Pengfei Huo

List of Publications by Year
in descending order

39 papers	1,626 citations	331670 21 h-index	330143 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. Journal of Chemical Physics, 2011, 135, 201101.	3.0	128
2	Efficient Energy Transfer in Light-Harvesting Systems, III: The Influence of the Eighth Bacteriochlorophyll on the Dynamics and Efficiency in FMO. Journal of Physical Chemistry Letters, 2011, 2, 3045-3052.	4.6	123
3	Cavity frequency-dependent theory for vibrational polariton chemistry. Nature Communications, 2021, 12, 1315.	12.8	122
4	Semiclassical Path Integral Dynamics: Photosynthetic Energy Transfer with Realistic Environment Interactions. Annual Review of Physical Chemistry, 2016, 67, 639-668.	10.8	116
5	Investigating New Reactivities Enabled by Polariton Photochemistry. Journal of Physical Chemistry Letters, 2019, 10, 5519-5529.	4.6	96
6	Polariton-Mediated Electron Transfer via Cavity Quantum Electrodynamics. Journal of Physical Chemistry B, 2020, 124, 6321-6340.	2.6	90
7	Consistent schemes for non-adiabatic dynamics derived from partial linearized density matrix propagation. Journal of Chemical Physics, 2012, 137, 22A535.	3.0	89
8	Theoretical Study of Coherent Excitation Energy Transfer in Cryptophyte Phycocyanin 645 at Physiological Temperature. Journal of Physical Chemistry Letters, 2011, 2, 825-833.	4.6	68
9	Communication: Predictive partial linearized path integral simulation of condensed phase electron transfer dynamics. Journal of Chemical Physics, 2013, 139, 151103.	3.0	64
10	Semi-classical path integral non-adiabatic dynamics: a partial linearized classical mapping Hamiltonian approach. Molecular Physics, 2012, 110, 1035-1052.	1.7	55
11	Breaking the Correlation between Energy Costs and Kinetic Barriers in Hydrogen Evolution via a Cobalt Pyridine-Diimine-Dioxime Catalyst. ACS Catalysis, 2016, 6, 6114-6123.	11.2	51
12	Ring Polymer Surface Hopping: Incorporating Nuclear Quantum Effects into Nonadiabatic Molecular Dynamics Simulations. Journal of Physical Chemistry Letters, 2017, 8, 3073-3080.	4.6	47
13	Coherent state mapping ring polymer molecular dynamics for non-adiabatic quantum propagations. Journal of Chemical Physics, 2017, 147, 214109.	3.0	46
14	Resolution of Gauge Ambiguities in Molecular Cavity Quantum Electrodynamics. Physical Review Letters, 2020, 125, 123602.	7.8	46
15	Influence of environment induced correlated fluctuations in electronic coupling on coherent excitation energy transfer dynamics in model photosynthetic systems. Journal of Chemical Physics, 2012, 136, 115102.	3.0	45
16	Polarized Fock States and the Dynamical Casimir Effect in Molecular Cavity Quantum Electrodynamics. Journal of Physical Chemistry Letters, 2020, 11, 9215-9223.	4.6	45
17	Quasi-Diabatic Representation for Nonadiabatic Dynamics Propagation. Journal of Chemical Theory and Computation, 2018, 14, 1828-1840.	5.3	42
18	Enhancing Singlet Fission Dynamics by Suppressing Destructive Interference between Charge-Transfer Pathways. Journal of Physical Chemistry Letters, 2017, 8, 2480-2488.	4.6	35

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19	Theory of Mode-Selective Chemistry through Polaritonic Vibrational Strong Coupling. Journal of Physical Chemistry Letters, 2021, 12, 6974-6982.	4.6	35
20	Theory of vibrational polariton chemistry in the collective coupling regime. Journal of Chemical Physics, 2022, 156, 014101.	3.0	34
21	Symmetric quasi-classical dynamics with quasi-diabatic propagation scheme. Journal of Chemical Physics, 2018, 149, 044115.	3.0	25
22	Quasi-Diabatic Scheme for Nonadiabatic On-the-Fly Simulations. Journal of Physical Chemistry Letters, 2019, 10, 7062-7070.	4.6	25
23	Ring polymer quantization of the photon field in polariton chemistry. Journal of Chemical Physics, 2021, 154, 044109.	3.0	22
24	Investigating photoinduced proton coupled electron transfer reaction using quasi diabatic dynamics propagation. Journal of Chemical Physics, 2018, 148, 244102.	3.0	19
25	State dependent ring polymer molecular dynamics for investigating excited nonadiabatic dynamics. Journal of Chemical Physics, 2019, 150, 244102.	3.0	18
26	Polariton induced conical intersection and berry phase. Physical Chemistry Chemical Physics, 2021, 23, 16868-16879.	2.8	18
27	Molecular Polaritons Generated from Strong Coupling between CdSe Nanoplatelets and a Dielectric Optical Cavity. Journal of Physical Chemistry Letters, 2021, 12, 5030-5038.	4.6	18
28	Linearized approximations for condensed phase non-adiabatic dynamics: Multi-layered baths and Brownian dynamics implementation. Chemical Physics, 2010, 370, 87-97.	1.9	17
29	Quasi-Diabatic Propagation Scheme for Direct Simulation of Proton-Coupled Electron Transfer Reaction. Journal of Physical Chemistry A, 2019, 123, 2470-2482.	2.5	16
30	Non-adiabatic Matsubara dynamics and non-adiabatic ring-polymer molecular dynamics. Journal of Chemical Physics, 2021, 154, 124124.	3.0	13
31	Electronic coherence and the kinetics of inter-complex energy transfer in light-harvesting systems. Physical Chemistry Chemical Physics, 2015, 17, 30914-30924.	2.8	12
32	Resolving ambiguities of the mode truncation in cavity quantum electrodynamics. Optics Letters, 2022, 47, 1446.	3.3	11
33	Ab initio symmetric quasi-classical approach to investigate molecular Tully models. Journal of Chemical Physics, 2021, 155, 084106.	3.0	10
34	Non-adiabatic ring polymer molecular dynamics with spin mapping variables. Journal of Chemical Physics, 2021, 154, 184106.	3.0	7
35	Incorporating Lindblad decay dynamics into mixed quantum-classical simulations. Journal of Chemical Physics, 2022, 157, .	3.0	7
36	Direct Nonadiabatic Simulations of the Photoinduced Charge Transfer Dynamics. Journal of Physical Chemistry A, 2021, 125, 628-635.	2.5	6

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37	Investigating Tunneling-Controlled Chemical Reactions through Ab Initio Ring Polymer Molecular Dynamics. Journal of Physical Chemistry Letters, 2021, 12, 6714-6721.	4.6	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