

Guangjiu Zhao

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93
papers

6,734
citations

31
h-index

82
g-index

95
ext. papers

7,347
ext. citations

5.5
avg, IF

6.34
L-index

#	Paper	IF	Citations
93	Hydrogen bonding in the electronic excited state. <i>Accounts of Chemical Research</i> , 2012 , 45, 404-13	24.3	958
92	Site-selective photoinduced electron transfer from alcoholic solvents to the chromophore facilitated by hydrogen bonding: a new fluorescence quenching mechanism. <i>Journal of Physical Chemistry B</i> , 2007 , 111, 8940-5	3.4	651
91	Early time hydrogen-bonding dynamics of photoexcited coumarin 102 in hydrogen-donating solvents: theoretical study. <i>Journal of Physical Chemistry A</i> , 2007 , 111, 2469-74	2.8	512
90	A near-IR reversible fluorescent probe modulated by selenium for monitoring peroxyxynitrite and imaging in living cells. <i>Journal of the American Chemical Society</i> , 2011 , 133, 11030-3	16.4	469
89	Site-specific solvation of the photoexcited protochlorophyllide a in methanol: formation of the hydrogen-bonded intermediate state induced by hydrogen-bond strengthening. <i>Biophysical Journal</i> , 2008 , 94, 38-46	2.9	425
88	Effects of hydrogen bonding on tuning photochemistry: concerted hydrogen-bond strengthening and weakening. <i>ChemPhysChem</i> , 2008 , 9, 1842-6	3.2	348
87	Ultrafast hydrogen bond strengthening of the photoexcited fluorenone in alcohols for facilitating the fluorescence quenching. <i>Journal of Physical Chemistry A</i> , 2007 , 111, 9218-23	2.8	330
86	Time-dependent density functional theory study on hydrogen-bonded intramolecular charge-transfer excited state of 4-dimethylamino-benzonitrile in methanol. <i>Journal of Computational Chemistry</i> , 2008 , 29, 2010-7	3.5	278
85	Role of intramolecular and intermolecular hydrogen bonding in both singlet and triplet excited states of aminofluorenones on internal conversion, intersystem crossing, and twisted intramolecular charge transfer. <i>Journal of Physical Chemistry A</i> , 2009 , 113, 14329-35	2.8	214
84	The effect of intermolecular hydrogen bonding on the fluorescence of a bimetallic platinum complex. <i>Journal of Physical Chemistry A</i> , 2010 , 114, 9007-13	2.8	202
83	Reconsideration of the excited-state double proton transfer (ESDPT) in 2-aminopyridine/acid systems: role of the intermolecular hydrogen bonding in excited states. <i>Physical Chemistry Chemical Physics</i> , 2009 , 11, 4385-90	3.6	193
82	Photoinduced intramolecular charge transfer and S2 fluorescence in thiophene-pi-conjugated donor-acceptor systems: experimental and TDDFT studies. <i>Chemistry - A European Journal</i> , 2008 , 14, 6935-47	4.8	190
81	pH-Controlled twisted intramolecular charge transfer (TICT) excited state via changing the charge transfer direction. <i>Physical Chemistry Chemical Physics</i> , 2010 , 12, 8914-8	3.6	162
80	Theoretical Insights into Hydrogen Bonding and Its Influence on the Structural and Spectral Properties of Aquo Palladium(II) Complexes: cis-[(dppp)Pd(H2O)2](2+), cis-[(dppp)Pd(H2O)(OSO2CF3)](+)(OSO2CF3)(-), and cis-[(dppp)Pd(H2O)2](2+)(OSO2CF3)(-). <i>Journal of Chemical Theory and Computation</i> , 2009 , 5, 1955-8	6.4	139
79	Photophysical properties of coordination-driven self-assembled metallosupramolecular rhomboids: experimental and theoretical investigations. <i>Journal of Physical Chemistry A</i> , 2010 , 114, 3418-22	2.8	122
78	Excited state electronic structures and photochemistry of heterocyclic annulated perylene (HAP) materials tuned by heteroatoms: S, Se, N, O, C, Si, and B. <i>Journal of Physical Chemistry A</i> , 2009 , 113, 4788-94	2.8	104
77	Modification of n-type organic semiconductor performance of perylene diimides by substitution in different positions: two-dimensional π -stacking and hydrogen bonding. <i>ChemSusChem</i> , 2012 , 5, 879-87	8.3	92

