Juan Sebastian Sandoval** (2016-2018), **Prakhar Swarp** (2018-present), **Wenxiang Ying** (2020-present), **Eric Koessler** (2020-present)
- Undergraduate Students: **Matt DeLorenzo** (2020-present), **Jack Marion** (2020-present), **Michael A. D. Taylor** (2019-2020, Graduate Student at the University of Rochester), **Sebastian. M. Vega** (2019, Undergraduate Student at the Universidad de Antioquia), **Shreif Abdallah** (2019, Undergraduate Student at the University of Rochester) **Rachel Clune** (2017-2018, Graduate Student at UC Berkeley), **Claire Dickerson** (2017-2018, Graduate Student at UCLA), **Zak Marshall-Carter** (2017-2018, Graduate Student at Boston University), **Alessandro Rognoni** (2017, Graduate Student at the University of Milan), **Matthew Aquilina** (2017, Graduate Student at the University of Cambridge), **Yoshimi Araki** (2017, Engineer at Honda Aircraft Company) , **Maria Castellanos** (2016, Graduate Student at MIT), **Matthew Carbone** (2015-2016, Graduate Student at Columbia)

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.

- Computational Chemistry (undergraduate and 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.

Additional Synergistic Activities

1. **University Activities**: Affiliated faculty member of the *Institute of Optics*; Affiliated faculty member of *Materials Science Graduate Program*; Affiliated faculty member of the *Condensed-matter program* at the Department of Physics, Affiliated faculty member of the *Center for Energy and Environment*; Dept. of Chemistry Graduate Recruiting Committee (2015-present); Dept. of Chemistry Graduate Study Committee (2016-present).
2. **Reviewer Activities**: National Science Foundation *ad-hoc* reviewer, Review Panel, Department of Energy *ad-hoc* Reviewer, DOE Center for Integrated Nanotechnologies *ad-hoc* Reviewer, Canada Foundation for Innovation Review Panel, Israel Science Foundation (ISF) *ad-hoc* Reviewer, 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, Proceedings of the National Academy of Sciences USA, ACS Nano,The Journal of Physical Chemistry A, Applied Physics Letters, Computer Physics Communications

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**).