

## List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

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	Post-Density Matrix Renormalization Group Methods for Describing Dynamic Electron Correlation with Large Active Spaces.. <i>Journal of Physical Chemistry Letters</i> , <b>2022</b> , 904-915	6.4	5
81	Stochastic Adaptive Single-Site Time-Dependent Variational Principle.. <i>Jacs Au</i> , <b>2022</b> , 2, 335-340		1
80	Low-Scaling Excited State Calculation Using the Block Interaction Product State.. <i>Journal of Physical Chemistry Letters</i> , <b>2022</b> , 462-470	6.4	1
79	Quantum dynamics simulation of intramolecular singlet fission in covalently linked tetracene dimer. <i>Journal of Chemical Physics</i> , <b>2021</b> , 155, 194101	3.9	2
78	Computational and data driven molecular material design assisted by low scaling quantum mechanics calculations and machine learning.. <i>Chemical Science</i> , <b>2021</b> , 12, 14987-15006	9.4	3
77	Free-triplet generation with improved efficiency in tetracene oligomers through spatially separated triplet pair states. <i>Nature Chemistry</i> , <b>2021</b> , 13, 559-567	17.6	16
76	Substructure shock-friction theory for molecular transport in liquids. <i>Journal of Molecular Liquids</i> , <b>2021</b> , 330, 115655	6	0
75	Simultaneous Optimization of Donor/Acceptor Pairs and Device Specifications for Nonfullerene Organic Solar Cells Using a QSPR Model with Morphological Descriptors. <i>Journal of Physical Chemistry Letters</i> , <b>2021</b> , 12, 4980-4986	6.4	7
74	Theoretical Study of Effects of Solvents, Ligands, and Anions on Separation of Trivalent Lanthanides and Actinides. <i>Inorganic Chemistry</i> , <b>2021</b> , 60, 9552-9562	5.1	2
73	Unraveling fundamental active units in carbon nitride for photocatalytic oxidation reactions. <i>Nature Communications</i> , <b>2021</b> , 12, 320	17.4	55
72	An ester bond underlies the mechanical strength of a pathogen surface protein. <i>Nature Communications</i> , <b>2021</b> , 12, 5082	17.4	7
71	Singlet Fission Dynamics in Tetracene Single Crystals Probed by Polarization-Dependent Two-Dimensional Electronic Spectroscopy. <i>Journal of Physical Chemistry A</i> , <b>2020</b> , 124, 10447-10456	2.8	6
70	The macroscopic viscosity approximation: A first-principle relationship between molecular diffusion and viscosity. <i>AIP Advances</i> , <b>2020</b> , 10, 035321	1.5	7
69	Multi-reference Epstein-Nesbet perturbation theory with density matrix renormalization group reference wavefunction. <i>Electronic Structure</i> , <b>2020</b> , 2, 014002	2.6	10
68	Single-Molecule MicroRNA Electrochemiluminescence Detection Using Cyclometalated Dinuclear Ir(III) Complex with Synergistic Effect. <i>Analytical Chemistry</i> , <b>2020</b> , 92, 1268-1275	7.8	9
67	Dopant-Free and Green-Solvent-Processable Hole-Transporting Materials for Highly Efficient Inverted Planar Perovskite Solar Cells. <i>Solar Rrl</i> , <b>2020</b> , 4, 2000327	7.1	6
66	Charge transfer via deep hole in the J51/N2200 blend. <i>Journal of Chemical Physics</i> , <b>2020</b> , 153, 054705	3.9	0

65	Automatic Selection of Active Orbitals from Generalized Valence Bond Orbitals. <i>Journal of Physical Chemistry A</i> , <b>2020</b> , 124, 8321-8329	2.8	7
64	Accelerated Discovery of Potential Organic Dyes for Dye-Sensitized Solar Cells by Interpretable Machine Learning Models and Virtual Screening. <i>Solar Rrl</i> , <b>2020</b> , 4, 2000110	7.1	15
63	Long Persistent Luminescence Enabled by Dissociation of Triplet Intermediate States in an Organic Guest/Host System. <i>Journal of Physical Chemistry Letters</i> , <b>2020</b> , 11, 3582-3588	6.4	7
