Panwang Zhou

List of Publications by Year
in descending order

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103 papers	3,274 citations	230014 27 h-index	190340 53 g-index
103 all docs	103 docs citations	103 times ranked	2518 citing authors

#	Article	IF	Citations
1	Theoretical exploration in the substituent effect on photophysical properties and excited-state intramolecular proton transfer process of benzo[a]imidazo[5,1,2-cd]indolizines. Journal of Photochemistry and Photobiology A: Chemistry, 2022, 422, 113570.	2.0	9
2	Blocking the dark state as sensing mechanism of 3-nitro-1,8-naphthalimide derivatives for detection of carbon monoxide in the living cells. Dyes and Pigments, 2022, 197, 109905.	2.0	10
3	ESIPTâ€based AIE luminogens: Design strategies, applications, and mechanisms. Aggregate, 2022, 3, .	5.2	100
4	Mechanistic Investigation on the Initial Thermal Decomposition of Energetic Materials FOX-7 and RDX in the Crystal and Gas Phase: An MM/DFT-Based ONIOM Calculation. Journal of Physical Chemistry A, 2022, 126, 1666-1673.	1.1	7
5	Intermolecular hydrogen-bonding-induced fluorescence of 3-hydroxyisonicotinealdehyde in different pH media. Journal of Luminescence, 2022, 247, 118878.	1.5	5
6	Regulation of excited-state intramolecular proton transfer process and photophysical properties for benzoxazole isothiocyanate fluorescent dyes by changing atomic electronegativity. Chinese Journal of Chemical Physics, 2022, 35, 331-337.	0.6	2
7	Memorial Viewpoint for Keli Han. Journal of Physical Chemistry A, 2022, 126, 3973-3975.	1.1	0
8	Unraveling the Key Role of the Benzyl Group in the Synthesis of CL-20 Precursor HBIW. ACS Omega, 2022, 7, 21912-21924.	1.6	3
9	Theoretical insights into the synthesis reaction mechanism of 1,2,3-triazole based on sakai reaction. Tetrahedron, 2021, 77, 131737.	1.0	7
10	Theoretical studies of the ultrafast deactivation mechanism of 8-oxo-guanine on the S1 and S2 electronic states in gas phase. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2021, 244, 118884.	2.0	2
11	New Cy5 photosensitizers for cancer phototherapy: a low singletâ€“triplet gap provides high quantum yield of singlet oxygen. Chemical Science, 2021, 12, 13809-13816.	3.7	19
12	A combined experimental and theoretical investigation of the excited-state dynamics of 2,4,6-trinitrotoluene (TNT) in DMSO solvent. Physical Chemistry Chemical Physics, 2021, 23, 20718-20723.	1.3	2
13	Unraveling the Mechanism for Tuning the Fluorescence of Fluorescein Derivatives: The Role of the Conical Intersection and nÏ€* State. Journal of Physical Chemistry Letters, 2021, 12, 6478-6485.	2.1	45
14	Effects of Intermolecular Hydrogen Bonding and Solvation on Enolâ€“Keto Tautomerism and Photophysics of Azomethineâ€“BODIPY Dyads. Journal of Physical Chemistry B, 2021, 125, 9296-9303.	1.2	13
15	Janus luminogens with bended intramolecular charge transfer: Toward molecular transistor and brain imaging. Matter, 2021, 4, 3286-3300.	5.0	12
16	Theoretical insights into the enhancement of 1-Methyl-2,4,5-trinitroimidazole yield by exchanging of group introduction order. Chemical Physics Letters, 2021, 779, 138834.	1.2	2
17	Achieving metal-free phosphorescence in dilute solutions for imaging hypoxia in cells and tumors. Materials Chemistry Frontiers, 2021, 5, 7170-7175.	3.2	12
18	Stacking Engineering: A Boosting Strategy for 2D Photocatalysts. Journal of Physical Chemistry Letters, 2021, 12, 10190-10196.	2.1	25

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19	Quasi-Two-Dimensional Perovskite Nanosheets Based on the Triplet Energy Acceptor Molecule with Pure Green Emission Light. Journal of Physical Chemistry C, 2021, 125, 23889-23894.	1.5	5
20	Intramolecular triplet energy transfer in two-dimensional hybrid perovskite nanosheets. Chemical Physics Letters, 2021, 785, 139132.	1.2	3
21	Marcus inverted region of charge transfer from low-dimensional semiconductor materials. Nature Communications, 2021, 12, 6333.	5.8	27
