Haobin Wang

List of Publications by Year
in descending order

86 papers	5,425 citations	66343 42 h-index	79698 73 g-index
86 all docs	86 docs citations	86 times ranked	2900 citing authors

#	Article	IF	Citations
1	Demonstration of a Stereospecific Photochemical Meta Effect. Photochem, 2022, 2, 69-76.	2.2	0
2	Importance of Appropriately Regularizing the ML-MCTDH Equations of Motion. Journal of Physical Chemistry A, 2021, 125, 3077-3087.	2.5	9
3	Chemical Bonding as a New Avenue for Controlling Excitedâ€State Properties and Excitation Energyâ€Transfer Processes in Zinc Phthalocyanineâ€“Fullerene Dyads. Chemistry - A European Journal, 2021, 27, 4159-4167.	3.3	10
4	Trisulfur-Radical-Anion-Triggered C(sp²)â€“H Amination of Electron-Deficient Alkenes. Organic Letters, 2020, 22, 9751-9756.	4.6	14
5	Phase-Separated Transcriptional Condensates Accelerate Target-Search Process Revealed by Live-Cell Single-Molecule Imaging. Cell Reports, 2020, 33, 108248.	6.4	88
6	Experimental and theoretical rationalization for the base pairing abilities of inosine, guanosine, adenosine, and their corresponding 8â€oxo â€7,8â€dihydropurine, and 8â€bromopurine analogues within Aâ€form duplexes of RNA. Biopolymers, 2020, 111, e23410.	2.4	6
7	Heat Transport in a Spin-Boson Model at Low Temperatures: A Multilayer Multiconfiguration Time-Dependent Hartree Study. Entropy, 2020, 22, 1099.	2.2	5
8	Memorial Viewpoint for William L. Hase. Journal of Physical Chemistry A, 2020, 124, 4183-4184.	2.5	0
9	Photocycloaddition of S,S-Dioxo-benzothiophene-2-methanol, Reactivity in the Solid State and in Solution: Mechanistic Studies and Diastereoselective Formation of Cyclobutyl Rings. Journal of Organic Chemistry, 2019, 84, 9714-9725.	3.2	10
10	A unified view of hierarchy approach and formula of differentiation. Journal of Chemical Physics, 2019, 151, 164110.	3.0	3
11	Computational study on the removal of photolabile protecting groups by photochemical reactions. Computational and Theoretical Chemistry, 2019, 1151, 1-11.	2.5	4
12	Metal-free cross-coupling of Ï€-conjugated triazenes with unactivated arenes via photoactivation. Organic Chemistry Frontiers, 2019, 6, 152-161.	4.5	22
13	Quantum Phase Transition in the Spin-Boson Model: A Multilayer Multiconfiguration Time-Dependent Hartree Study. Journal of Physical Chemistry A, 2019, 123, 1882-1893.	2.5	12
14	Nuclear condensates of the Polycomb protein chromobox 2 (CBX2) assemble through phase separation. Journal of Biological Chemistry, 2019, 294, 1451-1463.	3.4	261
15	Direct Aryloxylation/Alkyloxylation of Dialkyl Phosphonates for the Synthesis of Mixed Phosphonates. Angewandte Chemie - International Edition, 2018, 57, 6624-6628.	13.8	51
16	Approximate DFT-based methods for generating diabatic states and calculating electronic couplings: models of two and more states. Physical Chemistry Chemical Physics, 2018, 20, 2571-2584.	2.8	6
17	On regularizing the MCTDH equations of motion. Journal of Chemical Physics, 2018, 148, 124105.	3.0	32
18	A multilayer multiconfiguration time-dependent Hartree study of the nonequilibrium Anderson impurity model at zero temperature. Chemical Physics, 2018, 509, 13-19.	1.9	19

