Jianzhong Fan

List of Publications by Year
in descending order

82 papers	1,985 citations	279487 23 h-index	288905 40 g-index
82 all docs	82 docs citations	82 times ranked	1322 citing authors

#	Article	IF	Citations
1	Mechanical Insights into Aggregationâ€Induced Delayed Fluorescence Materials with Antiâ€Kasha Behavior. Advanced Science, 2019, 6, 1801629.	5.6	111
2	Aggregation Effects on the Optical Emission of 1,1,2,3,4,5-Hexaphenylsilole (HPS): A QM/MM Study. Journal of Physical Chemistry A, 2014, 118, 9094-9104.	1.1	110
3	Excited state properties of non-doped thermally activated delayed fluorescence emitters with aggregation-induced emission: a QM/MM study. Journal of Materials Chemistry C, 2017, 5, 8390-8399.	2.7	91
4	Theoretical Study of the Mechanism of Aggregation-Caused Quenching in Near-Infrared Thermally Activated Delayed Fluorescence Molecules: Hydrogen-Bond Effect. Journal of Physical Chemistry C, 2019, 123, 24705-24713.	1.5	89
5	Spectroscopic Signature of the Aggregation-Induced Emission Phenomena Caused by Restricted Nonradiative Decay: A Theoretical Proposal. Journal of Physical Chemistry C, 2015, 119, 5040-5047.	1.5	70
6	Excited State Properties of a Thermally Activated Delayed Fluorescence Molecule in Solid Phase Studied by Quantum Mechanics/Molecular Mechanics Method. Journal of Physical Chemistry C, 2018, 122, 2358-2366.	1.5	68
7	Highâ€Performance Ultraviolet Organic Lightâ€Emitting Diode Enabled by Highâ€Lying Reverse Intersystem Crossing. Angewandte Chemie - International Edition, 2021, 60, 22241-22247.	7.2	68
8	Using the isotope effect to probe an aggregation induced emission mechanism: theoretical prediction and experimental validation. Chemical Science, 2016, 7, 5573-5580.	3.7	67
9	Photomechanical Luminescence from Throughâ€Space Conjugated AIEgens. Angewandte Chemie - International Edition, 2020, 59, 8828-8832.	7.2	67
10	Unraveling the Important Role of Highâ€Lying Tripletâ€“Lowest Excited Singlet Transitions in Achieving Highly Efficient Deepâ€Blue AIEâ€Based OLEDs. Advanced Materials, 2021, 33, e2006953.	11.1	66
11	Theoretical insights on the electroluminescent mechanism of thermally activated delayed fluorescence emitters. Organic Electronics, 2017, 41, 17-25.	1.4	65
12	Aggregation-Induced Delayed Fluorescence Luminogens with Accelerated Reverse Intersystem Crossing for High-Performance OLEDs. , 2019, 1, 613-619.		51
13	Highly Efficient Near-Infrared Thermally Activated Delayed Fluorescence Molecules via Acceptor Tuning: Theoretical Molecular Design and Experimental Verification. Journal of Physical Chemistry Letters, 2021, 12, 1893-1903.	2.1	48
14	Decreasing the singletâ€“triplet gap for thermally activated delayed fluorescence molecules by structural modification on the donor fragment: First-principles study. Chemical Physics Letters, 2016, 652, 16-21.	1.2	43
15	Effects of intramolecular and intermolecular interactions on excited state properties of two isomeric Cu complexes with AIE and TADF mechanisms in solid phase: A QM/MM study. Organic Electronics, 2019, 71, 113-122.	1.4	40
16	An Effective Design Strategy for Robust Aggregationâ€Induced Delayed Fluorescence Luminogens to Improve Efficiency Stability of Nondoped and Doped OLEDs. Advanced Optical Materials, 2020, 8, 2001027.	3.6	38
17	Excited state dynamics for hybridized local and charge transfer state fluorescent emitters with aggregation-induced emission in the solid phase: a QM/MM study. Physical Chemistry Chemical Physics, 2017, 19, 29872-29879.	1.3	36
18	Towards boosting the exciton lifetime and efficiency of near-infrared aggregation induced emitters with hybridized local and charge transfer excited states: a multiscale study. Journal of Materials Chemistry C, 2019, 7, 8874-8887.	2.7	35