22	Dual fluorescence of 2-(2â€²-hydroxyphenyl) benzoxazole derivatives via the branched decays from the upper excited-state. Physical Chemistry Chemical Physics, 2021, 23, 27304-27311.	1.3	26
23	A new interpretation of the ESIPT mechanism of 2-(benzimidazol-2-yl)-3-hydroxychromone derivatives. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2020, 224, 117359.	2.0	34
24	Whether the excited state intramolecular proton transfer of 1-hydroxy-2-acetonaphthone will happen?. Journal of Luminescence, 2020, 217, 116825.	1.5	18
25	Effects of solvents on the excited state intramolecular proton transfer and hydrogen bond mechanisms of alizarin and its isomers. Journal of Molecular Liquids, 2020, 301, 112415.	2.3	56
26	DFT/TDDFT investigation on the Dâ€“Ïâ€“A type molecule probes 4-(5-R-thiophen-2-yl)-2-isobutyl-2H-[1,2,3]triazolo[4,5-e][1,2,4] triazolo[1,5-a]pyrimidines: fluorescence sensing mechanism and roles of weak interactions. Theoretical Chemistry Accounts, 2020, 139, 1.	0.5	6
27	A distinct excited-state proton transfer mechanism for 4-(N-Substituted-amino)-1H-pyrrolo[2,3-b]pyridines in aprotic and protic solvents. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2020, 231, 117800.	2.0	3
28	Quantifying the Fast Dynamics of HClO in Living Cells by a Fluorescence Probe Capable of Responding to Oxidation and Reduction Events within the Time Scale of Milliseconds. Analytical Chemistry, 2020, 92, 12987-12995.	3.2	21
29	Reply to â€œComment on â€˜Theoretical Insights into the Excited State Decays of a Donorâ€“Acceptor Dyad: Is the Twisted and Rehybridized Intramolecular Charge-Transfer State Involved?â€™â€•. Journal of Physical Chemistry B, 2020, 124, 10582-10584.	1.2	1
30	Sensing Mechanism of a Fluorescent Probe for Cysteine: Photoinduced Electron Transfer and Invalidity of Excited-State Intramolecular Proton Transfer. Journal of Physical Chemistry A, 2020, 124, 6920-6927.	1.1	34
31	Carbonyl Stretch as a Franckâ€“Condon Active Mode and Driving Force for Excited-State Decay of 8-Methoxy-4-methyl-2H-benzo[g]chromen-2-one from nÏ€* State. Journal of Physical Chemistry B, 2020, 124, 11472-11480.	1.2	19
32	Competition between tubular, planar and cage geometries: a complete picture of structural evolution of B_n (n = 31â€“50) clusters. Physical Chemistry Chemical Physics, 2020, 22, 12959-12966.	1.3	21
33	Theoretical Insights into the Excited State Decays of a Donorâ€“Acceptor Dyad: Is the Twisted and Rehybridized Intramolecular Charge-Transfer State Involved?. Journal of Physical Chemistry B, 2020, 124, 4564-4572.	1.2	20
34	Enhancing Intersystem Crossing to Achieve Thermally Activated Delayed Fluorescence in a Water-Soluble Fluorescein Derivative with a Flexible Propenyl Group. Journal of Physical Chemistry Letters, 2020, 11, 5692-5698.	2.1	18
35	Theoretical study on the ESIPT of fluorescent probe molecules N-(2-(4-(dimethylamino)phenyl)-3-hydroxy-4-oxo-4h -chromen-6-yl) butyramide in different solvents. Journal of Molecular Liquids, 2020, 314, 113614.	2.3	14
36	Thermochemistry and Initial Decomposition Pathways of Triazole Energetic Materials. Journal of Physical Chemistry A, 2020, 124, 2951-2960.	1.1	20

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37	Spin-Controlled Charge-Recombination Pathways across the Inorganic/Organic Interface. Journal of the American Chemical Society, 2020, 142, 4723-4731.	6.6	25
38	Unraveling the Mechanism of cyclo-N₅^{â€“} Production through Selective Câ€“N Bond Cleavage of Arylpentazole with Ferrous Bisglycinate and m-Chloroperbenzonic Acid: A Theoretical Perspective. Journal of Physical Chemistry Letters, 2020, 11, 1030-1037.	2.1	26
39	New Insights into the Excited State Dynamics of Quinolineâ€“Pyrazole Isomerism. Journal of Physical Chemistry B, 2020, 124, 3400-3407.	1.2	50
40	A theoretical study of the ESIPT mechanism of 3-hydroxyflavone derivatives: solvation effect and the importance of TICT for its dual fluorescence properties. Organic Chemistry Frontiers, 2019, 6, 3136-3143.	2.3	43
