

# Haobin Wang

## List of Publications by Year in descending order

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86  
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66343

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86  
all docs

86  
docs citations

86  
times ranked

2900  
citing authors

#	ARTICLE	IF	CITATIONS
1	Multilayer formulation of the multiconfiguration time-dependent Hartree theory. <i>Journal of Chemical Physics</i> , 2003, 119, 1289-1299.	3.0	729
2	Nuclear condensates of the Polycomb protein chromobox 2 (CBX2) assemble through phase separation. <i>Journal of Biological Chemistry</i> , 2019, 294, 1451-1463.	3.4	261
3	Self-consistent hybrid approach for complex systems: Application to the spin-boson model with Debye spectral density. <i>Journal of Chemical Physics</i> , 2001, 115, 2991-3005.	3.0	226
4	Multilayer Multiconfiguration Time-Dependent Hartree Theory. <i>Journal of Physical Chemistry A</i> , 2015, 119, 7951-7965.	2.5	165
5	Systematic convergence in the dynamical hybrid approach for complex systems: A numerically exact methodology. <i>Journal of Chemical Physics</i> , 2001, 115, 2979-2990.	3.0	163
6	Semiclassical study of electronically nonadiabatic dynamics in the condensed-phase: Spin-boson problem with Debye spectral density. <i>Journal of Chemical Physics</i> , 1999, 110, 4828-4840.	3.0	159
7	Monte Carlo Sampling for Classical Trajectory Simulations. <i>Advances in Chemical Physics</i> , 2007, , 171-201.	0.3	158
8	Quantum Dynamics of Photoinduced Electron-Transfer Reactions in Dye-Semiconductor Systems: First-Principles Description and Application to Coumarin 343-TiO <sub>2</sub> . <i>Journal of Physical Chemistry C</i> , 2007, 111, 11970-11981.	3.1	157
9	Numerically exact quantum dynamics for indistinguishable particles: The multilayer multiconfiguration time-dependent Hartree theory in second quantization representation. <i>Journal of Chemical Physics</i> , 2009, 131, 024114.	3.0	155
10	Modeling of ultrafast electron-transfer processes: Validity of multilevel Redfield theory. <i>Journal of Chemical Physics</i> , 2003, 119, 2761-2773.	3.0	151
11	Forward-backward initial value representation for the calculation of thermal rate constants for reactions in complex molecular systems. <i>Journal of Chemical Physics</i> , 2000, 112, 47-55.	3.0	128
12	From coherent motion to localization: dynamics of the spin-boson model at zero temperature. <i>New Journal of Physics</i> , 2008, 10, 115005.	2.9	114
13	Basis set approach to the quantum dissipative dynamics: Application of the multiconfiguration time-dependent Hartree method to the spin-boson problem. <i>Journal of Chemical Physics</i> , 2000, 113, 9948-9956.	3.0	102
14	Extended hierarchy equation of motion for the spin-boson model. <i>Journal of Chemical Physics</i> , 2015, 143, 224112.	3.0	94
15	Proton transfer reactions in model condensed-phase environments: Accurate quantum dynamics using the multilayer multiconfiguration time-dependent Hartree approach. <i>Journal of Chemical Physics</i> , 2007, 127, 144503.	3.0	93
16	Generalized Filinov transformation of the semiclassical initial value representation. <i>Journal of Chemical Physics</i> , 2001, 115, 6317-6326.	3.0	91
17	Bistability in a nonequilibrium quantum system with electron-phonon interactions. <i>Physical Review B</i> , 2013, 88, .	3.2	88
18	Phase-Separated Transcriptional Condensates Accelerate Target-Search Process Revealed by Live-Cell Single-Molecule Imaging. <i>Cell Reports</i> , 2020, 33, 108248.	6.4	88

