

Jianzhong Fan

List of Publications by Year in descending order

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82
papers

1,985
citations

279487

23
h-index

288905

40
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82
all docs

82
docs citations

82
times ranked

1322
citing authors

#	ARTICLE	IF	CITATIONS
1	Triplet exciton dynamics of pure organics with halogen substitution boosted two photon absorption and room temperature phosphorescence: A theoretical perspective. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2022, 270, 120786.	2.0	9
2	A QM/MM study on through space charge transfer-based thermally activated delayed fluorescence molecules in the solid state. <i>Journal of Materials Chemistry C</i> , 2022, 10, 517-531.	2.7	30
3	Theoretical Study on the Light-Emitting Mechanism of Multifunctional Thermally Activated Delayed Fluorescence Molecules. <i>Journal of Physical Chemistry C</i> , 2022, 126, 2437-2446.	1.5	10
4	Structure-property relationship study of blue thermally activated delayed fluorescence molecules with different donor and position substitutions: theoretical perspective and molecular design. <i>Journal of Materials Chemistry C</i> , 2022, 10, 4723-4736.	2.7	17
5	Theoretical perspective of relationship between molecular structure and luminescence properties for circularly polarized thermally activated delayed fluorescence. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2022, 275, 121164.	2.0	6
6	Insights on isomeric emitters with thermally activated delayed fluorescence: Comparison between solvent and crystal state. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2022, 278, 121328.	2.0	4
7	Substituent effects on the intermolecular interactions and emission behaviors in pyrene-based mechanochromic luminogens. <i>Journal of Materials Chemistry C</i> , 2022, 10, 9310-9318.	2.7	16
8	Theoretical studies on the excited-state properties of thermally activated delayed fluorescence molecules with aggregation induced emission. <i>Journal of Materials Chemistry C</i> , 2022, 10, 9377-9390.	2.7	7
9	Novel Deep Red Thermally Activated Delayed Fluorescence Molecule with Aggregation-Induced Emission Enhancement: Theoretical Design and Experimental Validation. <i>Journal of Physical Chemistry Letters</i> , 2022, 13, 4711-4720.	2.1	16
10	A theoretical perspective of the relationship between the structures and luminescence properties of red thermally activated delayed fluorescence molecules. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 17140-17154.	1.3	6
11	Theoretical insights into room temperature phosphorescence emission with anti-Kasha behavior in aggregate. <i>Dyes and Pigments</i> , 2022, 205, 110560.	2.0	8
12	Design strategy for blue thermally activated delayed fluorescence: Position and methyl substitutions. <i>Chemical Physics Letters</i> , 2021, 764, 138260.	1.2	6
13	Theoretical perspective on the luminescence mechanism of a hybridized local and charge transfer state emitter with aggregation induced emission: a QM/MM study. <i>CrystEngComm</i> , 2021, 23, 3582-3593.	1.3	4
14	Highly efficient T-shaped deep-red thermally activated delayed fluorescence emitters: substitution position effect. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 21883-21892.	1.3	20
15	Unraveling the Important Role of High-Lying Triplet-Lowest Excited Singlet Transitions in Achieving Highly Efficient Deep-Blue Alq ₃ -Based OLEDs. <i>Advanced Materials</i> , 2021, 33, e2006953.	11.1	66
16	Highly Efficient Near-Infrared Thermally Activated Delayed Fluorescence Molecules via Acceptor Tuning: Theoretical Molecular Design and Experimental Verification. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 1893-1903.	2.1	48
17	Responsive mechanism of 2-fluoro-5-nitrobenzoate based two-photon fluorescent probes for H ₂ Sn detection: A theoretical perspective. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2021, 250, 119244.	2.0	2
18	Sensing mechanism of fluorescent sensor to Cu ²⁺ based on inhibiting ultra-fast intramolecular proton transfer process. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2021, 254, 119685.	2.0	6