76	A TD-DFT study on the cyanide-chemosensing mechanism of 8-formyl-7-hydroxycoumarin. <i>Journal of Computational Chemistry</i> , 2011 , 32, 668-74	3.5	91
75	Fluorescence quenching phenomena facilitated by excited-state hydrogen bond strengthening for fluorenone derivatives in alcohols. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2010 , 209, 181-185	4.7	91
74	The charge transfer mechanism and spectral properties of a near-infrared heptamethine cyanine dye in alcoholic and aprotic solvents. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2007 , 187, 305-310	4.7	83
73	TD-DFT study on the sensing mechanism of a fluorescent chemosensor for fluoride: excited-state proton transfer. <i>Journal of Computational Chemistry</i> , 2010 , 31, 1759-65	3.5	77
72	Substituent effects on the intramolecular charge transfer and fluorescence of bimetallic platinum complexes. <i>Journal of Physical Chemistry A</i> , 2011 , 115, 6390-3	2.8	76
71	Photoinduced intramolecular charge-transfer state in thiophene- π -conjugated donor-acceptor molecules. <i>Journal of Molecular Structure</i> , 2008 , 876, 102-109	3.4	68
70	The ultrafast dynamics of near-infrared heptamethine cyanine dye in alcoholic and aprotic solvents. <i>Chemical Physics</i> , 2007 , 333, 179-185	2.3	64
69	A HClO-specific near-infrared fluorescent probe for determination of Myeloperoxidase activity and imaging mitochondrial HClO in living cells. <i>Biosensors and Bioelectronics</i> , 2016 , 86, 68-74	11.8	63
68	Photophysical properties of self-assembled multinuclear platinum metallacycles with different conformational geometries. <i>Journal of the American Chemical Society</i> , 2013 , 135, 6694-702	16.4	61
67	Dynamic simulation study on ultrafast excited-state torsional dynamics of 9,9'-bianthryl (BA) in gas phase: Real-time observation of novel oscillation behavior with the torsional coordinate. <i>Chemical Physics Letters</i> , 2008 , 453, 29-34	2.5	57
66	Phase Regulation Strategy of Perovskite Nanocrystals from 1D Orthomorphous NH ₄ PbI ₃ to 3D Cubic (NH ₄) ₂ PbBr ₄ Phase Enhances Photoluminescence. <i>Angewandte Chemie - International Edition</i> , 2019 , 58, 11642-11646	16.4	51
65	Photophysical Properties of a Post-Self-Assembly Host/Guest Coordination Cage: Visible Light Driven Core-to-Cage Charge Transfer. <i>Journal of Physical Chemistry Letters</i> , 2015 , 6, 1942-7	6.4	47
64	Lead-free sodium bismuth halide Cs ₂ NaBiX ₆ double perovskite nanocrystals with highly efficient photoluminescence. <i>Chemical Engineering Journal</i> , 2020 , 397, 125367	14.7	36
63	Photoabsorption of green and red fluorescent protein chromophore anions in vacuo. <i>Biophysical Chemistry</i> , 2007 , 129, 218-23	3.5	33
62	Molecular dynamics simulation exploration of unfolding and refolding of a ten-amino acid miniprotein. <i>Amino Acids</i> , 2012 , 43, 557-65	3.5	28
61	New lead bromide chiral perovskites with ultra-broadband white-light emission. <i>Journal of Materials Chemistry C</i> , 2020 , 8, 5673-5680	7.1	25
60	Combined TDDFT and AIM Insights into Photoinduced Excited State Intramolecular Proton Transfer (ESIPT) Mechanism in Hydroxyl- and Amino-Anthraquinone Solution. <i>Scientific Reports</i> , 2017 , 7, 13766	4.9	24
59	Theoretical exploration of laser-parameter effects on the generation of an isolated attosecond pulse from two-color high-order harmonic generation. <i>Physical Review A</i> , 2010 , 82,	2.6	23