41	Restriction of Flip-flop Motion as a Mechanism for Aggregation-Induced Emission. Journal of Physical Chemistry Letters, 2019, 10, 6929-6935.	2.1	80
42	New perspective on the fluorescence and sensing mechanism of TNP chemosensor 2-(4,5-bis(4-chlorophenyl)-1H-imidazol-2-yl)-4-chlorolphenol. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2019, 213, 309-317.	2.0	5
43	Theoretical perspective on the reaction mechanism from arylpentazenes to arylpentazoles: new insights into the enhancement of cyclo-N₅ production. Chemical Communications, 2019, 55, 2628-2631.	2.2	20
44	Theoretical insights into the sensing mechanism of a series of terpyridine-based chemosensors for TNP. Chemical Physics Letters, 2019, 725, 45-51.	1.2	15
45	The effects of the heteroatom and position on excited-state intramolecular proton transfer of new hydroxyphenyl benzoxazole derivatives: a time-dependent density functional theory study. Organic Chemistry Frontiers, 2019, 6, 1807-1815.	2.3	17
46	How Does the O⁶-Methylation Regulate the Excited-State Decay of Guanine Monomers. Journal of Physical Chemistry B, 2019, 123, 201-206.	1.2	6
47	Does the wavelength dependent photoisomerization process of the pâ€coumaric acid come out from the electronic state dependent pathways?. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2019, 211, 203-211.	2.0	5
48	Accurate description of excited state intramolecular proton transfer that involves zwitterionic state using optimally tuned rangeâ€separated timeâ€dependent density functional theory. International Journal of Quantum Chemistry, 2018, 118, e25618.	1.0	17
49	Mechanism of Fluorescence Quenching by Acylamino Twist in the Excited State for 1-(Acylamino)anthraquinones. Journal of Physical Chemistry A, 2018, 122, 2864-2870.	1.1	27
50	Reconsideration of the Detection and Fluorescence Mechanism of a Pyrene-Based Chemosensor for TNT. Journal of Physical Chemistry A, 2018, 122, 1400-1405.	1.1	32
51	Investigation on sensing mechanism of a fluorescent probe for TNP detection in aqueous solution. Tetrahedron, 2018, 74, 2684-2691.	1.0	21
52	The effect of benzoâ€annelation on intermolecular hydrogen bond and proton transfer of 2â€methylâ€3â€hydroxyâ€4(<scp>1H</scp>)â€quinolone in methanol: A <scp>TDâ€DFT</scp> study. Journal of Physical Organic Chemistry, 2018, 31, e3803.	n/a	5
53	Excited-State Proton Transfer Mechanism of 2,6-DiazaindolesÂ·(H₂O)_n (n = 2â€“4) Clusters. Journal of Physical Chemistry B, 2018, 122, 3988-3995.	1.2	50
54	Excited-state intramolecular proton transfer mechanism for 2-(quinolin-2-yl)-3-hydroxychromone: A detailed time-dependent density functional theory study. Journal of Molecular Liquids, 2018, 260, 447-457.	2.3	25

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55	Why the lowest electronic excitations of rhodamines are overestimated by timeâ€dependent density functional theory. International Journal of Quantum Chemistry, 2018, 118, e25780.	1.0	31
56	A binding model study on TNP fluorescent sensor 4,40-(9,9 dimethylfluorene-2,7-diyl)dibenzoic acid. Journal of Photochemistry and Photobiology A: Chemistry, 2018, 367, 282-289.	2.0	10
57	New insights into the sensing mechanism of a phosphonate pyrene chemosensor for TNT. Physical Chemistry Chemical Physics, 2018, 20, 19539-19545.	1.3	20
58	The photoinduced isomerization mechanism of the 2-(1-(methylimino)methyl)-6-chlorophenol (SMAC): Nonadiabatic surface hopping dynamics simulations. Journal of Chemical Physics, 2018, 149, 034309.	1.2	5
59	Solvation effect on the ESIPT mechanism of 2-(4â€²-amino-2â€²-hydroxyphenyl)-1H-imidazo-[4,5-c]pyridine. Journal of Photochemistry and Photobiology A: Chemistry, 2018, 367, 261-269.	2.0	38
60	Unraveling the Detailed Mechanism of Excited-State Proton Transfer. Accounts of Chemical Research, 2018, 51, 1681-1690.	7.6	432
61	On the mechanism of non-radiative decay of blue fluorescent protein chromophore: New insight from the excited-state molecular dynamics simulations and potential energy calculations. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2017, 186, 52-58.	2.0	9