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19	Accurate calculation of equilibrium reduced density matrix for the system-bath model: A multilayer multiconfiguration time-dependent Hartree approach and its comparison to a multi-electronic-state path integral molecular dynamics approach. Chinese Journal of Chemical Physics, 2018, 31, 446-456.	1.3	6
20	On the memory kernel and the reduced system propagator. Journal of Chemical Physics, 2018, 149, 104105.	3.0	28
21	Modeling of canonical and C2â€²-O-thiophenylmethyl modified hexamers of RNA. Insights into the nature of structural changes and thermal stability. New Journal of Chemistry, 2018, 42, 10177-10183.	2.8	1
22	Live-cell single-molecule dynamics of PcG proteins imposed by the DIPG H3.3K27M mutation. Nature Communications, 2018, 9, 2080.	12.8	63
23	On regularizing the ML-MCTDH equations of motion. Journal of Chemical Physics, 2018, 149, 044119.	3.0	31
24	Plasmonic circular dichroism of vesicle-like nanostructures by the template-less self-assembly of achiral Janus nanoparticles. Nanoscale, 2018, 10, 14586-14593.	5.6	10
25	Direct Aryloxylation/Alkyloxylation of Dialkyl Phosphonates for the Synthesis of Mixed Phosphonates. Angewandte Chemie, 2018, 130, 6734-6738.	2.0	15
26	A multilayer multiconfiguration time-dependent Hartree simulation of the reaction-coordinate spin-boson model employing an interaction picture. Journal of Chemical Physics, 2017, 146, 124112.	3.0	12
27	Quantum kinetic expansion in the spin-boson model: Matrix formulation and system-bath factorized initial state. Journal of Chemical Physics, 2017, 147, 244112.	3.0	2
28	Employing an interaction picture to remove artificial correlations in multilayer multiconfiguration time-dependent Hartree simulations. Journal of Chemical Physics, 2016, 145, 164105.	3.0	20
29	Synthesis, Thermal Stability, Biophysical Properties, and Molecular Modeling of Oligonucleotides of RNA Containing 2â€²-O-2-Thiophenylmethyl Groups. Journal of Organic Chemistry, 2016, 81, 8947-8958.	3.2	4
30	On the accuracy of the noninteracting electron approximation for vibrationally coupled electron transport. Chemical Physics, 2016, 481, 117-123.	1.9	6
31	Sub-Ohmic to super-Ohmic crossover behavior in nonequilibrium quantum systems with electron-phonon interactions. Physical Review B, 2015, 92, .	3.2	33
32	Extended hierarchy equation of motion for the spin-boson model. Journal of Chemical Physics, 2015, 143, 224112.	3.0	94
33	Multilayer Multiconfiguration Time-Dependent Hartree Theory. Journal of Physical Chemistry A, 2015, 119, 7951-7965.	2.5	165
34	Phonon dynamics in correlated quantum systems driven away from equilibrium. Physical Review B, 2014, 90, .	3.2	20
35	Nonequilibrium quantum systems with electron-phonon interactions: Transient dynamics and approach to steady state. Physical Review B, 2014, 89, .	3.2	86
36	Iterative Calculation of Energy Eigenstates Employing the Multilayer Multiconfiguration Time-Dependent Hartree Theory. Journal of Physical Chemistry A, 2014, 118, 9253-9261.	2.5	26