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19	Excited state dynamics of new-type thermally activated delayed fluorescence emitters: theoretical view of light-emitting mechanism. Molecular Physics, 2018, 116, 19-28.	0.8	34
20	Pressure-induced emission enhancement in hexaphenylsilole: a computational study. Journal of Materials Chemistry C, 2019, 7, 1388-1398.	2.7	33
21	Dynamics of Excited States for Fluorescent Emitters with Hybridized Local and Charge-Transfer Excited State in Solid Phase: A QM/MM Study. Journal of Physical Chemistry A, 2016, 120, 9422-9430.	1.1	30
22	A QM/MM study on through space charge transfer-based thermally activated delayed fluorescence molecules in the solid state. Journal of Materials Chemistry C, 2022, 10, 517-531.	2.7	30
23	Theoretical perspective for internal quantum efficiency of thermally activated delayed fluorescence emitter in solid phase: A QM/MM study. Organic Electronics, 2017, 51, 349-356.	1.4	27
24	Theoretical perspective for luminescent mechanism of thermally activated delayed fluorescence emitter with excited-state intramolecular proton transfer. Journal of Materials Chemistry C, 2020, 8, 98-108.	2.7	27
25	Effect of Intermolecular Excited-state Interaction on Vibrationally Resolved Optical Spectra in Organic Molecular Aggregates. Acta Chimica Sinica, 2016, 74, 902.	0.5	27
26	First-Principles Investigation on Triazine Based Thermally Activated Delayed Fluorescence Emitters. Chinese Journal of Chemical Physics, 2016, 29, 291-296.	0.6	25
27	Molecular stacking effect on photoluminescence quantum yield and charge mobility of organic semiconductors. Physical Chemistry Chemical Physics, 2017, 19, 30147-30156.	1.3	24
28	Theoretical Study on the Sensing Mechanism of Novel Hydrazine Sensor TAPHP and Its ESIPT and ICT Processes. Frontiers in Chemistry, 2019, 7, 932.	1.8	24
29	Bicolor switching mechanism of multifunctional light-emitting molecular material in solid phase. Organic Electronics, 2019, 71, 212-219.	1.4	23
30	Electroluminescent Mechanism of Thermally Activated Delayed Fluorescence Emitters: Conformational Effect. Journal of Physical Chemistry C, 2018, 122, 19953-19961.	1.5	22
31	The role of intermolecular interactions in regulating the thermally activated delayed fluorescence and charge transfer properties: a theoretical perspective. Journal of Materials Chemistry C, 2020, 8, 8601-8612.	2.7	22
32	Theoretical study on the light-emitting mechanism of circularly polarized luminescence molecules with both thermally activated delayed fluorescence and aggregation-induced emission. Physical Chemistry Chemical Physics, 2019, 21, 7288-7297.	1.3	20
33	Thermally activated delayed fluorescence emitters with dual conformations for white organic light-emitting diodes: mechanism and molecular design. Physical Chemistry Chemical Physics, 2020, 22, 1313-1323.	1.3	20
34	Suppression of aggregation caused quenching in U-shaped thermally activated delayed fluorescence molecules: Tert-butyl effect. Journal of Luminescence, 2020, 219, 116899.	1.5	20
35	Highly efficient T-shaped deep-red thermally activated delayed fluorescence emitters: substitution position effect. Physical Chemistry Chemical Physics, 2021, 23, 21883-21892.	1.3	20
36	Theoretical perspective of the excited state intramolecular proton transfer for a compound with aggregation induced emission in the solid phase. RSC Advances, 2017, 7, 44089-44096.	1.7	18