62	Effect of Methylation on the Photodynamical Behavior of Arylazoimidazoles: New Insight from Theoretical ab Initio Potential Energy Calculations and Molecular Dynamics Simulations. Journal of Physical Chemistry A, 2017, 121, 141-150.	1.1	12
63	pH-dependent absorption spectra of rhodopsin mutant E113Q: On the role of counterions and protein. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2017, 174, 25-31.	2.0	5
64	Non-adiabatic dynamics investigation of the radiationless decay mechanism of trans-urocanic acid in the S2 state. Journal of Chemical Physics, 2016, 145, 044316.	1.2	12
65	Synthesis and Characterization of Phenothiazineâ€Based Platinum(II)â€“Acetylide Photosensitizers for Efficient Dyeâ€Sensitized Solar Cells. Chemistry - A European Journal, 2016, 22, 3750-3757.	1.7	27
66	Excited-state proton transfer of 4-hydroxyl-1, 8-naphthalimide derivatives: A combined experimental and theoretical investigation. Journal of Luminescence, 2016, 177, 197-203.	1.5	15
67	Non-adiabatic dynamics simulation exploration of the wavelength-dependent photoinduced relaxation mechanism of trans-N-1-methyl-2-(tolylazo) imidazole in the gas phase. RSC Advances, 2016, 6, 64323-64331.	1.7	16
68	New Insight into the Photoisomerization Process of the Salicylidene Methylamine under Vacuum. Journal of Physical Chemistry A, 2016, 120, 7419-7426.	1.1	28
69	The Effects of Heteroatoms Si and S on Tuning the Optical Properties of Rhodamineâ€and Fluoresceinâ€Based Fluorescence Probes: A Theoretical Analysis. ChemPhysChem, 2016, 17, 3139-3145.	1.0	37
70	The charge mobilities in fused ring Oligothiophenes and their derivatives: influence of molecular structures. Journal of Molecular Modeling, 2016, 22, 182.	0.8	1
71	Molecular engineering of starburst triarylamine donor with selenophene containing Ï€-linker for dye-sensitized solar cells. Journal of Materials Chemistry C, 2016, 4, 713-726.	2.7	23
72	Effect of the Hydrogen Bond on Photochemical Synthesis of Silver Nanoparticles. Journal of Physical Chemistry A, 2015, 119, 12579-12585.	1.1	10

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73	New Excited-State Proton Transfer Mechanisms for 1,8-Dihydroxydibenzo[a,h]phenazine. Journal of Physical Chemistry A, 2015, 119, 681-688.	1.1	190
74	The Charge Transfer Phenomenon in Benzeneâ€“Pyreneâ€“Sulfoxide/Methanol System: Role of the Intermolecular Hydrogen Bond in Excited States. Journal of Cluster Science, 2015, 26, 1463-1472.	1.7	33
75	Competitive excited-state single or double proton transfer mechanisms for bis-2,5-(2-benzoxazolyl)-hydroquinone and its derivatives. Physical Chemistry Chemical Physics, 2015, 17, 11990-11999.	1.3	243
76	Photoisomerization mechanism of 1,1â€²-dimethyl-2,2â€²-pyridocyanine in the gas phase and in solution. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2015, 136, 1157-1166.	2.0	5
77	New Insights into the Dual Fluorescence of Methyl Salicylate: Effects of Intermolecular Hydrogen Bonding and Solvation. Journal of Physical Chemistry B, 2015, 119, 2125-2131.	1.2	163
78	Non-adiabatic dynamics of isolated green fluorescent protein chromophore anion. Journal of Chemical Physics, 2014, 141, 235101.	1.2	41
79	Photochemical dynamics simulations for transâ€“cis photoisomerizations of azobenzene and bridged azobenzene. Computational and Theoretical Chemistry, 2014, 1031, 13-21.	1.1	24
80	The photoisomerization of 11â€cisâ€retinal protonated schiff base in gas phase: Insight from spinâ€flip density functional theory. Journal of Computational Chemistry, 2014, 35, 109-120.	1.5	38
81	A DFT/TDDFT study of the excited state intramolecular proton transfer based sensing mechanism for the aqueous fluoride chemosensor BTTPB. RSC Advances, 2014, 4, 254-259.	1.7	73
82	Probing ultrafast excited state dynamics and nonlinear absorption properties of three star-shaped conjugated oligomers with 1,3,5-triazine core. RSC Advances, 2014, 4, 10960.	1.7	28
