Haibo

List of Publications by Year in descending order

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83	2,745	172457	206112
papers	citations	29 h-index	48 g-index

83	83	83	3854
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Low-Scaling Excited State Calculation Using the Block Interaction Product State. Journal of Physical Chemistry Letters, 2022, 13, 462-470.	4.6	8
2	Post-Density Matrix Renormalization Group Methods for Describing Dynamic Electron Correlation with Large Active Spaces. Journal of Physical Chemistry Letters, 2022, 13, 904-915.	4.6	19
3	Stochastic Adaptive Single-Site Time-Dependent Variational Principle. Jacs Au, 2022, 2, 335-340.	7.9	11
4	Performance Prediction and Experimental Optimization Assisted by Machine Learning for Organic Photovoltaics. Advanced Intelligent Systems, 2022, 4, .	6.1	13
5	An ultrafast-response and high-detectivity self-powered perovskite photodetector based on a triazine-derived star-shaped small molecule as a dopant-free hole transporting layer. Journal of Materials Chemistry C, 2021, 9, 7632-7642.	5.5	15
6	Unraveling fundamental active units in carbon nitride for photocatalytic oxidation reactions. Nature Communications, 2021, 12, 320.	12.8	150
7	Free-triplet generation with improved efficiency in tetracene oligomers through spatially separated triplet pair states. Nature Chemistry, 2021, 13, 559-567.	13.6	46
8	Substructure shock-friction theory for molecular transport in liquids. Journal of Molecular Liquids, 2021, 330, 115655.	4.9	1
9	Simultaneous Optimization of Donor/Acceptor Pairs and Device Specifications for Nonfullerene Organic Solar Cells Using a QSPR Model with Morphological Descriptors. Journal of Physical Chemistry Letters, 2021, 12, 4980-4986.	4.6	16
10	Mechanisms of a Cyclobutane-Fused Lactone Hydrolysis in Alkaline and Acidic Conditions. Molecules, 2021, 26, 3519.	3.8	0
11	Theoretical Study of Effects of Solvents, Ligands, and Anions on Separation of Trivalent Lanthanides and Actinides. Inorganic Chemistry, 2021, 60, 9552-9562.	4.0	14
12	An ester bond underlies the mechanical strength of a pathogen surface protein. Nature Communications, 2021, 12, 5082.	12.8	20
13	Quantum dynamics simulation of intramolecular singlet fission in covalently linked tetracene dimer. Journal of Chemical Physics, 2021, 155, 194101.	3.0	15
14	Computational and data driven molecular material design assisted by low scaling quantum mechanics calculations and machine learning. Chemical Science, 2021, 12, 14987-15006.	7.4	16
15	Single-Molecule MicroRNA Electrochemiluminescence Detection Using Cyclometalated Dinuclear Ir(III) Complex with Synergistic Effect. Analytical Chemistry, 2020, 92, 1268-1275.	6.5	23
16	Dopantâ€Free and Greenâ€Solventâ€Processable Holeâ€Transporting Materials for Highly Efficient Inverted Planar Perovskite Solar Cells. Solar Rrl, 2020, 4, 2000327.	5.8	16
17	Charge transfer via deep hole in the J51/N2200 blend. Journal of Chemical Physics, 2020, 153, 054705.	3.0	1
18	Automatic Selection of Active Orbitals from Generalized Valence Bond Orbitals. Journal of Physical Chemistry A, 2020, 124, 8321-8329.	2.5	14