62	Ultrafast hole transfer mediated by polaron pairs in all-polymer photovoltaic blends. <i>Nature Communications</i> , <b>2019</b> , 10, 398	17.4	39
61	A molecular contact theory for simulating polarization: application to dielectric constant prediction. <i>Physical Chemistry Chemical Physics</i> , <b>2019</b> , 21, 14846-14857	3.6	8
60	A Bifunctional Saddle-Shaped Small Molecule as a Dopant-Free Hole Transporting Material and Interfacial Layer for Efficient and Stable Perovskite Solar Cells. <i>Solar Rrl</i> , <b>2019</b> , 3, 1900011	7.1	27
59	Exciton-Phonon Interaction Model for Singlet Fission in Prototypical Molecular Crystals. <i>Journal of Chemical Theory and Computation</i> , <b>2019</b> , 15, 3721-3729	6.4	22
58	Axial ligands tailoring the ORR activity of cobalt porphyrin. <i>Science Bulletin</i> , <b>2019</b> , 64, 1158-1166	10.6	30
57	Designing promising molecules for organic solar cells via machine learning assisted virtual screening. <i>Journal of Materials Chemistry A</i> , <b>2019</b> , 7, 17480-17488	13	50
56	Boosting Luminescence Energy Transfer Efficiency in Upconversion Nanoparticles with an Energy-Concentrating Zone. <i>Angewandte Chemie - International Edition</i> , <b>2019</b> , 58, 12117-12122	16.4	31
55	Unraveling Correlations between Molecular Properties and Device Parameters of Organic Solar Cells Using Machine Learning. <i>Journal of Physical Chemistry Letters</i> , <b>2019</b> , 10, 7277-7284	6.4	32
54	Carbon Dioxide (CO) Fixation: Linearly Bridged Zn Paddlewheel Nodes by CO in a Metal-Organic Framework. <i>Inorganic Chemistry</i> , <b>2019</b> , 58, 16040-16046	5.1	7
53	High-Performance Inverted Planar Perovskite Solar Cells Enhanced by Thickness Tuning of New Dopant-Free Hole Transporting Layer. <i>Small</i> , <b>2019</b> , 15, e1904715	11	30
52	Direct Extracellular Electron Transfer of the Pili Relevant to Interaromatic Distances. <i>BioMed Research International</i> , <b>2019</b> , 2019, 6151587	3	3
51	Strong optical response and light emission from a monolayer molecular crystal. <i>Nature Communications</i> , <b>2019</b> , 10, 5589	17.4	36
50	Time-dependent density matrix renormalization group quantum dynamics for realistic chemical systems. <i>Journal of Chemical Physics</i> , <b>2019</b> , 151, 224101	3.9	27
49	Uniform and ultrathin high- $\kappa$ gate dielectrics for two-dimensional electronic devices. <i>Nature Electronics</i> , <b>2019</b> , 2, 563-571	28.4	93
48	Full Quantum Dynamics Simulation of a Realistic Molecular System Using the Adaptive Time-Dependent Density Matrix Renormalization Group Method. <i>Journal of Physical Chemistry Letters</i> , <b>2018</b> , 9, 413-419	6.4	27

47	Unexpected solvent effects on the UV/Vis absorption spectra of <i>p</i> -cresol in toluene and benzene: in contrast with non-aromatic solvents. <i>Royal Society Open Science</i> , <b>2018</b> , 5, 171928	3.3	9
46	Externally-Contracted Multireference Configuration Interaction Method Using a DMRG Reference Wave Function. <i>Journal of Chemical Theory and Computation</i> , <b>2018</b> , 14, 4747-4755	6.4	20
45	The time-dependent density matrix renormalisation group method. <i>Molecular Physics</i> , <b>2018</b> , 116, 854-868	6.7	9
44	Dissolution and homogeneous photocatalysis of polymeric carbon nitride. <i>Chemical Science</i> , <b>2018</b> , 9, 7912-7915	9.4	29
43	Chlorinated Wide-Bandgap Donor Polymer Enabling Annealing Free Nonfullerene Solar Cells with the Efficiency of 11.5. <i>Journal of Physical Chemistry Letters</i> , <b>2018</b> , 9, 6955-6962	6.4	50
42	Toward Predicting Efficiency of Organic Solar Cells via Machine Learning and Improved Descriptors. <i>Advanced Energy Materials</i> , <b>2018</b> , 8, 1801032	21.8	95