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19	Structure-property relationship for triarylboron-based thermally activated delayed fluorescence molecules: A theoretical perspective. <i>Materials Science and Engineering B: Solid-State Materials for Advanced Technology</i> , 2021, 270, 115203.	1.7	3
20	High-Performance Ultraviolet Organic Light-Emitting Diode Enabled by High-Lying Reverse Intersystem Crossing. <i>Angewandte Chemie</i> , 2021, 133, 22415-22421.	1.6	10
21	High-Performance Ultraviolet Organic Light-Emitting Diode Enabled by High-Lying Reverse Intersystem Crossing. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 22241-22247.	7.2	68
22	Theoretical insights on the luminescent mechanism of an efficient aggregation-induced nondoped delayed fluorescence emitter using QM / MM method. <i>International Journal of Quantum Chemistry</i> , 2021, 121, e26490.	1.0	3
23	Intermolecular interaction on excited-state properties of fluoro-substituted thermally activated delayed fluorescence molecules with aggregation-induced emission: a theoretical perspective. <i>Molecular Physics</i> , 2021, 119, e1862931.	0.8	3
24	Effects of Secondary Acceptors on Excited-State Properties of Sky-Blue Thermally Activated Delayed Fluorescence Molecules: Luminescence Mechanism and Molecular Design. <i>Journal of Physical Chemistry A</i> , 2021, 125, 175-186.	1.1	12
25	Structural Isomerization Effect on the Triplet Energy Consumption Process of Organic Room-Temperature Phosphorescence Molecules: A QM/MM Study. <i>Journal of Physical Chemistry C</i> , 2021, 125, 27810-27819.	1.5	10
26	Thermally activated delayed fluorescence emitters with dual conformations for white organic light-emitting diodes: mechanism and molecular design. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 1313-1323.	1.3	20
27	Theoretical perspective for luminescent mechanism of thermally activated delayed fluorescence emitter with excited-state intramolecular proton transfer. <i>Journal of Materials Chemistry C</i> , 2020, 8, 98-108.	2.7	27
28	Substitution effect on luminescent property of thermally activated delayed fluorescence molecule with aggregation induced emission: A QM/MM study. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2020, 229, 117964.	2.0	15
29	Suppression of aggregation caused quenching in U-shaped thermally activated delayed fluorescence molecules: Tert-butyl effect. <i>Journal of Luminescence</i> , 2020, 219, 116899.	1.5	20
30	Photomechanical Luminescence from Through-Space Conjugated AIEgens. <i>Angewandte Chemie</i> , 2020, 132, 8913-8917.	1.6	12
31	Photomechanical Luminescence from Through-Space Conjugated AIEgens. <i>Angewandte Chemie - International Edition</i> , 2020, 59, 8828-8832.	7.2	67
32	Synthesis of fulvene-containing boron complexes with aggregation-induced emission and mechanochromic luminescence. <i>Chemical Communications</i> , 2020, 56, 14435-14438.	2.2	6
33	Dual Functionalization of Electron Transport Layer via Tailoring Molecular Structure for High-Performance Perovskite Light-Emitting Diodes. <i>ACS Applied Materials & Interfaces</i> , 2020, 12, 37346-37353.	4.0	17
34	The photophysical properties and imaging application of a new polarity-sensitive fluorescent probe. <i>Analyst</i> , 2020, 145, 6556-6561.	1.7	14
35	Tunable lifetimes and efficiencies of room temperature phosphorescent liquids by modulating the length and number of alkyl chains. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 19746-19757.	1.3	8
36	An Effective Design Strategy for Robust Aggregation-Induced Delayed Fluorescence Luminogens to Improve Efficiency Stability of Nondoped and Doped OLEDs. <i>Advanced Optical Materials</i> , 2020, 8, 2001027.	3.6	38