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19	Singlet Fission Dynamics in Tetracene Single Crystals Probed by Polarization-Dependent Two-Dimensional Electronic Spectroscopy. Journal of Physical Chemistry A, 2020, 124, 10447-10456.	2.5	14
20	The macroscopic viscosity approximation: A first-principle relationship between molecular diffusion and viscosity. AIP Advances, 2020, 10, 035321.	1.3	11
21	Multi-reference Epsteinâ€“Nesbet perturbation theory with density matrix renormalization group reference wavefunction. Electronic Structure, 2020, 2, 014002.	2.8	15
22	Accelerated Discovery of Potential Organic Dyes for Dyeâ€Sensitized Solar Cells by Interpretable Machine Learning Models and Virtual Screening. Solar Rrl, 2020, 4, 2000110.	5.8	35
23	Long Persistent Luminescence Enabled by Dissociation of Triplet Intermediate States in an Organic Guest/Host System. Journal of Physical Chemistry Letters, 2020, 11, 3582-3588.	4.6	12
24	Axial ligands tailoring the ORR activity of cobalt porphyrin. Science Bulletin, 2019, 64, 1158-1166.	9.0	57
25	Designing promising molecules for organic solar cells via machine learning assisted virtual screening. Journal of Materials Chemistry A, 2019, 7, 17480-17488.	10.3	80
26	Boosting Luminance Energy Transfer Efficiency in Upconversion Nanoparticles with an Energyâ€Concentrating Zone. Angewandte Chemie - International Edition, 2019, 58, 12117-12122.	13.8	56
27	Unraveling Correlations between Molecular Properties and Device Parameters of Organic Solar Cells Using Machine Learning. Journal of Physical Chemistry Letters, 2019, 10, 7277-7284.	4.6	65
28	Carbon Dioxide (CO₂) Fixation: Linearly Bridged Zn₂ Paddlewheel Nodes by CO₂ in a Metalâ€“Organic Framework. Inorganic Chemistry, 2019, 58, 16040-16046.	4.0	7
29	Highâ€Performance Inverted Planar Perovskite Solar Cells Enhanced by Thickness Tuning of New Dopantâ€Free Hole Transporting Layer. Small, 2019, 15, e1904715.	10.0	47
30	Ultrafast hole transfer mediated by polaron pairs in all-polymer photovoltaic blends. Nature Communications, 2019, 10, 398.	12.8	56
31	A molecular contact theory for simulating polarization: application to dielectric constant prediction. Physical Chemistry Chemical Physics, 2019, 21, 14846-14857.	2.8	8
32	A Bifunctional Saddleâ€Shaped Small Molecule as a Dopantâ€Free Hole Transporting Material and Interfacial Layer for Efficient and Stable Perovskite Solar Cells. Solar Rrl, 2019, 3, 1900011.	5.8	34
33	Excitonâ€“Phonon Interaction Model for Singlet Fission in Prototypical Molecular Crystals. Journal of Chemical Theory and Computation, 2019, 15, 3721-3729.	5.3	31
34	Direct Extracellular Electron Transfer of the Geobacter sulfurreducens Pili Relevant to Interaromatic Distances. BioMed Research International, 2019, 2019, 1-12.	1.9	8
35	Strong optical response and light emission from a monolayer molecular crystal. Nature Communications, 2019, 10, 5589.	12.8	59
36	Time-dependent density matrix renormalization group quantum dynamics for realistic chemical systems. Journal of Chemical Physics, 2019, 151, 224101.	3.0	45

