

Kai Zhang

List of Publications by Year in descending order

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Version: 2024-02-01

35
papers

692
citations

516710

16
h-index

610901

24
g-index

35
all docs

35
docs citations

35
times ranked

379
citing authors

#	ARTICLE	IF	CITATIONS
1	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.	3.1	89
2	High-Performance Ultraviolet Organic Light-Emitting Diode Enabled by High-Lying Reverse Intersystem Crossing. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 22241-22247.	13.8	68
3	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.	4.6	48
4	Positive impact of chromophore flexibility on the efficiency of red thermally activated delayed fluorescence materials. <i>Materials Horizons</i> , 2021, 8, 1297-1303.	12.2	41
5	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.	2.6	40
6	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.	5.5	35
7	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.	5.5	30
8	An extended π -backbone for highly efficient near-infrared thermally activated delayed fluorescence with enhanced horizontal molecular orientation. <i>Materials Horizons</i> , 2022, 9, 772-779.	12.2	26
9	Bicolor switching mechanism of multifunctional light-emitting molecular material in solid phase. <i>Organic Electronics</i> , 2019, 71, 212-219.	2.6	23
10	Carry-On Nitric-Oxide Luggage for Enhanced Chemotherapeutic Efficacy. <i>Nano Letters</i> , 2020, 20, 5275-5283.	9.1	23
11	Interrupted intramolecular donor-acceptor interaction compensated by strong through-space electronic coupling for highly efficient near-infrared TADF with emission over 800Ånm. <i>Chemical Engineering Journal</i> , 2022, 430, 132744.	12.7	23
12	Positive isotope effect in thermally activated delayed fluorescence emitters based on deuterium-substituted donor units. <i>Chemical Engineering Journal</i> , 2022, 430, 132822.	12.7	21
13	Highly efficient T-shaped deep-red thermally activated delayed fluorescence emitters: substitution position effect. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 21883-21892.	2.8	20
14	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.	3.1	18
15	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.	2.5	18
16	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.	5.5	17
17	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.	4.6	16
18	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.	3.9	12

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19	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.	2.5	12
20	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.	3.9	11
21	Insights on aggregation induced room temperature phosphorescence properties: A QM/MM study. <i>Journal of Luminescence</i> , 2020, 221, 117046.	3.1	11
22	High-Performance Ultraviolet Organic Light-Emitting Diode Enabled by High-Lying Reverse Intersystem Crossing. <i>Angewandte Chemie</i> , 2021, 133, 22415-22421.	2.0	10
23	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.	3.1	10
24	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.	3.1	10
25	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.	3.9	9
26	Determination of Fe ³⁺ upon Special "Upconversion Luminescence" of Dopamine. <i>ACS Omega</i> , 2019, 4, 9918-9924.	3.5	8
27	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.	2.8	8
28	Theoretical insights into room temperature phosphorescence emission with anti-Kasha behavior in aggregate. <i>Dyes and Pigments</i> , 2022, 205, 110560.	3.7	8
29	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.	5.5	7
30	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.	2.8	6
31	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.	3.9	4
32	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.	1.7	3
33	Highly efficient thermally activated delayed fluorescence emitters with suppressed energy loss and a fast reverse intersystem crossing process. <i>Journal of Materials Chemistry C</i> , 2022, 10, 3685-3690.	5.5	3
34	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.	3.9	2
35	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.	3.9	2