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37	Dynamical Simulation of Electron Transfer Processes in Alkanethiolate Self-Assembled Monolayers at the Au(111) Surface. Journal of Physical Chemistry C, 2013, 117, 25334-25342.	3.1	15
38	Multilayer Multiconfiguration Time-Dependent Hartree Study of Vibrationally Coupled Electron Transport Using the Scattering-State Representation. Journal of Physical Chemistry A, 2013, 117, 7431-7441.	2.5	39
39	Numerically exact, time-dependent study of correlated electron transport in model molecular junctions. Journal of Chemical Physics, 2013, 138, 134704.	3.0	58
40	Bistability in a nonequilibrium quantum system with electron-phonon interactions. Physical Review B, 2013, 88, .	3.2	88
41	Quantum dynamics of electron-transfer reactions: photoinduced intermolecular electron transfer in a porphyrinâ€“quinone complex. Molecular Physics, 2012, 110, 751-763.	1.7	25
42	Dynamics of a two-level system coupled to a bath of spins. Journal of Chemical Physics, 2012, 137, 22A504.	3.0	22
43	Dynamics of electron transfer in complex glassy environment modeled by the Coleâ€“Davidson spectral density. Molecular Physics, 2012, 110, 581-594.	1.7	9
44	Bistability signatures in nonequilibrium charge transport through molecular quantum dots. Physical Review B, 2012, 86, .	3.2	65
45	Orbital-Symmetry-Dependent Electron Transfer through Molecules Assembled on Metal Substrates. Journal of Physical Chemistry Letters, 2012, 3, 436-440.	4.6	35
46	COMPUTATIONAL STUDY OF BRIDGE-MEDIATED INTERVALENCE ELECTRON TRANSFER II: COUPLINGS IN DIFFERENT METALLOCENE COMPLEXES. Journal of Theoretical and Computational Chemistry, 2012, 11, 1341-1356.	1.8	2
47	Numerically exact, time-dependent treatment of vibrationally coupled electron transport in single-molecule junctions. Journal of Chemical Physics, 2011, 135, 244506.	3.0	71
48	Computational study of topological effects on intramolecular electron transfer in mixed-valence compounds. Frontiers of Chemistry in China: Selected Publications From Chinese Universities, 2011, 6, 280-286.	0.4	0
49	Computational Study of Bridge-Assisted Intervalence Electron Transfer. Journal of Physical Chemistry A, 2010, 114, 6039-6046.	2.5	50
50	From coherent motion to localization: II. Dynamics of the spin-boson model with sub-Ohmic spectral density at zero temperature. Chemical Physics, 2010, 370, 78-86.	1.9	70
51	Computational Study of Ferrocene-Based Molecular Frameworks with 2,5-Diethynylpyridine as a Chemical Bridge. Materials, 2010, 3, 2668-2683.	2.9	37
52	Theoretical Study of Photoinduced Electron-Transfer Processes in the Dyeâ^'Semiconductor System Alizarinâ^'TiO₂. Journal of Physical Chemistry C, 2010, 114, 18481-18493.	3.1	69
53	Meirâ€“Wingreen formula for heat transport in a spin-boson nanojunction model. Journal of Chemical Physics, 2010, 133, 084503.	3.0	39
54	Dynamics of electron transfer reactions in the presence of mode mixing: Comparison of a generalized master equation approach with the numerically exact simulation. Journal of Chemical Physics, 2009, 131, 094109.	3.0	21

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55	Numerically exact quantum dynamics for indistinguishable particles: The multilayer multiconfiguration time-dependent Hartree theory in second quantization representation. Journal of Chemical Physics, 2009, 131, 024114.	3.0	155
56	Heat transport through model molecular junctions: A multilayer multiconfiguration time-dependent Hartree approach. Chemical Physics Letters, 2008, 460, 325-330.	2.6	78
57	Nonperturbative quantum simulation of time-resolved nonlinear spectra: Methodology and application to electron transfer reactions in the condensed phase. Chemical Physics, 2008, 347, 139-151.	1.9	45
58	A Langevin equation approach to electron transfer reactions in the diabatic basis. Journal of Chemical Physics, 2008, 129, 144502.	3.0	10
59	Nanoparticle-Mediated Intervalence Transfer. Journal of the American Chemical Society, 2008, 130, 12156-12162.	13.7	59
60	Dynamical Simulation of Photoinduced Electron Transfer Reactions in Dyeâ^'Semiconductor Systems with Different Anchor Groups. Journal of Physical Chemistry C, 2008, 112, 12326-12333.	3.1	81
61	Effects of intense femtosecond pumping on ultrafast electronic-vibrational dynamics in molecular systems with relaxation. Journal of Chemical Physics, 2008, 129, 214303.	3.0	45
62	From coherent motion to localization: dynamics of the spin-boson model at zero temperature. New Journal of Physics, 2008, 10, 115005.	2.9	114
63	Proton transfer reactions in model condensed-phase environments: Accurate quantum dynamics using the multilayer multiconfiguration time-dependent Hartree approach. Journal of Chemical Physics, 2007, 127, 144503.	3.0	93
64	Correlated electron-nuclear dynamics in ultrafast photoinduced electron-transfer reactions at dye-semiconductor interfaces. Physical Review B, 2007, 76, .	3.2	40
65	Quantum Dynamical Simulation of Electron-Transfer Reactions in an Anharmonic Environment. Journal of Physical Chemistry A, 2007, 111, 10369-10375.	2.5	74
66	Monte Carlo Sampling for Classical Trajectory Simulations. Advances in Chemical Physics, 2007, , 171-201.	0.3	158
67	Quantum Dynamics of Photoinduced Electron-Transfer Reactions in Dyeâ^'Semiconductor Systems:â€‰ First-Principles Description and Application to Coumarin 343â^'TiO₂. Journal of Physical Chemistry C, 2007, 111, 11970-11981.	3.1	157
68	Theoretical Study of Ultrafast Heterogeneous Electron Transfer Reactions at Dyeâ^'Semiconductor Interfaces:Â Coumarin 343 at Titanium Oxideâ€. Journal of Physical Chemistry A, 2006, 110, 1364-1374.	2.5	80
69	Computational study of titanium (IV) complexes with organic chromophores. International Journal of Quantum Chemistry, 2006, 106, 1291-1303.	2.0	47
70	Quantum dynamical simulation of ultrafast molecular processes in the condensed phase. Chemical Physics, 2006, 322, 210-222.	1.9	48
71	Quantum-mechanical evaluation of the Boltzmann operator in correlation functions for large molecular systems: A multilayer multiconfiguration time-dependent Hartree approach. Journal of Chemical Physics, 2006, 124, 034114.	3.0	72
72	Calculation of reactive flux correlation functions for systems in a condensed phase environment: A multilayer multiconfiguration time-dependent Hartree approach. Journal of Chemical Physics, 2006, 125, 174502.	3.0	66

