Haibo

List of Publications by Citations

82 papers	1,815 citations	26 h-index	39 g-index
83 ext. papers	2,273 ext. citations	7.1 avg, IF	5.39 L-index

#	Paper	IF	Citations
82	Simultaneous Noncovalent Modification and Exfoliation of 2D Carbon Nitride for Enhanced Electrochemiluminescent Biosensing. *Journal of the American Chemical Society*, **2017**, 139, 11698-11701	16.4	202
81	Toward Predicting Efficiency of Organic Solar Cells via Machine Learning and Improved Descriptors. *Advanced Energy Materials*, **2018**, 8, 1801032	21.8	95
80	Uniform and ultrathin high-[illegible]gate dielectrics for two-dimensional electronic devices. *Nature Electronics*, **2019**, 2, 563-571	28.4	93
79	Trends in the electronic and geometric structure of non-fullerene based acceptors for organic solar cells. *Energy and Environmental Science*, **2017**, 10, 395-401	35.4	77
78	Unraveling fundamental active units in carbon nitride for photocatalytic oxidation reactions. *Nature Communications*, **2021**, 12, 320	17.4	55
77	Designing promising molecules for organic solar cells via machine learning assisted virtual screening. *Journal of Materials Chemistry A*, **2019**, 7, 17480-17488	13	50
76	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	6.4	50
75	Single-Molecule Mechanics of Catechol-Iron Coordination Bonds. *ACS Biomaterials Science and Engineering*, **2017**, 3, 979-989	5.5	49
74	Direct optical generation of long-range charge-transfer states in organic photovoltaics. *Advanced Materials*, **2014**, 26, 6163-7	24	49
73	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	6.4	41
72	Ultrafast hole transfer mediated by polaron pairs in all-polymer photovoltaic blends. *Nature Communications*, **2019**, 10, 398	17.4	39
71	Strong optical response and light emission from a monolayer molecular crystal. *Nature Communications*, **2019**, 10, 5589	17.4	36
70	Three novel isomeric zinc metal-organic frameworks from a tetracarboxylate linker. *Inorganic Chemistry*, **2012**, 51, 7066-74	5.1	35
69	Unraveling Correlations between Molecular Properties and Device Parameters of Organic Solar Cells Using Machine Learning. *Journal of Physical Chemistry Letters*, **2019**, 10, 7277-7284	6.4	32
68	Boosting Luminance Energy Transfer Efficiency in Upconversion Nanoparticles with an Energy-Concentrating Zone. *Angewandte Chemie - International Edition*, **2019**, 58, 12117-12122	16.4	31
67	Assessment of various natural orbitals as the basis of large active space density-matrix renormalization group calculations. *Journal of Chemical Physics*, **2013**, 138, 224105	3.9	31
66	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	3.9	31

65	Axial ligands tailoring the ORR activity of cobalt porphyrin. *Science Bulletin*, **2019**, 64, 1158-1166	10.6	30
64	High-Performance Inverted Planar Perovskite Solar Cells Enhanced by Thickness Tuning of New Dopant-Free Hole Transporting Layer. *Small*, **2019**, 15, e1904715	11	30
63	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	3.8	29
62	Dissolution and homogeneous photocatalysis of polymeric carbon nitride. *Chemical Science*, **2018**, 9, 7912-7915	9.4	29
61	A Bifunctional Saddle-Shaped Small Molecule as a Dopant-Free Hole Transporting Material and Interfacial Layer for Efficient and Stable Perovskite Solar Cells. *Solar Rrl*, **2019**, 3, 1900011	7.1	27
60	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	6.4	27
59	Electronic Structure Properties of Two-Dimensional □Conjugated Polymers. *Macromolecules*, **2016**, 49, 1305-1312	5.5	27
58	Electronic Excited States in Amorphous MEH-PPV Polymers from Large-Scale First Principles Calculations. *Journal of Chemical Theory and Computation*, **2014**, 10, 1272-82	6.4	27
57	Time-dependent density matrix renormalization group quantum dynamics for realistic chemical systems. *Journal of Chemical Physics*, **2019**, 151, 224101	3.9	27
56	Single Molecule Study of Force-Induced Rotation of Carbon-Carbon Double Bonds in Polymers. *ACS Nano*, **2017**, 11, 194-203	16.7	25
55	Dynamical simulations of polaron transport in conjugated polymers with the inclusion of electron-electron interactions. *Journal of Physical Chemistry A*, **2009**, 113, 1360-7	2.8	23
54	Solvent effect on light-emitting property of Si nanocrystals. *Physics Letters, Section A: General, Atomic and Solid State Physics*, **2005**, 334, 447-452	2.3	23
53	Exciton-Phonon Interaction Model for Singlet Fission in Prototypical Molecular Crystals. *Journal of Chemical Theory and Computation*, **2019**, 15, 3721-3729	6.4	22
52	Implementation of renormalized excitonic method at ab initio level. *Journal of Computational Chemistry*, **2012**, 33, 34-43	3.5	21
51	Externally-Contracted Multireference Configuration Interaction Method Using a DMRG Reference Wave Function. *Journal of Chemical Theory and Computation*, **2018**, 14, 4747-4755	6.4	20
50	2-(Anthracenyl)-4,5-bis(2,5-dimethyl(3-thienyl))-1-imidazole: regulatable stacking structures, reversible grinding- and heating-induced emission switching, and solid-state photodimerization behavior. *Chemical Science*, **2016**, 7, 451-456	9.4	19
49	A new fragment-based approach for calculating electronic excitation energies of large systems. *Journal of Chemical Physics*, **2012**, 136, 024113	3.9	19
48	Static polarizability and second hyperpolarizability of closed- and open-shell pi-conjugated polymers. *Journal of Chemical Physics*, **2007**, 126, 044903	3.9	19

