

Pengfei Huo

List of Publications by Year in descending order

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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	Theory of vibrational polariton chemistry in the collective coupling regime. <i>Journal of Chemical Physics</i> , 2022, 156, 014101.	3.0	34
2	Resolving ambiguities of the mode truncation in cavity quantum electrodynamics. <i>Optics Letters</i> , 2022, 47, 1446.	3.3	11
3	Incorporating Lindblad decay dynamics into mixed quantum-classical simulations. <i>Journal of Chemical Physics</i> , 2022, 157, .	3.0	7
4	Polariton induced conical intersection and berry phase. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 16868-16879.	2.8	18
5	Ring polymer quantization of the photon field in polariton chemistry. <i>Journal of Chemical Physics</i> , 2021, 154, 044109.	3.0	22
6	Direct Nonadiabatic Simulations of the Photoinduced Charge Transfer Dynamics. <i>Journal of Physical Chemistry A</i> , 2021, 125, 628-635.	2.5	6
7	Cavity frequency-dependent theory for vibrational polariton chemistry. <i>Nature Communications</i> , 2021, 12, 1315.	12.8	122
8	Non-adiabatic Matsubara dynamics and non-adiabatic ring-polymer molecular dynamics. <i>Journal of Chemical Physics</i> , 2021, 154, 124124.	3.0	13
9	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.	4.6	18
10	Non-adiabatic ring polymer molecular dynamics with spin mapping variables. <i>Journal of Chemical Physics</i> , 2021, 154, 184106.	3.0	7
11	Theory of Mode-Selective Chemistry through Polaritonic Vibrational Strong Coupling. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 6974-6982.	4.6	35
12	Investigating Tunneling-Controlled Chemical Reactions through Ab Initio Ring Polymer Molecular Dynamics. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 6714-6721.	4.6	2
13	Ab initio symmetric quasi-classical approach to investigate molecular Tully models. <i>Journal of Chemical Physics</i> , 2021, 155, 084106.	3.0	10
14	Polarized Fock States and the Dynamical Casimir Effect in Molecular Cavity Quantum Electrodynamics. <i>Journal of Physical Chemistry Letters</i> , 2020, 11, 9215-9223.	4.6	45
15	Resolution of Gauge Ambiguities in Molecular Cavity Quantum Electrodynamics. <i>Physical Review Letters</i> , 2020, 125, 123602.	7.8	46
16	Polariton-Mediated Electron Transfer via Cavity Quantum Electrodynamics. <i>Journal of Physical Chemistry B</i> , 2020, 124, 6321-6340.	2.6	90
17	State dependent ring polymer molecular dynamics for investigating excited nonadiabatic dynamics. <i>Journal of Chemical Physics</i> , 2019, 150, 244102.	3.0	18
18	Quasi-Diabatic Scheme for Nonadiabatic On-the-Fly Simulations. <i>Journal of Physical Chemistry Letters</i> , 2019, 10, 7062-7070.	4.6	25

#	ARTICLE	IF	CITATIONS
19	Investigating New Reactivities Enabled by Polariton Photochemistry. <i>Journal of Physical Chemistry Letters</i> , 2019, 10, 5519-5529.	4.6	96
20	Quasi-Adiabatic Propagation Scheme for Direct Simulation of Proton-Coupled Electron Transfer Reaction. <i>Journal of Physical Chemistry A</i> , 2019, 123, 2470-2482.	2.5	16
21	Investigating Polaritonic Photochemistry Through Quantum Dynamics Simulations. , 2019, , .		0
22	Quasi-Adiabatic Representation for Nonadiabatic Dynamics Propagation. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 1828-1840.	5.3	42
23	Symmetric quasi-classical dynamics with quasi-adiabatic propagation scheme. <i>Journal of Chemical Physics</i> , 2018, 149, 044115.	3.0	25
24	Investigating photoinduced proton coupled electron transfer reaction using quasi adiabatic dynamics propagation. <i>Journal of Chemical Physics</i> , 2018, 148, 244102.	3.0	19
25	Ring Polymer Surface Hopping: Incorporating Nuclear Quantum Effects into Nonadiabatic Molecular Dynamics Simulations. <i>Journal of Physical Chemistry Letters</i> , 2017, 8, 3073-3080.	4.6	47
26	Enhancing Singlet Fission Dynamics by Suppressing Destructive Interference between Charge-Transfer Pathways. <i>Journal of Physical Chemistry Letters</i> , 2017, 8, 2480-2488.	4.6	35
27	Coherent state mapping ring polymer molecular dynamics for non-adiabatic quantum propagations. <i>Journal of Chemical Physics</i> , 2017, 147, 214109.	3.0	46
28	Chapter 8 Excitation Energy Transfer in Light-Harvesting Systems: Theory, Models, and Application. , 2017, , 293-336.		2
29	Semiclassical Path Integral Dynamics: Photosynthetic Energy Transfer with Realistic Environment Interactions. <i>Annual Review of Physical Chemistry</i> , 2016, 67, 639-668.	10.8	116
30	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.	11.2	51
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.	2.8	12
32	Communication: Predictive partial linearized path integral simulation of condensed phase electron transfer dynamics. <i>Journal of Chemical Physics</i> , 2013, 139, 151103.	3.0	64
33	Consistent schemes for non-adiabatic dynamics derived from partial linearized density matrix propagation. <i>Journal of Chemical Physics</i> , 2012, 137, 22A535.	3.0	89
34	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.	3.0	45
35	Semi-classical path integral non-adiabatic dynamics: a partial linearized classical mapping Hamiltonian approach. <i>Molecular Physics</i> , 2012, 110, 1035-1052.	1.7	55
36	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.	4.6	68

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37	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
38	Communication: Partial linearized density matrix dynamics for dissipative, non-adiabatic quantum evolution. Journal of Chemical Physics, 2011, 135, 201101.	3.0	128
39	Linearized approximations for condensed phase non-adiabatic dynamics: Multi-layered baths and Brownian dynamics implementation. Chemical Physics, 2010, 370, 87-97.	1.9	17