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19	Nonequilibrium quantum systems with electron-phonon interactions: Transient dynamics and approach to steady state. <i>Physical Review B</i> , 2014, 89, .	3.2	86
20	Theoretical Study of Ultrafast Photoinduced Electron Transfer Processes in Mixed-Valence Systems. <i>Journal of Physical Chemistry A</i> , 2003, 107, 2126-2136.	2.5	81
21	Dynamical Simulation of Photoinduced Electron Transfer Reactions in Dye <sup>+</sup> Semiconductor Systems with Different Anchor Groups. <i>Journal of Physical Chemistry C</i> , 2008, 112, 12326-12333.	3.1	81
22	Theoretical Study of Ultrafast Heterogeneous Electron Transfer Reactions at Dye <sup>+</sup> Semiconductor Interfaces: A Coumarin 343 at Titanium Oxide. <i>Journal of Physical Chemistry A</i> , 2006, 110, 1364-1374.	2.5	80
23	Combining semiclassical time evolution and quantum Boltzmann operator to evaluate reactive flux correlation function for thermal rate constants of complex systems. <i>Journal of Chemical Physics</i> , 2002, 116, 7335-7349.	3.0	79
24	Theoretical study of ultrafast heterogeneous electron transfer reactions at dye <sup>+</sup> semiconductor interfaces. <i>Chemical Physics</i> , 2004, 304, 169-181.	1.9	79
25	Heat transport through model molecular junctions: A multilayer multiconfiguration time-dependent Hartree approach. <i>Chemical Physics Letters</i> , 2008, 460, 325-330.	2.6	78
26	Quantum Dynamical Simulation of Electron-Transfer Reactions in an Anharmonic Environment. <i>Journal of Physical Chemistry A</i> , 2007, 111, 10369-10375.	2.5	74
27	Quantum-mechanical evaluation of the Boltzmann operator in correlation functions for large molecular systems: A multilayer multiconfiguration time-dependent Hartree approach. <i>Journal of Chemical Physics</i> , 2006, 124, 034114.	3.0	72
28	Numerically exact, time-dependent treatment of vibrationally coupled electron transport in single-molecule junctions. <i>Journal of Chemical Physics</i> , 2011, 135, 244506.	3.0	71
29	From coherent motion to localization: II. Dynamics of the spin-boson model with sub-Ohmic spectral density at zero temperature. <i>Chemical Physics</i> , 2010, 370, 78-86.	1.9	70
30	Semiclassical description of diffraction and its quenching by the forward <sup>+</sup> backward version of the initial value representation. <i>Journal of Chemical Physics</i> , 2001, 114, 2572-2579.	3.0	69
31	Theoretical Study of Photoinduced Electron-Transfer Processes in the Dye <sup>+</sup> Semiconductor System Alizarin <sup>+</sup> TiO <sub>2</sub> . <i>Journal of Physical Chemistry C</i> , 2010, 114, 18481-18493.	3.1	69
32	Calculation of reactive flux correlation functions for systems in a condensed phase environment: A multilayer multiconfiguration time-dependent Hartree approach. <i>Journal of Chemical Physics</i> , 2006, 125, 174502.	3.0	66
33	Bistability signatures in nonequilibrium charge transport through molecular quantum dots. <i>Physical Review B</i> , 2012, 86, .	3.2	65
34	Live-cell single-molecule dynamics of PcG proteins imposed by the DIPG H3.3K27M mutation. <i>Nature Communications</i> , 2018, 9, 2080.	12.8	63
35	Nanoparticle-Mediated Intervalence Transfer. <i>Journal of the American Chemical Society</i> , 2008, 130, 12156-12162.	13.7	59
36	Numerically exact, time-dependent study of correlated electron transport in model molecular junctions. <i>Journal of Chemical Physics</i> , 2013, 138, 134704.	3.0	58