47	Spin distribution in neutral polyene radicals: Pariser-Parr-Pople model studied with the density matrix renormalization group method. *Journal of Chemical Physics*, **2005**, 122, 104909	3.9	19
46	Hydration structure of Na+, K+, F and Cl in ambient and supercritical water: A quantum mechanics/molecular mechanics study. *International Journal of Quantum Chemistry*, **2014**, 114, 1006-1011	2.1	17
45	Theoretical study of very high spin organic pi-conjugated polyradicals. *Journal of Physical Chemistry A*, **2007**, 111, 9471-8	2.8	17
44	Calculating excited states of molecular aggregates by the renormalized excitonic method. *Journal of Physical Chemistry A*, **2013**, 117, 3655-65	2.8	16
43	"Triplet-excited region" in polyene oligomers revisited: Pariser-Parr-Pople model studied with the density matrix renormalization group method. *Journal of Chemical Physics*, **2004**, 120, 9316-20	3.9	16
42	Free-triplet generation with improved efficiency in tetracene oligomers through spatially separated triplet pair states. *Nature Chemistry*, **2021**, 13, 559-567	17.6	16
41	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	3.9	15
40	Theoretical study of the lowest pi-->pi* excitation energies for neutral and doped polyenes. *Journal of Chemical Physics*, **2005**, 123, 084303	3.9	15
39	Accelerated Discovery of Potential Organic Dyes for Dye-Sensitized Solar Cells by Interpretable Machine Learning Models and Virtual Screening. *Solar Rrl*, **2020**, 4, 2000110	7.1	15
38	Density-matrix renormalization group algorithm with multi-level active space. *Journal of Chemical Physics*, **2015**, 143, 034105	3.9	13
37	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	6.4	13
36	Density dependence of the entropy and the solvation shell structure in supercritical water via molecular dynamics simulation. *Journal of Chemical Physics*, **2012**, 136, 214501	3.9	13
35	Effect of electron-electron interactions on the charge carrier transitions in trans-polyacetylene. *Journal of Physical Chemistry A*, **2010**, 114, 5439-44	2.8	13
34	Dynamical simulations of charged soliton transport in conjugated polymers with the inclusion of electron-electron interactions. *Journal of Chemical Physics*, **2008**, 129, 244705	3.9	13
33	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	3.9	11
32	Multi-reference Epstein Nesbet perturbation theory with density matrix renormalization group reference wavefunction. *Electronic Structure*, **2020**, 2, 014002	2.6	10
31	Unexpected solvent effects on the UV/Vis absorption spectra of -cresol in toluene and benzene: in contrast with non-aromatic solvents. *Royal Society Open Science*, **2018**, 5, 171928	3.3	9
30	Single-Molecule MicroRNA Electrochemiluminescence Detection Using Cyclometalated Dinuclear Ir(III) Complex with Synergistic Effect. *Analytical Chemistry*, **2020**, 92, 1268-1275	7.8	9