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37	Strategy to modulate the singlet-triplet energy gap for spiro-based thermally activated delayed fluorescence molecules. Journal of Luminescence, 2019, 209, 372-378.	1.5	18
38	Solid-State Effect Induced Thermally Activated Delayed Fluorescence with Tunable Emission: A Multiscale Study. Journal of Physical Chemistry A, 2020, 124, 8540-8550.	1.1	18
39	Dual Functionalization of Electron Transport Layer via Tailoring Molecular Structure for High-Performance Perovskite Light-Emitting Diodes. ACS Applied Materials & Interfaces, 2020, 12, 37346-37353.	4.0	17
40	Structureâ€“property relationship study of blue thermally activated delayed fluorescence molecules with different donor and position substitutions: theoretical perspective and molecular design. Journal of Materials Chemistry C, 2022, 10, 4723-4736.	2.7	17
41	Substituent effects on the intermolecular interactions and emission behaviors in pyrene-based mechanochromic luminogens. Journal of Materials Chemistry C, 2022, 10, 9310-9318.	2.7	16
42	Novel Deep Red Thermally Activated Delayed Fluorescence Molecule with Aggregation-Induced Emission Enhancement: Theoretical Design and Experimental Validation. Journal of Physical Chemistry Letters, 2022, 13, 4711-4720.	2.1	16
43	Substitution effect on luminescent property of thermally activated delayed fluorescence molecule with aggregation induced emission: A QM/MM study. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2020, 229, 117964.	2.0	15
44	The photophysical properties and imaging application of a new polarity-sensitive fluorescent probe. Analyst, The, 2020, 145, 6556-6561.	1.7	14
45	Theoretical Study on Thermally Activated Delayed Fluorescence Emitters in White Organic Light-Emitting Diodes: Emission Mechanism and Molecular Design. Journal of Physical Chemistry A, 2020, 124, 7526-7537.	1.1	14
46	Effect of intermolecular interaction on excited-state properties of thermally activated delayed fluorescence molecules in solid phase: A QM/MM study. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2019, 209, 248-255.	2.0	12
47	Photomechanical Luminescence from Throughâ€Space Conjugated AIEgens. Angewandte Chemie, 2020, 132, 8913-8917.	1.6	12
48	Effects of Secondary Acceptors on Excited-State Properties of Sky-Blue Thermally Activated Delayed Fluorescence Molecules: Luminescence Mechanism and Molecular Design. Journal of Physical Chemistry A, 2021, 125, 175-186.	1.1	12
49	Solid-state effect on luminescent properties of thermally activated delayed fluorescence molecule with aggregation induced emission: A theoretical perspective. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2020, 241, 118634.	2.0	11
50	Insights on aggregation induced room temperature phosphorescence properties: A QM/MM study. Journal of Luminescence, 2020, 221, 117046.	1.5	11
51	Highâ€Performance Ultraviolet Organic Lightâ€Emitting Diode Enabled by Highâ€Lying Reverse Intersystem Crossing. Angewandte Chemie, 2021, 133, 22415-22421.	1.6	10
52	Theoretical Study on the Light-Emitting Mechanism of Multifunctional Thermally Activated Delayed Fluorescence Molecules. Journal of Physical Chemistry C, 2022, 126, 2437-2446.	1.5	10
53	Structural Isomerization Effect on the Triplet Energy Consumption Process of Organic Room-Temperature Phosphorescence Molecules: A QM/MM Study. Journal of Physical Chemistry C, 2021, 125, 27810-27819.	1.5	10
54	Triplet exciton dynamics of pure organics with halogen substitution boosted two photon absorption and room temperature phosphorescence: A theoretical perspective. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2022, 270, 120786.	2.0	9