83	Experimental and theoretical study on the sensing mechanism of a fluorescence probe for hypochloric acid: a Seâ‹¯N nonbonding interaction modulated twisting process. Physical Chemistry Chemical Physics, 2014, 16, 3749.	1.3	39
84	Stability and Raman Spectroscopy of Alkane Guest Molecules (C_{n}H_{m},) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 5¹²6² and 5¹²6⁴ Water Cavities by Density Functional Theory Calculations. Wuli Huaxue Xuebao/ Acta Physico - Chimica Sinica, 2014, 30, 1437-1446.	2.2	8
85	Sensing mechanism for a fluoride chemosensor: invalidity of excited-state proton transfer mechanism. Physical Chemistry Chemical Physics, 2013, 15, 16183.	1.3	85
86	Fluoride Anion Sensing Mechanism of 2-Ureido-4[1H]-pyrimidinone Quadruple Hydrogen-Bonded Supramolecular Assembly: Photoinduced Electron Transfer and Partial Configuration Change. Journal of Physical Chemistry B, 2013, 117, 5212-5221.	1.2	76
87	White Light Assisted Photosensitized Synthesis of Ag Nanoparticles: Excited-State Hydrogen Bonding Roles. Journal of Physical Chemistry C, 2013, 117, 11858-11865.	1.5	13
88	The Rate Constant Calculations for the Reaction H(2 S)+NH(X ³ Î£) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 14 Chinese Physics Letters, 2012, 29, 063401.	1.3	2
89	FACILITATED PHOTOLYSIS OF 9-FLUORENOL IN ALCOHOLS BY EXCITED-STATE HYDROGEN BOND REORGANIZATION. Journal of Theoretical and Computational Chemistry, 2012, 11, 493-504.	1.8	5
90	Quantum wave packet calculation of the O(3P)+H2 reaction on the new potential energy surfaces for the two lowest states. Computational and Theoretical Chemistry, 2012, 986, 25-29.	1.1	6

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91	Theoretical Study on Photoisomerization Effect with a Reversible Nonlinear Optical Switch for Dithiazolylarylene. Journal of Physical Chemistry A, 2012, 116, 5392-5397.	1.1	35
92	The invalidity of the photo-induced electron transfer mechanism for fluorescein derivatives. Physical Chemistry Chemical Physics, 2012, 14, 15191.	1.3	79
93	Mechanisms of ultrafast fluorescence depletion spectroscopy and applications to measure slovation dynamics of coummarin 153 in methanol. Journal of Luminescence, 2012, 132, 2275-2280.	1.5	6
94	Solvent Effects on 3-Keto-1H-pyrido[3,2,1-kl]phenothiazine Fluorescence in Polar and Protic Solvents. Journal of Physical Chemistry B, 2011, 115, 10692-10698.	1.2	29
95	Photo-induced intramolecular charge transfer from antenna to anchor groups in phenoxazine dyes. Chemical Physics Letters, 2011, 512, 66-69.	1.2	19
96	Promoting Effect of Electrostatic Interaction between a Cobalt Catalyst and a Xanthene Dye on Visible-Light-Driven Electron Transfer and Hydrogen Production. Journal of Physical Chemistry C, 2011, 115, 15089-15096.	1.5	73
97	DFT investigation on mechanism of dirhodium tetracarboxylate-catalyzed O-H insertion of diazo compounds with H2O. Open Chemistry, 2010, 8, 223-228.	1.0	4
98	Photophysical Properties of 4â€²-(p-aminophenyl)-2,2â€²:6â€²,2â€³-terpyridine. Chinese Journal of Chemical Physics, 2010, 23, 558-564.	0.6	5
99	Rotational reorientation dynamics of Rhodamine 700 in different excited states. Journal of Luminescence, 2009, 129, 283-289.	1.5	14
100	Experimental and theoretical study of the rotational reorientation dynamics of 7-animocoumarin derivatives in polar solvents: hydrogen-bonding effects. Physical Chemistry Chemical Physics, 2009, 11, 9440.	1.3	65
101	The effect of hydrogen-bond in alcoholic solvent on the solvation ultrafast dynamics of oxazine 750 dye. Science Bulletin, 2008, 53, 1951-1954.	4.3	6
102	Rotational Reorientation Dynamics of Oxazine 750 in Polar Solvents. Journal of Physical Chemistry A, 2008, 112, 3646-3655.	1.1	20
103	Preparation and biodistribution of 99mTc-tricarbonyl complex with 4-[(2-methoxyphenyl)piperazin-1-yl]-dithioformate as a potential 5-HT1A receptor imaging agent. Applied Radiation and Isotopes, 2007, 65, 287-292.	0.7	26