29	The time-dependent density matrix renormalisation group method. *Molecular Physics*, **2018**, 116, 854-868.	1.7	9
28	A molecular contact theory for simulating polarization: application to dielectric constant prediction. *Physical Chemistry Chemical Physics*, **2019**, 21, 14846-14857	3.6	8
27	The macroscopic viscosity approximation: A first-principle relationship between molecular diffusion and viscosity. *AIP Advances*, **2020**, 10, 035321	1.5	7
26	Carbon Dioxide (CO) Fixation: Linearly Bridged Zn Paddlewheel Nodes by CO in a Metal-Organic Framework. *Inorganic Chemistry*, **2019**, 58, 16040-16046	5.1	7
25	Automatic Selection of Active Orbitals from Generalized Valence Bond Orbitals. *Journal of Physical Chemistry A*, **2020**, 124, 8321-8329	2.8	7
24	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	6.4	7
23	Opposite Anisotropy Effects of Singlet and Triplet Exciton Diffusion in Tetracene Crystal. *ChemistryOpen*, **2016**, 5, 201-205	2.3	7
22	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	6.4	7
21	An ester bond underlies the mechanical strength of a pathogen surface protein. *Nature Communications*, **2021**, 12, 5082	17.4	7
20	A fragmentation-based approach for evaluating the intra-chain excitonic couplings in conjugated polymers. *Chemical Physics Letters*, **2017**, 679, 152-157	2.5	6
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	2.8	6
18	Theoretical investigation of static characterization on nonlinear elementary excitations in trans-polyacetylene. *Journal of Physical Chemistry B*, **2006**, 110, 26488-96	3.4	6
17	Dopant-Free and Green-Solvent-Processable Hole-Transporting Materials for Highly Efficient Inverted Planar Perovskite Solar Cells. *Solar Rrl*, **2020**, 4, 2000327	7.1	6
16	Cyclometalated Ir(iii) complexes [Ir(tpy)(bbibH)Cl][PF] and [Ir(tpy)(bmbib)Cl][PF]: intramolecular □ interactions leading to facile synthesis and enhanced luminescence. *Dalton Transactions*, **2018**, 47, 9779-9786	4.2	6
15	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	3.6	5
14	Post-Density Matrix Renormalization Group Methods for Describing Dynamic Electron Correlation with Large Active Spaces.. *Journal of Physical Chemistry Letters*, **2022**, 904-915	6.4	5
13	Computational and data driven molecular material design assisted by low scaling quantum mechanics calculations and machine learning.. *Chemical Science*, **2021**, 12, 14987-15006	9.4	3
12	Direct Extracellular Electron Transfer of the Pili Relevant to Interaromatic Distances. *BioMed Research International*, **2019**, 2019, 6151587	3	3

11	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*,	7.1	3
10	BLOCK DENSITY MATRIX RENORMALIZATION GROUP WITH EFFECTIVE INTERACTIONS. *Journal of Theoretical and Computational Chemistry*, **2009**, 08, 837-848	1.8	2
9	Quantum dynamics simulation of intramolecular singlet fission in covalently linked tetracene dimer. *Journal of Chemical Physics*, **2021**, 155, 194101	3.9	2
8	Theoretical Study of Effects of Solvents, Ligands, and Anions on Separation of Trivalent Lanthanides and Actinides. *Inorganic Chemistry*, **2021**, 60, 9552-9562	5.1	2
7	Performance Prediction and Experimental Optimization Assisted by Machine Learning for Organic Photovoltaics. *Advanced Intelligent Systems*,2100261	6	2
6	Stochastic Adaptive Single-Site Time-Dependent Variational Principle.. *Jacs Au*, **2022**, 2, 335-340		1
5	Low-Scaling Excited State Calculation Using the Block Interaction Product State.. *Journal of Physical Chemistry Letters*, **2022**, 462-470	6.4	1
4	Charge transfer via deep hole in the J51/N2200 blend. *Journal of Chemical Physics*, **2020**, 153, 054705	3.9	0
3	Substructure shock-friction theory for molecular transport in liquids. *Journal of Molecular Liquids*, **2021**, 330, 115655	6	0
2	Response to "Comment on "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"[J. Chem. Phys. 138, 217101 (2013)]. *Journal of Chemical Physics*, **2013**, 138, 217102	3.9	
1	Theoretical Investigation of Mono- and Di-Chloro-Substitient Effects on the Insulation and Greenhouse Properties of Octafluorocyclobutane. *Frontiers in Chemistry*, **2016**, 4, 47	5	