58	Experimental and theoretical study on the photophysical properties of 90° and 60° bimetallic platinum complexes. <i>Journal of Physical Chemistry A</i> , 2012 , 116, 9911-8	2.8	20
57	Hydrogen-bond facilitated intramolecular proton transfer in excited state and fluorescence quenching mechanism of flavonoid compounds in aqueous solution. <i>Journal of Molecular Liquids</i> , 2020 , 302, 112562	6	16
56	DFT/TDDFT theoretical investigation on the excited-state intermolecular hydrogen bonding interactions, photoinduced charge transfer, and vibrational spectroscopic properties of deprotonated deoxyadenosine monophosphate [dAMP-H] ⁻ anion in aqueous solution: Upon photoexcitation of hydrogen-bonded model complexes [dAMP-H] ⁻ ··· H ₂ O (n = 0, 1, 2, 3, 4). Attosecond pulse generation by applying a weak static electric field to a few-cycle pulse. <i>New Journal of Physics</i> , 2011 , 13, 093035	6	15
55	Photoluminescence spectral broadening, chirality transfer and amplification of chiral perovskite materials (R-X-p-mBZA)PbBr (X = H, F, Cl, Br) regulated by van der Waals and halogen atoms interactions. <i>Physical Chemistry Chemical Physics</i> , 2020 , 22, 17299-17305	2.9	14
54	Rational Design of a Profluorescent Substrate for S-adenosylhomocysteine Hydrolase and its Applications in Bioimaging and Inhibitor Screening. <i>ACS Applied Materials & Interfaces</i> , 2016 , 8, 25818-25824	9.5	12
53	Steady-state and time-resolved spectroscopic investigations on the existence of stable methanol/AOT/n-heptane reverse micelles. <i>Journal of Colloid and Interface Science</i> , 2014 , 423, 1-6	3.6	13
52	Influence of the Halogenated Substituent on Charge Transfer Mobility of Aniline Tetramer and Derivatives: Remarkable Anisotropic Mobilities. <i>Journal of Physical Chemistry C</i> , 2017 , 121, 17633-17640	3.8	13
51	Time-dependent density functional theory (TDDFT) study on the electronic spectroscopic blue-shift phenomenon and photoinduced charge transfer of firefly luciferin anion in aqueous solution: Insight into the excited-state hydrogen bond weakening mechanism. <i>Journal of Luminescence</i> , 2018 , 195, 116-119	3.8	12
50	Ultrafast Nonadiabatic Photoisomerization Dynamics Mechanism for the UV Photoprotection of Stilbenoids in Grape Skin. <i>Chemistry - an Asian Journal</i> , 2020 , 15, 1478-1483	4.5	11
49	Mechanism for tunable broadband white photoluminescence of one-dimensional (C ₄ N ₂ H ₁₄) ₂ Pb _{1-x} Mn _x Br ₄ perovskite microcrystals. <i>Journal of Luminescence</i> , 2020 , 221, 117045	3.8	11
48	Influence of collision energy on the dynamics of the reaction H (2S) + NH (X ³ Π-rN (4S) + H ₂ (X ¹ Π +g) by the state-to-state quantum mechanical study. <i>Theoretical Chemistry Accounts</i> , 2014 , 133, 1	1.9	11
47	Theoretical and spectroscopic investigation on ultrafast nonadiabatic photoprotective mechanism of novel ultraviolet protective compounds inspired by natural sunscreens. <i>Journal of Luminescence</i> , 2020 , 223, 117228	3.8	11
46	Circularly Polarized Luminescence from Solvent-Free Chiral Organic Liquids. <i>Angewandte Chemie - International Edition</i> , 2021 , 60, 3745-3751	16.4	11
45	Charge-transfer mobility and electrical conductivity of PANI as conjugated organic semiconductors. <i>Journal of Chemical Physics</i> , 2017 , 147, 114905	3.9	10
44	The promotion effects of thionation and isomerization on charge carrier mobility in naphthalene diimide crystals. <i>Physical Chemistry Chemical Physics</i> , 2017 , 19, 28175-28181	3.6	9
43	A novel aggregation induced emission (AIE) fluorescence probe by combining tetraphenylethylene and 2',3'-O-isopropylideneadenosine for localizing Golgi apparatus. <i>Sensors and Actuators B: Chemical</i> , 2021 , 329, 129245	8.5	9
42	Phase Regulation Strategy of Perovskite Nanocrystals from 1D Orthomorphous NH ₄ PbI ₃ to 3D Cubic (NH ₄) _{0.5} Cs _{0.5} Pb(I _{0.5} Br _{0.5}) ₃ Phase Enhances Photoluminescence. <i>Angewandte Chemie</i> , 2019 , 131, 11768-11772	3.6	8
41			