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73	Theoretical study of ultrafast heterogeneous electron transfer reactions at dyeâ€“semiconductor interfaces. Chemical Physics, 2004, 304, 169-181.	1.9	79
74	Multilayer formulation of the multiconfiguration time-dependent Hartree theory. Journal of Chemical Physics, 2003, 119, 1289-1299.	3.0	729
75	Modeling of ultrafast electron-transfer processes: Validity of multilevel Redfield theory. Journal of Chemical Physics, 2003, 119, 2761-2773.	3.0	151
76	Theoretical Study of Ultrafast Photoinduced Electron Transfer Processes in Mixed-Valence Systems. Journal of Physical Chemistry A, 2003, 107, 2126-2136.	2.5	81
77	Combining semiclassical time evolution and quantum Boltzmann operator to evaluate reactive flux correlation function for thermal rate constants of complex systems. Journal of Chemical Physics, 2002, 116, 7335-7349.	3.0	79
78	Self-consistent hybrid approach for simulating electron transfer reactions in condensed phases. Israel Journal of Chemistry, 2002, 42, 167-182.	2.3	23
79	Quantum dynamical simulation of ultrafast photoinduced electron transfer processes in a mixed-valence compound. Chemical Physics Letters, 2002, 358, 298-306.	2.6	34
80	Self-consistent hybrid approach for complex systems: Application to the spin-boson model with Debye spectral density. Journal of Chemical Physics, 2001, 115, 2991-3005.	3.0	226
81	Systematic convergence in the dynamical hybrid approach for complex systems: A numerically exact methodology. Journal of Chemical Physics, 2001, 115, 2979-2990.	3.0	163
82	Semiclassical description of diffraction and its quenching by the forwardâ€“backward version of the initial value representation. Journal of Chemical Physics, 2001, 114, 2572-2579.	3.0	69
83	Generalized Filinov transformation of the semiclassical initial value representation. Journal of Chemical Physics, 2001, 115, 6317-6326.	3.0	91
84	Basis set approach to the quantum dissipative dynamics: Application of the multiconfiguration time-dependent Hartree method to the spin-boson problem. Journal of Chemical Physics, 2000, 113, 9948-9956.	3.0	102
85	Forwardâ€“backward initial value representation for the calculation of thermal rate constants for reactions in complex molecular systems. Journal of Chemical Physics, 2000, 112, 47-55.	3.0	128
86	Semiclassical study of electronically nonadiabatic dynamics in the condensed-phase: Spin-boson problem with Debye spectral density. Journal of Chemical Physics, 1999, 110, 4828-4840.	3.0	159