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37	Solid-State Effect Induced Thermally Activated Delayed Fluorescence with Tunable Emission: A Multiscale Study. <i>Journal of Physical Chemistry A</i> , 2020, 124, 8540-8550.	1.1	18
38	Theoretical Study on Thermally Activated Delayed Fluorescence Emitters in White Organic Light-Emitting Diodes: Emission Mechanism and Molecular Design. <i>Journal of Physical Chemistry A</i> , 2020, 124, 7526-7537.	1.1	14
39	Syntheses and structures of two novel fluorescent metal-organic frameworks generated from a tridentate donor-acceptor motif ligand. <i>Acta Crystallographica Section C, Structural Chemistry</i> , 2020, 76, 605-615.	0.2	1
40	Solid-state effect on luminescent properties of thermally activated delayed fluorescence molecule with aggregation induced emission: A theoretical perspective. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2020, 241, 118634.	2.0	11
41	Perspective for aggregation-induced delayed fluorescence mechanism: A QM/MM study*. <i>Chinese Physics B</i> , 2020, 29, 088504.	0.7	7
42	Insights on aggregation induced room temperature phosphorescence properties: A QM/MM study. <i>Journal of Luminescence</i> , 2020, 221, 117046.	1.5	11
43	The role of intermolecular interactions in regulating the thermally activated delayed fluorescence and charge transfer properties: a theoretical perspective. <i>Journal of Materials Chemistry C</i> , 2020, 8, 8601-8612.	2.7	22
44	Towards boosting the exciton lifetime and efficiency of near-infrared aggregation induced emitters with hybridized local and charge transfer excited states: a multiscale study. <i>Journal of Materials Chemistry C</i> , 2019, 7, 8874-8887.	2.7	35
45	Pressure-induced emission enhancement in hexaphenylsilole: a computational study. <i>Journal of Materials Chemistry C</i> , 2019, 7, 1388-1398.	2.7	33
46	Aggregation-Induced Delayed Fluorescence Luminogens with Accelerated Reverse Intersystem Crossing for High-Performance OLEDs. , 2019, 1, 613-619.		51
47	Substitution induced tunable emission of an airplane-like pyrene-based fluorophore: First-principles study. <i>Chemical Physics Letters</i> , 2019, 734, 136726.	1.2	3
48	Theoretical Study of the Mechanism of Aggregation-Caused Quenching in Near-Infrared Thermally Activated Delayed Fluorescence Molecules: Hydrogen-Bond Effect. <i>Journal of Physical Chemistry C</i> , 2019, 123, 24705-24713.	1.5	89
49	Theoretical study and experimental validation on the optical emission processes in free and locked pyrazine derivatives. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2019, 223, 117296.	2.0	3
50	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. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2019, 223, 117321.	2.0	8
51	Bicolor switching mechanism of multifunctional light-emitting molecular material in solid phase. <i>Organic Electronics</i> , 2019, 71, 212-219.	1.4	23
52	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. <i>Organic Electronics</i> , 2019, 71, 113-122.	1.4	40
53	Theoretical arrangement of thermally activated delayed fluorescence as host for fluorescent emitter with blue to red emission. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2019, 219, 44-52.	2.0	2
54	Theoretical study on the optical emission processes in geminally locked tetraphenylethylene derivatives. <i>Chemical Physics Letters</i> , 2019, 727, 25-30.	1.2	1