40	Theoretical investigation of the competitive mechanism between dissociation and ionization of H ₂ in intense field. <i>Journal of Physical Chemistry A</i> , 2014 , 118, 9173-81	2.8	8
39	Theoretical modeling of the hydrated serotonin in solution: Insight into intermolecular hydrogen bonding dynamics and spectral shift in the electronic excited states. <i>Journal of Molecular Liquids</i> , 2019 , 288, 111093	6	7
38	Tunable dual fluorescence emissions with high photoluminescence quantum yields modulated by Na ion dispersion method for purely solid state N-doped carbon dots. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2020 , 397, 112548	4.7	7
37	Excited state intramolecular proton transfer (ESIPT) luminescence mechanism for 4-N,N-diethylamino-3-hydroxyflavone in propylene carbonate, acetonitrile and the mixed solvents. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2020 , 224, 117416	4.4	7
36	Thermally Activated Delayed Fluorescence Enabled by Reversed Conformational Distortion for Blue Emitters. <i>Journal of Physical Chemistry Letters</i> , 2021 , 12, 9501-9507	6.4	7
35	Stereodynamics of chemical reactions: quasi-classical, quantum and mixed quantum-classical theories. <i>Open Physics</i> , 2012 , 10,	1.3	6
34	Anisotropic charge carrier transport of optoelectronic functional selenium-containing organic semiconductor materials. <i>Journal of Computational Chemistry</i> , 2020 , 41, 976-985	3.5	6
33	A novel lysosome-localized fluorescent probe with aggregation-induced emission without alkalinizing effect. <i>SmartMat</i> ,	22.8	6
32	New insights into ESIPT mechanism of three sunscreen compounds in solution: A combined experimental and theoretical study. <i>Colloids and Surfaces B: Biointerfaces</i> , 2021 , 207, 112039	6	6
31	Defect passivation and lattice distortion enhance solid-state photoluminescence of two-dimensional perovskites. <i>2D Materials</i> , 2020 , 7, 031008	5.9	5
30	Photophysical investigation of methyl 2-hydroxy-3-naphthoate (MHN23) in different self-organized supramolecular assemblies of micelles and niosomes formed by nonionic surfactant. <i>Journal of Alloys and Compounds</i> , 2016 , 686, 656-661	5.7	5
29	Unveiling the theoretical mechanism of purely organic room temperature phosphorescence emission and heteroatomic effects on singlet-triplet intersystem crossing for isopropylthioxanthone derivatives. <i>Journal of Luminescence</i> , 2021 , 232, 117864	3.8	5
28	Codoping of Lead-Free Double Perovskites Promotes Near-Infrared Photoluminescence. <i>Angewandte Chemie - International Edition</i> , 2021 , 60, 540-542	16.4	5
27	Nonadiabatic dynamics Mechanisms of natural UV Photoprotection compounds chlorogenic acid and isochlorogenic acid a: Double conjugated structures but single photoexcited channel. <i>Journal of Molecular Liquids</i> , 2021 , 324, 114725	6	5
26	Influence of wavelength on nonadiabatic effects in circularly polarized strong-field ionization. <i>Physical Review A</i> , 2015 , 92,	2.6	4
25	Nonadiabatic Dynamics Mechanism of Chalcone Analogue Sunscreen FPPO-HBr: Excited State Intramolecular Proton Transfer Followed by Conformation Twisting. <i>Journal of Physical Chemistry B</i> , 2021 , 125, 9572-9578	3.4	4
24	Efficient Photoluminescence of Manganese-Doped Two-Dimensional Chiral Alloyed Perovskites.. <i>Journal of Physical Chemistry Letters</i> , 2021 , 12, 12129-12134	6.4	4
23	Unveiling the photoluminescence regulation of colloidal perovskite quantum dots via defect passivation and lattice distortion by potassium cations doping: Not the more the better. <i>Journal of Colloid and Interface Science</i> , 2021 , 596, 199-205	9.3	3