41	Cyclometalated Ir(III) complexes [Ir(tpy)(bbibH)Cl][PF <sub>6</sub> ] and [Ir(tpy)(bmbib)Cl][PF <sub>6</sub> ]: intramolecular $\pi$ interactions leading to facile synthesis and enhanced luminescence. <i>Dalton Transactions</i> , <b>2018</b> , 47, 9779-9786	4.3	6
40	Trends in the electronic and geometric structure of non-fullerene based acceptors for organic solar cells. <i>Energy and Environmental Science</i> , <b>2017</b> , 10, 395-401	35.4	77
39	Single-Molecule Mechanics of Catechol-Iron Coordination Bonds. <i>ACS Biomaterials Science and Engineering</i> , <b>2017</b> , 3, 979-989	5.5	49
38	A fragmentation-based approach for evaluating the intra-chain excitonic couplings in conjugated polymers. <i>Chemical Physics Letters</i> , <b>2017</b> , 679, 152-157	2.5	6
37	Efficient Reconstruction of CAS-CI-Type Wave Functions for a DMRG State Using Quantum Information Theory and a Genetic Algorithm. <i>Journal of Chemical Theory and Computation</i> , <b>2017</b> , 13, 4699-4710	6.4	13
36	Simultaneous Noncovalent Modification and Exfoliation of 2D Carbon Nitride for Enhanced Electrochemiluminescent Biosensing. <i>Journal of the American Chemical Society</i> , <b>2017</b> , 139, 11698-11701	16.4	202
35	Aggregation-induced visible light absorption makes reactant 1,2-diisocyanobenzenes act as photosensitizers in double radical isocyanide insertions. <i>Physical Chemistry Chemical Physics</i> , <b>2017</b> , 19, 31443-31451	3.6	5
34	Single Molecule Study of Force-Induced Rotation of Carbon-Carbon Double Bonds in Polymers. <i>ACS Nano</i> , <b>2017</b> , 11, 194-203	16.7	25
33	Ultrafast Long-Range Charge Separation in Organic Photovoltaics: Promotion by Off-Diagonal Vibronic Couplings and Entropy Increase. <i>Journal of Physical Chemistry Letters</i> , <b>2016</b> , 7, 4830-4835	6.4	41
32	Electronic Structure Properties of Two-Dimensional $\pi$ -Conjugated Polymers. <i>Macromolecules</i> , <b>2016</b> , 49, 1305-1312	5.5	27
31	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. <i>Chemical Science</i> , <b>2016</b> , 7, 451-456	9.4	19
30	Theoretical Investigation of Mono- and Di-Chloro-Substituent Effects on the Insulation and Greenhouse Properties of Octafluorocyclobutane. <i>Frontiers in Chemistry</i> , <b>2016</b> , 4, 47	5	

29	Opposite Anisotropy Effects of Singlet and Triplet Exciton Diffusion in Tetracene Crystal. <i>ChemistryOpen</i> , <b>2016</b> , 5, 201-205	2.3	7
28	Density-matrix renormalization group algorithm with multi-level active space. <i>Journal of Chemical Physics</i> , <b>2015</b> , 143, 034105	3.9	13
27	Hydration structure of Na <sup>+</sup> , K <sup>+</sup> , F <sup>-</sup> and Cl <sup>-</sup> in ambient and supercritical water: A quantum mechanics/molecular mechanics study. <i>International Journal of Quantum Chemistry</i> , <b>2014</b> , 114, 1006-1011	4.1	17
26	Direct optical generation of long-range charge-transfer states in organic photovoltaics. <i>Advanced Materials</i> , <b>2014</b> , 26, 6163-7	2.4	49
25	Electronic Excited States in Amorphous MEH-PPV Polymers from Large-Scale First Principles Calculations. <i>Journal of Chemical Theory and Computation</i> , <b>2014</b> , 10, 1272-82	6.4	27
24	Modulating the Exciton Dissociation Rate by up to More than Two Orders of Magnitude by Controlling the Alignment of LUMO + 1 in Organic Photovoltaics. <i>Journal of Physical Chemistry C</i> , <b>2014</b> , 118, 27272-27280	3.8	29
23	Calculating excited states of molecular aggregates by the renormalized excitonic method. <i>Journal of Physical Chemistry A</i> , <b>2013</b> , 117, 3655-65	2.8	16
22	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)]. <i>Journal of Chemical Physics</i> , <b>2013</b> , 138, 217102	3.9	