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37	Direct Aryloxylation/Alkyloxylation of Dialkyl Phosphonates for the Synthesis of Mixed Phosphonates. <i>Angewandte Chemie - International Edition</i> , 2018, 57, 6624-6628.	13.8	51
38	Computational Study of Bridge-Assisted Intervale Electron Transfer. <i>Journal of Physical Chemistry A</i> , 2010, 114, 6039-6046.	2.5	50
39	Quantum dynamical simulation of ultrafast molecular processes in the condensed phase. <i>Chemical Physics</i> , 2006, 322, 210-222.	1.9	48
40	Computational study of titanium (IV) complexes with organic chromophores. <i>International Journal of Quantum Chemistry</i> , 2006, 106, 1291-1303.	2.0	47
41	Nonperturbative quantum simulation of time-resolved nonlinear spectra: Methodology and application to electron transfer reactions in the condensed phase. <i>Chemical Physics</i> , 2008, 347, 139-151.	1.9	45
42	Effects of intense femtosecond pumping on ultrafast electronic-vibrational dynamics in molecular systems with relaxation. <i>Journal of Chemical Physics</i> , 2008, 129, 214303.	3.0	45
43	Correlated electron-nuclear dynamics in ultrafast photoinduced electron-transfer reactions at dye-semiconductor interfaces. <i>Physical Review B</i> , 2007, 76, .	3.2	40
44	Meirâ€™Wingreen formula for heat transport in a spin-boson nanojunction model. <i>Journal of Chemical Physics</i> , 2010, 133, 084503.	3.0	39
45	Multilayer Multiconfiguration Time-Dependent Hartree Study of Vibrationally Coupled Electron Transport Using the Scattering-State Representation. <i>Journal of Physical Chemistry A</i> , 2013, 117, 7431-7441.	2.5	39
46	Computational Study of Ferrocene-Based Molecular Frameworks with 2,5-Diethynylpyridine as a Chemical Bridge. <i>Materials</i> , 2010, 3, 2668-2683.	2.9	37
47	Orbital-Symmetry-Dependent Electron Transfer through Molecules Assembled on Metal Substrates. <i>Journal of Physical Chemistry Letters</i> , 2012, 3, 436-440.	4.6	35
48	Quantum dynamical simulation of ultrafast photoinduced electron transfer processes in a mixed-valence compound. <i>Chemical Physics Letters</i> , 2002, 358, 298-306.	2.6	34
49	Sub-Ohmic to super-Ohmic crossover behavior in nonequilibrium quantum systems with electron-phonon interactions. <i>Physical Review B</i> , 2015, 92, .	3.2	33
50	On regularizing the MCTDH equations of motion. <i>Journal of Chemical Physics</i> , 2018, 148, 124105.	3.0	32
51	On regularizing the ML-MCTDH equations of motion. <i>Journal of Chemical Physics</i> , 2018, 149, 044119.	3.0	31
52	On the memory kernel and the reduced system propagator. <i>Journal of Chemical Physics</i> , 2018, 149, 104105.	3.0	28
53	Iterative Calculation of Energy Eigenstates Employing the Multilayer Multiconfiguration Time-Dependent Hartree Theory. <i>Journal of Physical Chemistry A</i> , 2014, 118, 9253-9261.	2.5	26
54	Quantum dynamics of electron-transfer reactions: photoinduced intermolecular electron transfer in a porphyrinâ€™quinone complex. <i>Molecular Physics</i> , 2012, 110, 751-763.	1.7	25

