

# Pengfei Huo

## List of Publications by Year in descending order

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39  
papers

1,626  
citations

331538

21  
h-index

330025

37  
g-index

59  
all docs

59  
docs citations

59  
times ranked

1025  
citing authors

#	ARTICLE	IF	CITATIONS
1	Communication: Partial linearized density matrix dynamics for dissipative, non-adiabatic quantum evolution. <i>Journal of Chemical Physics</i> , 2011, 135, 201101.	1.2	128
2	Efficient Energy Transfer in Light-Harvesting Systems, III: The Influence of the Eighth Bacteriochlorophyll on the Dynamics and Efficiency in FMO. <i>Journal of Physical Chemistry Letters</i> , 2011, 2, 3045-3052.	2.1	123
3	Cavity frequency-dependent theory for vibrational polariton chemistry. <i>Nature Communications</i> , 2021, 12, 1315.	5.8	122
4	Semiclassical Path Integral Dynamics: Photosynthetic Energy Transfer with Realistic Environment Interactions. <i>Annual Review of Physical Chemistry</i> , 2016, 67, 639-668.	4.8	116
5	Investigating New Reactivities Enabled by Polariton Photochemistry. <i>Journal of Physical Chemistry Letters</i> , 2019, 10, 5519-5529.	2.1	96
6	Polariton-Mediated Electron Transfer via Cavity Quantum Electrodynamics. <i>Journal of Physical Chemistry B</i> , 2020, 124, 6321-6340.	1.2	90
7	Consistent schemes for non-adiabatic dynamics derived from partial linearized density matrix propagation. <i>Journal of Chemical Physics</i> , 2012, 137, 22A535.	1.2	89
8	Theoretical Study of Coherent Excitation Energy Transfer in Cryptophyte Phycocyanin 645 at Physiological Temperature. <i>Journal of Physical Chemistry Letters</i> , 2011, 2, 825-833.	2.1	68
9	Communication: Predictive partial linearized path integral simulation of condensed phase electron transfer dynamics. <i>Journal of Chemical Physics</i> , 2013, 139, 151103.	1.2	64
10	Semi-classical path integral non-adiabatic dynamics: a partial linearized classical mapping Hamiltonian approach. <i>Molecular Physics</i> , 2012, 110, 1035-1052.	0.8	55
11	Breaking the Correlation between Energy Costs and Kinetic Barriers in Hydrogen Evolution via a Cobalt Pyridine-Diimine-Dioxime Catalyst. <i>ACS Catalysis</i> , 2016, 6, 6114-6123.	5.5	51
12	Ring Polymer Surface Hopping: Incorporating Nuclear Quantum Effects into Nonadiabatic Molecular Dynamics Simulations. <i>Journal of Physical Chemistry Letters</i> , 2017, 8, 3073-3080.	2.1	47
13	Coherent state mapping ring polymer molecular dynamics for non-adiabatic quantum propagations. <i>Journal of Chemical Physics</i> , 2017, 147, 214109.	1.2	46
14	Resolution of Gauge Ambiguities in Molecular Cavity Quantum Electrodynamics. <i>Physical Review Letters</i> , 2020, 125, 123602.	2.9	46
15	Influence of environment induced correlated fluctuations in electronic coupling on coherent excitation energy transfer dynamics in model photosynthetic systems. <i>Journal of Chemical Physics</i> , 2012, 136, 115102.	1.2	45
16	Polarized Fock States and the Dynamical Casimir Effect in Molecular Cavity Quantum Electrodynamics. <i>Journal of Physical Chemistry Letters</i> , 2020, 11, 9215-9223.	2.1	45
17	Quasi-Adiabatic Representation for Nonadiabatic Dynamics Propagation. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 1828-1840.	2.3	42
18	Enhancing Singlet Fission Dynamics by Suppressing Destructive Interference between Charge-Transfer Pathways. <i>Journal of Physical Chemistry Letters</i> , 2017, 8, 2480-2488.	2.1	35

#	ARTICLE	IF	CITATIONS
19	Theory of Mode-Selective Chemistry through Polaritonic Vibrational Strong Coupling. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 6974-6982.	2.1	35
20	Theory of vibrational polariton chemistry in the collective coupling regime. <i>Journal of Chemical Physics</i> , 2022, 156, 014101.	1.2	34
21	Symmetric quasi-classical dynamics with quasi-diabatic propagation scheme. <i>Journal of Chemical Physics</i> , 2018, 149, 044115.	1.2	25
22	Quasi-Diabatic Scheme for Nonadiabatic On-the-Fly Simulations. <i>Journal of Physical Chemistry Letters</i> , 2019, 10, 7062-7070.	2.1	25
23	Ring polymer quantization of the photon field in polariton chemistry. <i>Journal of Chemical Physics</i> , 2021, 154, 044109.	1.2	22
24	Investigating photoinduced proton coupled electron transfer reaction using quasi diabatic dynamics propagation. <i>Journal of Chemical Physics</i> , 2018, 148, 244102.	1.2	19
25	State dependent ring polymer molecular dynamics for investigating excited nonadiabatic dynamics. <i>Journal of Chemical Physics</i> , 2019, 150, 244102.	1.2	18
26	Polariton induced conical intersection and berry phase. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 16868-16879.	1.3	18
27	Molecular Polaritons Generated from Strong Coupling between CdSe Nanoplatelets and a Dielectric Optical Cavity. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 5030-5038.	2.1	18
28	Linearized approximations for condensed phase non-adiabatic dynamics: Multi-layered baths and Brownian dynamics implementation. <i>Chemical Physics</i> , 2010, 370, 87-97.	0.9	17
29	Quasi-Diabatic Propagation Scheme for Direct Simulation of Proton-Coupled Electron Transfer Reaction. <i>Journal of Physical Chemistry A</i> , 2019, 123, 2470-2482.	1.1	16
30	Non-adiabatic Matsubara dynamics and non-adiabatic ring-polymer molecular dynamics. <i>Journal of Chemical Physics</i> , 2021, 154, 124124.	1.2	13
31	Electronic coherence and the kinetics of inter-complex energy transfer in light-harvesting systems. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 30914-30924.	1.3	12
32	Resolving ambiguities of the mode truncation in cavity quantum electrodynamics. <i>Optics Letters</i> , 2022, 47, 1446.	1.7	11
33	Ab initio symmetric quasi-classical approach to investigate molecular Tully models. <i>Journal of Chemical Physics</i> , 2021, 155, 084106.	1.2	10
34	Non-adiabatic ring polymer molecular dynamics with spin mapping variables. <i>Journal of Chemical Physics</i> , 2021, 154, 184106.	1.2	7
35	Incorporating Lindblad decay dynamics into mixed quantum-classical simulations. <i>Journal of Chemical Physics</i> , 2022, 157, .	1.2	7
36	Direct Nonadiabatic Simulations of the Photoinduced Charge Transfer Dynamics. <i>Journal of Physical Chemistry A</i> , 2021, 125, 628-635.	1.1	6

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37	Investigating Tunneling-Controlled Chemical Reactions through Ab Initio Ring Polymer Molecular Dynamics. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 6714-6721.	2.1	2
38	Chapter 8 Excitation Energy Transfer in Light-Harvesting Systems: Theory, Models, and Application. , 2017, , 293-336.		2
39	Investigating Polaritonic Photochemistry Through Quantum Dynamics Simulations. , 2019, , .		0