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37	Uniform and ultrathin high-Îº gate dielectrics for two-dimensional electronic devices. Nature Electronics, 2019, 2, 563-571.	26.0	204
38	Full Quantum Dynamics Simulation of a Realistic Molecular System Using the Adaptive Time-Dependent Density Matrix Renormalization Group Method. Journal of Physical Chemistry Letters, 2018, 9, 413-419.	4.6	34
39	Unexpected solvent effects on the UV/Vis absorption spectra of o -cresol in toluene and benzene: in contrast with non-aromatic solvents. Royal Society Open Science, 2018, 5, 171928.	2.4	16
40	The time-dependent density matrix renormalisation group method. Molecular Physics, 2018, 116, 854-868.	1.7	12
41	Dissolution and homogeneous photocatalysis of polymeric carbon nitride. Chemical Science, 2018, 9, 7912-7915.	7.4	42
42	Chlorinated Wide-Bandgap Donor Polymer Enabling Annealing Free Nonfullerene Solar Cells with the Efficiency of 11.5%. Journal of Physical Chemistry Letters, 2018, 9, 6955-6962.	4.6	70
43	Toward Predicting Efficiency of Organic Solar Cells via Machine Learning and Improved Descriptors. Advanced Energy Materials, 2018, 8, 1801032.	19.5	154
44	Cyclometalated Ir(<scp>iii</scp>) complexes [Ir(tpy)(bbibH₂)Cl][PF₆] and [Ir(tpy)(bmbib)Cl][PF₆]: intramolecular Ì€â‹¯Ï€ interactions leading to facile synthesis and enhanced luminescence. Dalton Transactions, 2018, 47, 9779-9786.	3.3	9
45	Externally-Contracted Multireference Configuration Interaction Method Using a DMRG Reference Wave Function. Journal of Chemical Theory and Computation, 2018, 14, 4747-4755.	5.3	26
46	Trends in the electronic and geometric structure of non-fullerene based acceptors for organic solar cells. Energy and Environmental Science, 2017, 10, 395-401.	30.8	94
47	Single-Molecule Mechanics of Catechol-Iron Coordination Bonds. ACS Biomaterials Science and Engineering, 2017, 3, 979-989.	5.2	67
48	A fragmentation-based approach for evaluating the intra-chain excitonic couplings in conjugated polymers. Chemical Physics Letters, 2017, 679, 152-157.	2.6	9
49	Efficient Reconstruction of CAS-CI-Type Wave Functions for a DMRG State Using Quantum Information Theory and a Genetic Algorithm. Journal of Chemical Theory and Computation, 2017, 13, 4699-4710.	5.3	18
50	Simultaneous Noncovalent Modification and Exfoliation of 2D Carbon Nitride for Enhanced Electrochemiluminescent Biosensing. Journal of the American Chemical Society, 2017, 139, 11698-11701.	13.7	247
51	Aggregation-induced visible light absorption makes reactant 1,2-diisocyanoarenes act as photosensitizers in double radical isocyanide insertions. Physical Chemistry Chemical Physics, 2017, 19, 31443-31451.	2.8	6
52	Single Molecule Study of Force-Induced Rotation of Carbonâ€“Carbon Double Bonds in Polymers. ACS Nano, 2017, 11, 194-203.	14.6	34
53	Theoretical Investigation of Mono- and Di-Chloro-Substitient Effects on the Insulation and Greenhouse Properties of Octafluorocyclobutane. Frontiers in Chemistry, 2016, 4, 47.	3.6	0
54	Opposite Anisotropy Effects of Singlet and Triplet Exciton Diffusion in Tetracene Crystal. ChemistryOpen, 2016, 5, 201-205.	1.9	9