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55	Theoretical study on the light-emitting mechanism of circularly polarized luminescence molecules with both thermally activated delayed fluorescence and aggregation-induced emission. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 7288-7297.	1.3	20
56	Strategy to modulate the singlet-triplet energy gap for spiro-based thermally activated delayed fluorescence molecules. <i>Journal of Luminescence</i> , 2019, 209, 372-378.	1.5	18
57	Effect of intermolecular interaction on excited-state properties of thermally activated delayed fluorescence molecules in solid phase: A QM/MM study. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2019, 209, 248-255.	2.0	12
58	Mechanical Insights into Aggregation-Induced Delayed Fluorescence Materials with Anti-Kasha Behavior. <i>Advanced Science</i> , 2019, 6, 1801629.	5.6	111
59	Theoretical Study on the Sensing Mechanism of Novel Hydrazine Sensor TAPHP and Its ESIPT and ICT Processes. <i>Frontiers in Chemistry</i> , 2019, 7, 932.	1.8	24
60	Structure-property relationship of phosphine oxide based thermally activated delayed fluorescence molecules: First-principles study. <i>Organic Electronics</i> , 2018, 59, 7-14.	1.4	6
61	Excited State Properties of a Thermally Activated Delayed Fluorescence Molecule in Solid Phase Studied by Quantum Mechanics/Molecular Mechanics Method. <i>Journal of Physical Chemistry C</i> , 2018, 122, 2358-2366.	1.5	68
62	Excited state dynamics of new-type thermally activated delayed fluorescence emitters: theoretical view of light-emitting mechanism. <i>Molecular Physics</i> , 2018, 116, 19-28.	0.8	34
63	Influence of electron donating ability on reverse intersystem crossing rate for one kind of thermally activated delayed fluorescence molecules. <i>Chinese Journal of Chemical Physics</i> , 2018, 31, 291-299.	0.6	3
64	Electroluminescent Mechanism of Thermally Activated Delayed Fluorescence Emitters: Conformational Effect. <i>Journal of Physical Chemistry C</i> , 2018, 122, 19953-19961.	1.5	22
65	Influence of donor and acceptor groups on the S-T energy gap for thermally activated delayed fluorescence emitters. <i>Molecular Physics</i> , 2017, 115, 809-814.	0.8	8
66	Theoretical insights on the electroluminescent mechanism of thermally activated delayed fluorescence emitters. <i>Organic Electronics</i> , 2017, 41, 17-25.	1.4	65
67	Excited state dynamics for hybridized local and charge transfer state fluorescent emitters with aggregation-induced emission in the solid phase: a QM/MM study. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 29872-29879.	1.3	36
68	Theoretical perspective for internal quantum efficiency of thermally activated delayed fluorescence emitter in solid phase: A QM/MM study. <i>Organic Electronics</i> , 2017, 51, 349-356.	1.4	27
69	Molecular stacking effect on photoluminescence quantum yield and charge mobility of organic semiconductors. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 30147-30156.	1.3	24
70	Theoretical perspective of the excited state intramolecular proton transfer for a compound with aggregation induced emission in the solid phase. <i>RSC Advances</i> , 2017, 7, 44089-44096.	1.7	18
71	Excited state properties of non-doped thermally activated delayed fluorescence emitters with aggregation-induced emission: a QM/MM study. <i>Journal of Materials Chemistry C</i> , 2017, 5, 8390-8399.	2.7	91
72	Luminescent properties of thermally activated delayed fluorescence molecule with intramolecular π - π interaction between donor and acceptor. <i>Chinese Physics B</i> , 2017, 26, 118503.	0.7	7

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73	First-Principles Investigation on Triazine Based Thermally Activated Delayed Fluorescence Emitters. <i>Chinese Journal of Chemical Physics</i> , 2016, 29, 291-296.	0.6	25
74	Modulating excited state properties of thermally activated delayed fluorescence molecules by tuning the connecting pattern. <i>Theoretical Chemistry Accounts</i> , 2016, 135, 1.	0.5	7
75	Decreasing the singlet-triplet gap for thermally activated delayed fluorescence molecules by structural modification on the donor fragment: First-principles study. <i>Chemical Physics Letters</i> , 2016, 652, 16-21.	1.2	43
76	Using the isotope effect to probe an aggregation induced emission mechanism: theoretical prediction and experimental validation. <i>Chemical Science</i> , 2016, 7, 5573-5580.	3.7	67
77	Efficient modulation of optical and electrical properties of X-shaped thermally activated delayed fluorescence emitters by substitution. <i>Journal of Molecular Modeling</i> , 2016, 22, 173.	0.8	2
78	Dynamics of Excited States for Fluorescent Emitters with Hybridized Local and Charge-Transfer Excited State in Solid Phase: A QM/MM Study. <i>Journal of Physical Chemistry A</i> , 2016, 120, 9422-9430.	1.1	30
79	Effect of Intermolecular Excited-state Interaction on Vibrationally Resolved Optical Spectra in Organic Molecular Aggregates. <i>Acta Chimica Sinica</i> , 2016, 74, 902.	0.5	27
80	Theoretical Analysis on Optical Limiting Properties of Newly Synthesized Graphene Oxide-Porphyrin Composites. <i>Chinese Journal of Chemical Physics</i> , 2015, 28, 257-262.	0.6	4
81	Spectroscopic Signature of the Aggregation-Induced Emission Phenomena Caused by Restricted Nonradiative Decay: A Theoretical Proposal. <i>Journal of Physical Chemistry C</i> , 2015, 119, 5040-5047.	1.5	70
82	Aggregation Effects on the Optical Emission of 1,1,2,3,4,5-Hexaphenylsilole (HPS): A QM/MM Study. <i>Journal of Physical Chemistry A</i> , 2014, 118, 9094-9104.	1.1	110