Chuan-Kui Wang

List of Publications by Year
in descending order

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95	1,541	304743	395702
papers	citations	22 h-index	33 g-index

95	95	95	1198
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	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.	5.5	91
2	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.	3.1	89
3	Accurate K-edge X-ray photoelectron and absorption spectra of g-C₃N₄ nanosheets by first-principles simulations and reinterpretations. Physical Chemistry Chemical Physics, 2019, 21, 22819-22830.	2.8	70
4	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.	3.1	68
5	Propagation of a strong x-ray pulse: Pulse compression, stimulated Raman scattering, amplified spontaneous emission, lasing without inversion, and four-wave mixing. Physical Review A, 2010, 81, .	2.5	65
6	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.	4.6	48
7	Modulation of Rectification in Diblock Co-oligomer Diodes by Adjusting Anchoring Groups for Both Symmetric and Asymmetric Electrodes. Journal of Physical Chemistry C, 2012, 116, 22009-22014.	3.1	40
8	Auger effect in the presence of strong x-ray pulses. Physical Review A, 2010, 81, .	2.5	38
9	Theoretical Studies on Protonation-Induced Inversion of the Rectifying Direction in Dipyrimidinylâ€“Diphenyl Diblock Molecular Junctions. Journal of Physical Chemistry C, 2012, 116, 3773-3778.	3.1	36
10	Designing molecular rectifiers and spin valves using metallocene-functionalized undecanethiolates: one transition metal atom matters. Journal of Materials Chemistry C, 2018, 6, 2105-2112.	5.5	36
11	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.	5.5	35
12	Giant Rectification Ratios of Azulene-like Dipole Molecular Junctions Induced by Chemical Doping in Armchair-Edged Graphene Nanoribbon Electrodes. Journal of Physical Chemistry C, 2014, 118, 18713-18720.	3.1	34
13	Excited state dynamics of new-type thermally activated delayed fluorescence emitters: theoretical view of light-emitting mechanism. Molecular Physics, 2018, 116, 19-28.	1.7	34
14	Fabricating Atom-Sized Gaps by Field-Aided Atom Migration in Nanoscale Junctions. Physical Review Applied, 2018, 9, .	3.8	31
15	Rotational Doppler effect in x-ray photoionization. Physical Review A, 2010, 82, .	2.5	30
16	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.	2.5	30
17	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.	5.5	30
18	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.	5.5	27

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19	An extended Ï€-backbone for highly efficient near-infrared thermally activated delayed fluorescence with enhanced horizontal molecular orientation. Materials Horizons, 2022, 9, 772-779.	12.2	26
20	First-Principles Study on Formation and Electron-Transport Properties of Single Oligothiophene Molecular Junctions. Journal of Physical Chemistry C, 2011, 115, 15586-15591.	3.1	25
21	Bias Dependence of Rectifying Direction in a Diblock Co-oligomer Molecule with Graphene Nanoribbon Electrodes. Journal of Physical Chemistry C, 2013, 117, 20951-20957.	3.1	25
22	Electroluminescent Mechanism of Thermally Activated Delayed Fluorescence Emitters: Conformational Effect. Journal of Physical Chemistry C, 2018, 122, 19953-19961.	3.1	22
23	Local structures of nitrogen-doped graphdiynes determined by computational X-ray spectroscopy. Carbon, 2019, 149, 672-678.	10.3	22
24	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.	5.5	22
25	Theoretical Isomer Identification of Three C₅₆ Fullerenes and Their Chlorinated Derivatives by XPS and NEXAFS Spectra. Journal of Physical Chemistry C, 2016, 120, 13779-13786.	3.1	21
26	A method to study electronic transport properties of molecular junction: one-dimension transmission combined with three-dimension correction approximation (OTCTCA). Scientific Reports, 2016, 6, 21946.	3.3	20
27	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.	2.8	20
28	Highly efficient T-shaped deep-red thermally activated delayed fluorescence emitters: substitution position effect. Physical Chemistry Chemical Physics, 2021, 23, 21883-21892.	2.8	20
29	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.	3.6	18
30	Solid-State Effect Induced Thermally Activated Delayed Fluorescence with Tunable Emission: A Multiscale Study. Journal of Physical Chemistry A, 2020, 124, 8540-8550.	2.5	18
31	Manipulating Current Spin Polarization in Magnetic Single-Molecule Junctions via Destructive Quantum Interference. Journal of Physical Chemistry C, 2020, 124, 12144-12152.	3.1	18
32	Theoretical Identification of Three C₆₆ Fullerene Isomers and Related Chlorinated Derivatives by X-ray Photoelectron Spectroscopy and Near-edge X-ray Absorption Fine Structure Spectroscopy. Journal of Physical Chemistry A, 2016, 120, 9932-9940.	2.5	17
33	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.	5.5	17
34	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.	4.6	16
35	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.	3.9	15
36	A theoretical library of N1s core binding energies of polynitrogen molecules and ions in the gas phase. Physical Chemistry Chemical Physics, 2022, 24, 8196-8207.	2.8	15