22	Inversing supramolecular chirality and boosting circularly polarized luminescence of pyrene moieties a gel matrix. <i>Soft Matter</i> , 2021 , 17, 4328-4334	3.6	3
21	Environmental-Friendly Lead-Free Chiral Mn-Based Metal Halides with Efficient Circularly Polarized Photoluminescence at Room Temperature. <i>Journal of Alloys and Compounds</i> , 2022 , 164892	5.7	3
20	Combined ultrafast spectroscopic and TDDFT theoretical studies on dual fluorescence emissions promoted by ligand-to-metal charge transfer (LMCT) excited states of tungsten-containing organometallic complexes. <i>Chemical Physics Letters</i> , 2020 , 748, 137396	2.5	2
19	Quantum wavepacket exploration of isolated high-order harmonic attosecond pulse generation: from two-color scheme to three-color scheme. <i>Journal of Modern Optics</i> , 2011 , 58, 954-961	1.1	2
18	Conformational torsion, intramolecular hydrogen bonding and solvent effects in intersystem crossing of singlet-triplet excited states for heavy-atom-free organic long persistent luminescence. <i>Journal of Molecular Liquids</i> , 2021 , 326, 115291	6	2
17	Elaborating the influence of substituent on energy gap and spin-orbit coupling of singlet-triplet excited states of novel organic light-emitting anthraquinone compounds in solution. <i>Journal of Luminescence</i> , 2021 , 234, 117964	3.8	2
16	Highly efficient photoluminescence of 2D perovskites enabled by dimensional increasing. <i>2D Materials</i> , 2021 , 8, 021003	5.9	2
15	Excited state trans-cis photoisomerization via non-adiabatic dynamics of novel UVB protective sunscreens. <i>Journal of Luminescence</i> , 2021 , 238, 118215	3.8	2
14	Suppression of Energy Metabolism in Cancer Cells with Nutrient-Sensing Nanodrugs.. <i>Nano Letters</i> , 2022 ,	11.5	2
13	Carrier envelope phase retrieval of a multi-cycle pulse by heterodyne mixing of a pulse containing a few cycles. <i>Laser Physics</i> , 2013 , 23, 025301	1.2	1
12	The Hydrogen Bond Effect on Excited State Mechanism for 2-Isopropyl Thioxanone in Protic Solvents: Experimental and Theoretical Investigation. <i>Journal of Molecular Liquids</i> , 2021 , 117012	6	1
11	Codoping of Lead-Free Double Perovskites Promotes Near-Infrared Photoluminescence. <i>Angewandte Chemie</i> , 2021 , 133, 548-550	3.6	1
10	Non-adiabatic Dynamics Mechanism in Excited State of Novel UV Protective Sunscreen in Rice: Conical Intersection Promotes Internal Conversion. <i>Journal of Cluster Science</i> , 2021 , 32, 967-973	3	1
9	Achieving metal-free phosphorescence in dilute solutions for imaging hypoxia in cells and tumors. <i>Materials Chemistry Frontiers</i> , 2021 , 5, 7170-7175	7.8	1
8	Ultrafast nonadiabatic mechanism of plant sunscreens biflavonoids with two excited-state intramolecular proton transfer structures. <i>Journal of Luminescence</i> , 2022 , 246, 118816	3.8	1
7	Excitons competition regulation via organic cation-site and halogen-site co-halogenation of (X-p-PEA)Pb(Cl/Br) perovskites. <i>Journal of Colloid and Interface Science</i> , 2021 , 588, 494-500	9.3	0
6	Site-Selective Photoinduced Electron Transfer of Excited-State Intermolecular Hydrogen-Bonded Cluster in Solution. <i>Journal of Cluster Science</i> , 2021 , 32, 93-99	3	0
5	Coordination-promoted photoluminescence induced by configuration twisting regulation. <i>Journal of Luminescence</i> , 2021 , 231, 117783	3.8	0

- 4 New insights into the excited state intramolecular proton transfer (ESIPT) competition mechanism for different intramolecular hydrogen bonds of Kaempferol and Quercetin in solution. *Journal of Luminescence*, **2022**, 248, 118914 3.8 0
- 3 Excited-State Dynamics of Intermolecular Dihydrogen Bond in Different Systems **2019**, 137-153
- 2 Excited state electronic structures and photochemistry of different oxidation states of 2,2-Azobis(3-ethylbenzothiazoline-6-sulfonic acid) (ABTS). *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2021**, 253, 119503 4.4
- 1 Unveiling the nonadiabatic photoisomerization mechanism of hemicyanines for UV photoprotection. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2021**, 260, 119949 4.4