21	Assessment of various natural orbitals as the basis of large active space density-matrix renormalization group calculations. <i>Journal of Chemical Physics</i> , <b>2013</b> , 138, 224105	3.9	31
20	Solvent effect on electronic absorption, fluorescence, and phosphorescence of acetone in water: revisited by quantum mechanics/molecular mechanics (QM/MM) simulations. <i>Journal of Chemical Physics</i> , <b>2013</b> , 138, 224505	3.9	11
19	Implementation of renormalized excitonic method at ab initio level. <i>Journal of Computational Chemistry</i> , <b>2012</b> , 33, 34-43	3.5	21
18	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. <i>Journal of Chemical Physics</i> , <b>2012</b> , 137, 214504	3.9	15
17	Three novel isomeric zinc metal-organic frameworks from a tetracarboxylate linker. <i>Inorganic Chemistry</i> , <b>2012</b> , 51, 7066-74	5.1	35
16	Density dependence of the entropy and the solvation shell structure in supercritical water via molecular dynamics simulation. <i>Journal of Chemical Physics</i> , <b>2012</b> , 136, 214501	3.9	13
15	A new fragment-based approach for calculating electronic excitation energies of large systems. <i>Journal of Chemical Physics</i> , <b>2012</b> , 136, 024113	3.9	19
14	Density dependence of hydrogen bonding and the translational-orientational structural order in supercritical water: a molecular dynamics study. <i>Journal of Chemical Physics</i> , <b>2011</b> , 135, 054504	3.9	31
13	Effect of electron-electron interactions on the charge carrier transitions in trans-polyacetylene. <i>Journal of Physical Chemistry A</i> , <b>2010</b> , 114, 5439-44	2.8	13
12	BLOCK DENSITY MATRIX RENORMALIZATION GROUP WITH EFFECTIVE INTERACTIONS. <i>Journal of Theoretical and Computational Chemistry</i> , <b>2009</b> , 08, 837-848	1.8	2

11	Dynamical simulations of polaron transport in conjugated polymers with the inclusion of electron-electron interactions. <i>Journal of Physical Chemistry A</i> , <b>2009</b> , 113, 1360-7	2.8	23
10	Dynamical simulations of charged soliton transport in conjugated polymers with the inclusion of electron-electron interactions. <i>Journal of Chemical Physics</i> , <b>2008</b> , 129, 244705	3.9	13
9	Theoretical study of very high spin organic pi-conjugated polyradicals. <i>Journal of Physical Chemistry A</i> , <b>2007</b> , 111, 9471-8	2.8	17
8	Static polarizability and second hyperpolarizability of closed- and open-shell pi-conjugated polymers. <i>Journal of Chemical Physics</i> , <b>2007</b> , 126, 044903	3.9	19
7	Theoretical investigation of static characterization on nonlinear elementary excitations in trans-polyacetylene. <i>Journal of Physical Chemistry B</i> , <b>2006</b> , 110, 26488-96	3.4	6
6	Solvent effect on light-emitting property of Si nanocrystals. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , <b>2005</b> , 334, 447-452	2.3	23
5	Spin distribution in neutral polyene radicals: Pariser-Parr-Pople model studied with the density matrix renormalization group method. <i>Journal of Chemical Physics</i> , <b>2005</b> , 122, 104909	3.9	19
4	Theoretical study of the lowest pi-->pi* excitation energies for neutral and doped polyenes. <i>Journal of Chemical Physics</i> , <b>2005</b> , 123, 084303	3.9	15
3	"Triplet-excited region" in polyene oligomers revisited: Pariser-Parr-Pople model studied with the density matrix renormalization group method. <i>Journal of Chemical Physics</i> , <b>2004</b> , 120, 9316-20	3.9	16
2	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. <i>Journal of Materials Chemistry C</i> ,	7.1	3
1	Performance Prediction and Experimental Optimization Assisted by Machine Learning for Organic Photovoltaics. <i>Advanced Intelligent Systems</i> , 2100261	6	2