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55	Self-consistent hybrid approach for simulating electron transfer reactions in condensed phases. Israel Journal of Chemistry, 2002, 42, 167-182.	2.3	23
56	Dynamics of a two-level system coupled to a bath of spins. Journal of Chemical Physics, 2012, 137, 22A504.	3.0	22
57	Metal-free cross-coupling of $\pi$ -conjugated triazenes with unactivated arenes via photoactivation. Organic Chemistry Frontiers, 2019, 6, 152-161.	4.5	22
58	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
59	Phonon dynamics in correlated quantum systems driven away from equilibrium. Physical Review B, 2014, 90, .	3.2	20
60	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
61	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
62	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
63	Direct Aryloxylation/Alkyloxylation of Dialkyl Phosphonates for the Synthesis of Mixed Phosphonates. Angewandte Chemie, 2018, 130, 6734-6738.	2.0	15
64	Trisulfur-Radical-Anion-Triggered $C(sp^2)$ -H Amination of Electron-Deficient Alkenes. Organic Letters, 2020, 22, 9751-9756.	4.6	14
65	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
66	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
67	A Langevin equation approach to electron transfer reactions in the diabatic basis. Journal of Chemical Physics, 2008, 129, 144502.	3.0	10
68	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
69	Photocycloaddition of $S_2$ , $S_2$ -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
70	Chemical Bonding as a New Avenue for Controlling Excited-State Properties and Excitation Energy Transfer Processes in Zinc Phthalocyanine-Fullerene Dyads. Chemistry - A European Journal, 2021, 27, 4159-4167.	3.3	10
71	Dynamics of electron transfer in complex glassy environment modeled by the Cole-Davidson spectral density. Molecular Physics, 2012, 110, 581-594.	1.7	9
72	Importance of Appropriately Regularizing the ML-MCTDH Equations of Motion. Journal of Physical Chemistry A, 2021, 125, 3077-3087.	2.5	9

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73	On the accuracy of the noninteracting electron approximation for vibrationally coupled electron transport. <i>Chemical Physics</i> , 2016, 481, 117-123.	1.9	6
74	Approximate DFT-based methods for generating diabatic states and calculating electronic couplings: models of two and more states. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 2571-2584.	2.8	6
75	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. <i>Chinese Journal of Chemical Physics</i> , 2018, 31, 446-456.	1.3	6
76	Experimental and theoretical rationalization for the base pairing abilities of inosine, guanosine, adenosine, and their corresponding 8-oxo-7,8-dihydropurine, and 8-bromopurine analogues within A-form duplexes of RNA. <i>Biopolymers</i> , 2020, 111, e23410.	2.4	6
77	Heat Transport in a Spin-Boson Model at Low Temperatures: A Multilayer Multiconfiguration Time-Dependent Hartree Study. <i>Entropy</i> , 2020, 22, 1099.	2.2	5
78	Synthesis, Thermal Stability, Biophysical Properties, and Molecular Modeling of Oligonucleotides of RNA Containing 2-thiophenylmethyl Groups. <i>Journal of Organic Chemistry</i> , 2016, 81, 8947-8958.	3.2	4
79	Computational study on the removal of photolabile protecting groups by photochemical reactions. <i>Computational and Theoretical Chemistry</i> , 2019, 1151, 1-11.	2.5	4
80	A unified view of hierarchy approach and formula of differentiation. <i>Journal of Chemical Physics</i> , 2019, 151, 164110.	3.0	3
81	COMPUTATIONAL STUDY OF BRIDGE-MEDIATED INTERVALENCE ELECTRON TRANSFER II: COUPLINGS IN DIFFERENT METALLOCENE COMPLEXES. <i>Journal of Theoretical and Computational Chemistry</i> , 2012, 11, 1341-1356.	1.8	2
82	Quantum kinetic expansion in the spin-boson model: Matrix formulation and system-bath factorized initial state. <i>Journal of Chemical Physics</i> , 2017, 147, 244112.	3.0	2
83	Modeling of canonical and C2-thiophenylmethyl modified hexamers of RNA. Insights into the nature of structural changes and thermal stability. <i>New Journal of Chemistry</i> , 2018, 42, 10177-10183.	2.8	1
84	Computational study of topological effects on intramolecular electron transfer in mixed-valence compounds. <i>Frontiers of Chemistry in China: Selected Publications From Chinese Universities</i> , 2011, 6, 280-286.	0.4	0
85	Memorial Viewpoint for William L. Hase. <i>Journal of Physical Chemistry A</i> , 2020, 124, 4183-4184.	2.5	0
86	Demonstration of a Stereospecific Photochemical Meta Effect. <i>Photochem</i> , 2022, 2, 69-76.	2.2	0