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55	Ultrafast Long-Range Charge Separation in Organic Photovoltaics: Promotion by Off-Diagonal Vibronic Couplings and Entropy Increase. Journal of Physical Chemistry Letters, 2016, 7, 4830-4835.	4.6	50
56	Electronic Structure Properties of Two-Dimensional Ï€-Conjugated Polymers. Macromolecules, 2016, 49, 1305-1312.	4.8	32
57	2-(Anthracenyl)-4,5-bis(2,5-dimethyl(3-thienyl))-1H-imidazole: regulatable stacking structures, reversible grinding- and heating-induced emission switching, and solid-state photodimerization behavior. Chemical Science, 2016, 7, 451-456.	7.4	27
58	Density-matrix renormalization group algorithm with multi-level active space. Journal of Chemical Physics, 2015, 143, 034105.	3.0	17
59	Modulating the Exciton Dissociation Rate by up to More than Two Orders of Magnitude by Controlling the Alignment of LUMO + 1 in Organic Photovoltaics. Journal of Physical Chemistry C, 2014, 118, 27272-27280.	3.1	34
60	Hydration structure of Na⁺, K⁺, F^{â^'}, and Cl^{â^'} in ambient and supercritical water: A quantum mechanics/molecular mechanics study. International Journal of Quantum Chemistry, 2014, 114, 1006-1011.	2.0	23
61	Direct Optical Generation of Longâ€Range Chargeâ€Transfer States in Organic Photovoltaics. Advanced Materials, 2014, 26, 6163-6167.	21.0	57
62	Electronic Excited States in Amorphous MEH-PPV Polymers from Large-Scale First Principles Calculations. Journal of Chemical Theory and Computation, 2014, 10, 1272-1282.	5.3	30
63	Calculating Excited States of Molecular Aggregates by the Renormalized Excitonic Method. Journal of Physical Chemistry A, 2013, 117, 3655-3665.	2.5	19
64	Response to â€œComment on â€˜Solvatochromic shifts of polar and non-polar molecules in ambient and supercritical water: A sequential quantum mechanics/molecular mechanics study including solute-solvent electron exchange-correlationâ€â€™ [J. Chem. Phys. 138, 217101 (2013)]. Journal of Chemical Physics, 2013, 138, 217102.	3.0	0
65	Assessment of various natural orbitals as the basis of large active space density-matrix renormalization group calculations. Journal of Chemical Physics, 2013, 138, 224105.	3.0	37
66	Solvent effect on electronic absorption, fluorescence, and phosphorescence of acetone in water: Revisited by quantum mechanics/molecular mechanics (QM/MM) simulations. Journal of Chemical Physics, 2013, 138, 224505.	3.0	13
67	A new fragment-based approach for calculating electronic excitation energies of large systems. Journal of Chemical Physics, 2012, 136, 024113.	3.0	24
68	Solvatochromic shifts of polar and non-polar molecules in ambient and supercritical water: A sequential quantum mechanics/molecular mechanics study including solute-solvent electron exchange-correlation. Journal of Chemical Physics, 2012, 137, 214504.	3.0	16
69	Three Novel Isomeric Zinc Metalâ€“Organic Frameworks from a Tetracarboxylate Linker. Inorganic Chemistry, 2012, 51, 7066-7074.	4.0	36
70	Density dependence of the entropy and the solvation shell structure in supercritical water via molecular dynamics simulation. Journal of Chemical Physics, 2012, 136, 214501.	3.0	13
71	Implementation of renormalized excitonic method at ab initio level. Journal of Computational Chemistry, 2012, 33, 34-43.	3.3	23
72	Density dependence of hydrogen bonding and the translational-orientational structural order in supercritical water: A molecular dynamics study. Journal of Chemical Physics, 2011, 135, 054504.	3.0	32

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73	Effect of Electronâ^'Electron Interactions on the Charge Carrier Transitions intrans-Polyacetylene. Journal of Physical Chemistry A, 2010, 114, 5439-5444.	2.5	13
74	BLOCK DENSITY MATRIX RENORMALIZATION GROUP WITH EFFECTIVE INTERACTIONS. Journal of Theoretical and Computational Chemistry, 2009, 08, 837-848.	1.8	2
75	Dynamical Simulations of Polaron Transport in Conjugated Polymers with the Inclusion of Electronâ^'Electron Interactions. Journal of Physical Chemistry A, 2009, 113, 1360-1367.	2.5	26
76	Dynamical simulations of charged soliton transport in conjugated polymers with the inclusion of electron-electron interactions. Journal of Chemical Physics, 2008, 129, 244705.	3.0	13
77	Static polarizability and second hyperpolarizability of closed- and open-shell Ï€-conjugated polymers. Journal of Chemical Physics, 2007, 126, 044903.	3.0	20
78	Theoretical Study of Very High Spin Organic Ï€-Conjugated Polyradicals. Journal of Physical Chemistry A, 2007, 111, 9471-9478.	2.5	19
79	Theoretical Investigation of Static Characterization on Nonlinear Elementary Excitations intrans-Polyacetylene. Journal of Physical Chemistry B, 2006, 110, 26488-26496.	2.6	6
80	Solvent effect on light-emitting property of Si nanocrystals. Physics Letters, Section A: General, Atomic and Solid State Physics, 2005, 334, 447-452.	2.1	23
81	Spin distribution in neutral polyene radicals: Pariserâ€"Parrâ€"Pople model studied with the density matrix renormalization group method. Journal of Chemical Physics, 2005, 122, 104909.	3.0	19
82	Theoretical study of the lowest Ï€â†'Ï€* excitation energies for neutral and doped polyenes. Journal of Chemical Physics, 2005, 123, 084303.	3.0	16
83	â€œTriplet-excited regionâ€•in polyene oligomers revisited: Pariserâ€"Parrâ€"Pople model studied with the density matrix renormalization group method. Journal of Chemical Physics, 2004, 120, 9316-9320.	3.0	16