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55	Influence of donor and acceptor groups on the S-T energy gap for thermally activated delayed fluorescence emitters. Molecular Physics, 2017, 115, 809-814.	0.8	8
56	The mechanism of the excited-state proton transfer of Salicylaldehyde azine and 2,2'-[1,4-Phenylenebis{(E)- nitrilomethylidyne}] bisphenol: Via single or double proton transfer. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2019, 223, 117321.	2.0	8
57	Tunable lifetimes and efficiencies of room temperature phosphorescent liquids by modulating the length and number of alkyl chains. Physical Chemistry Chemical Physics, 2020, 22, 19746-19757.	1.3	8
58	Theoretical insights into room temperature phosphorescence emission with anti-Kasha behavior in aggregate. Dyes and Pigments, 2022, 205, 110560.	2.0	8
59	Modulating excited state properties of thermally activated delayed fluorescence molecules by tuning the connecting pattern. Theoretical Chemistry Accounts, 2016, 135, 1.	0.5	7
60	Luminescent properties of thermally activated delayed fluorescence molecule with intramolecular Ï€ â€“ Ï€ interaction between donor and acceptor. Chinese Physics B, 2017, 26, 118503.	0.7	7
61	Perspective for aggregation-induced delayed fluorescence mechanism: A QM/MM study*. Chinese Physics B, 2020, 29, 088504.	0.7	7
62	Theoretical studies on the excited-state properties of thermally activated delayed fluorescence molecules with aggregation induced emission. Journal of Materials Chemistry C, 2022, 10, 9377-9390.	2.7	7
63	Structure-property relationship of phosphine oxide based thermally activated delayed fluorescence molecules: First-principles study. Organic Electronics, 2018, 59, 7-14.	1.4	6
64	Synthesis of fulvene-containing boron complexes with aggregation-induced emission and mechanochromic luminescence. Chemical Communications, 2020, 56, 14435-14438.	2.2	6
65	Design strategy for blue thermally activated delayed fluorescence: Position and methyl substitutions. Chemical Physics Letters, 2021, 764, 138260.	1.2	6
66	Sensing mechanism of fluorescent sensor to Cu2+ based on inhibiting ultra-fast intramolecular proton transfer process. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2021, 254, 119685.	2.0	6
67	Theoretical perspective of relationship between molecular structure and luminescence properties for circularly polarized thermally activated delayed fluorescence. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2022, 275, 121164.	2.0	6
68	A theoretical perspective of the relationship between the structures and luminescence properties of red thermally activated delayed fluorescence molecules. Physical Chemistry Chemical Physics, 2022, 24, 17140-17154.	1.3	6
69	Theoretical Analysis on Optical Limiting Properties of Newly Synthesized Graphene Oxide-Porphyrin Composites. Chinese Journal of Chemical Physics, 2015, 28, 257-262.	0.6	4
70	Theoretical perspective on the luminescence mechanism of a hybridized local and charge transfer state emitter with aggregation induced emission: a QM/MM study. CrystEngComm, 2021, 23, 3582-3593.	1.3	4
71	Insights on isomeric emitters with thermally activated delayed fluorescence: Comparison between solvent and crystal state. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2022, 278, 121328.	2.0	4
72	Influence of electron donating ability on reverse intersystem crossing rate for one kind of thermally activated delayed fluorescence molecules. Chinese Journal of Chemical Physics, 2018, 31, 291-299.	0.6	3

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73	Substitution induced tunable emission of an airplane-like pyrene-based fluorophore: First-principles study. Chemical Physics Letters, 2019, 734, 136726.	1.2	3
74	Theoretical study and experimental validation on the optical emission processes in â€œfreeâ€•and â€œlockedâ€•pyrazine derivatives. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2019, 223, 117296.	2.0	3
75	Structure-property relationship for triarylboron-based thermally activated delayed fluorescence molecules: A theoretical perspective. Materials Science and Engineering B: Solid-State Materials for Advanced Technology, 2021, 270, 115203.	1.7	3
76	Theoretical insights on the luminescent mechanism of an efficient aggregationâ€induced nondoped delayed fluorescence emitter using QM / MM method. International Journal of Quantum Chemistry, 2021, 121, e26490.	1.0	3
77	Intermolecular interaction on excited-state properties of fluoro-substituted thermally activated delayed fluorescence molecules with aggregation-induced emission: a theoretical perspective. Molecular Physics, 2021, 119, e1862931.	0.8	3
78	Efficient modulation of optical and electrical properties of X-shaped thermally activated delayed fluorescence emitters by substitution. Journal of Molecular Modeling, 2016, 22, 173.	0.8	2
79	Theoretical arrangement of thermally activated delayed fluorescence as host for fluorescent emitter with blue to red emission. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2019, 219, 44-52.	2.0	2
80	Responsive mechanism of 2-fluoro-5-nitrobenzoate based two-photon fluorescent probes for H2Sn detection: A theoretical perspective. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2021, 250, 119244.	2.0	2
81	Theoretical study on the optical emission processes in geminally locked tetraphenylethylene derivatives. Chemical Physics Letters, 2019, 727, 25-30.	1.2	1
82	Syntheses and structures of two novel fluorescent metalâ€“organic frameworks generated from a tridentate donorâ€“acceptor motif ligand. Acta Crystallographica Section C, Structural Chemistry, 2020, 76, 605-615.	0.2	1