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37	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.	2.5	14
38	An ultra-sensitive gas sensor based on a two-dimensional manganese porphyrin monolayer. Physical Chemistry Chemical Physics, 2021, 23, 11852-11862.	2.8	13
39	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.	3.9	12
40	Theoretical identification of seven C₈₀ fullerene isomers by XPS and NEXAFS spectroscopy. Physical Chemistry Chemical Physics, 2017, 19, 32647-32654.	2.8	12
41	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.	2.5	12
42	Spin Polarization at Organic-Ferromagnetic Interface: Effect of Contact Configuration. Chinese Journal of Chemical Physics, 2016, 29, 344-348.	1.3	11
43	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.	3.9	11
44	Theoretical Study on the Light-Emitting Mechanism of Multifunctional Thermally Activated Delayed Fluorescence Molecules. Journal of Physical Chemistry C, 2022, 126, 2437-2446.	3.1	10
45	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.	3.1	10
46	Stable Universal 1â€•and 2â€Input Singleâ€Molecule Logic Gates. Advanced Materials, 2022, 34, e2202135.	21.0	10
47	Optical limiting and dynamical two-photon absorption of porphyrin with ruthenium outlying complexes for a picosecond pulse train. European Physical Journal D, 2016, 70, 1.	1.3	9
48	Towards Rectifying Performance at the Molecular Scale. Topics in Current Chemistry, 2017, 375, 85.	5.8	9
49	Monitoring Hydrogen/Deuterium Tautomerization in Transient Isomers of Single Porphine by Highly Localized Plasmonic Field. Journal of Physical Chemistry C, 2019, 123, 11081-11093.	3.1	9
50	Controlling Rectification Performance by Tuning Moleculeâ€“Electrode Coupling Strength in Ferrocenyl-Undecanethiolate Molecular Diodes. Journal of Physical Chemistry C, 2019, 123, 1559-1565.	3.1	9
51	Surface decoration of phosphorene nanoribbons with 4d transition metal atoms for spintronics. Physical Chemistry Chemical Physics, 2020, 22, 16063-16071.	2.8	9
52	Dimerization and Isomerism Effects on Two-Photon Absorption of Tetraphenylethene Derivatives and Molecular Design for Two-Photon Absorption Materials. Journal of Physical Chemistry B, 2016, 120, 9708-9715.	2.6	8
53	Effect of H2O Adsorption on Negative Differential Conductance Behavior of Single Junction. Scientific Reports, 2017, 7, 4195.	3.3	8
54	Theoretical N K-edge NEXAFS spectroscopy study for configuration of a dipolar molecule on graphene. Materials Chemistry and Physics, 2018, 207, 309-314.	4.0	8

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55	Theoretical Identification of the Six Stable C₈₄ Isomers by IR, XPS, and NEXAFS Spectra. Journal of Physical Chemistry A, 2018, 122, 1019-1026.	2.5	8
56	Two-photon absorption properties of D-A-D type chromophores containing tetraphenylethylene and triphenylamine moieties: a close look at the effects of the strength, position and number of donors. Molecular Physics, 2019, 117, 672-680.	1.7	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.	2.8	8
58	Identification of Four C₄₀ Isomers by Means of a Theoretical XPS/NEXAFS Spectra Study. Journal of Physical Chemistry A, 2018, 122, 4750-4755.	2.5	7
59	Bias and molecular-length dependent oddâ€“even effect of rectification in 4â€²-methyl-2,2â€²-bipyridyl-terminated n-alkanethiolate single-molecule diodes. Journal of Materials Chemistry C, 2019, 7, 9000-9007.	5.5	7
60	Solvent effect on the photophysical properties of thermally activated delayed fluorescence molecules. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2020, 225, 117473.	3.9	7
61	Effect of a Hydrogen Bond on Molecular Probing Properties in the Solvent. Journal of Physical Chemistry A, 2020, 124, 520-528.	2.5	7
62	Protonation control of spin transport properties in magnetic single-molecule junctions. Journal of Materials Science, 2020, 55, 16311-16322.	3.7	7
63	Two-photon-induced x-ray emission in neon atoms. Physical Review A, 2010, 82, .	2.5	6
64	Obvious modulation of rectifying performance by conjugation breaking of the bridging fragment in donorâ€“bridgeâ€“acceptor molecular diodes. RSC Advances, 2017, 7, 14200-14205.	3.6	6
65	Trapping effect and trajectory control of surface plasmon polaritons in a metal-dielectric-metal waveguide. Physical Review A, 2020, 102, .	2.5	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.	3.9	6
67	Design of multifunctional spin logic gates based on manganese porphyrin molecules connected to graphene electrodes. Physical Chemistry Chemical Physics, 2022, 24, 1849-1859.	2.8	6
68	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.	3.9	6
69	Assignments of Inelastic Electron Tunneling Spectra of Semifluorinated Alkanethiol Molecular Junctions. Journal of Physical Chemistry C, 2011, 115, 20301-20306.	3.1	5
70	Protonation Effect on One- and Two-photon Absorption Property of a Newly Synthesized Octupolar Chromophore. Chinese Journal of Chemical Physics, 2012, 25, 666-670.	1.3	5
71	Isomerism and coordination mode effects on two-photon absorption of tris(picolyl)amine-based fluorescent probes for zinc ions. Chinese Physics B, 2018, 27, 103301.	1.4	5
72	Multistate magnetoresistance in zigzag-edge trigonal graphene magnetic junctions. Journal of Materials Science, 2019, 54, 5551-5560.	3.7	5

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73	Theoretical study of nano onion-like fullerenes C20@C80 on XPS and NEXAFS spectra. Molecular Physics, 2019, 117, 794-803.	1.7	5
74	Theoretical studies on structures and spectral properties for two C86 isomers and their chlorinated derivatives. Molecular Physics, 2019, 117, 507-515.	1.7	5
75	Decoding Forming Processes of Different Contact Configurations in Au- and Ag-Electrode Single-Molecule Junctions. Journal of Physical Chemistry C, 2021, 125, 27290-27297.	3.1	5
76	Theoretical Studies on One-photon and Two-photon Absorption Properties of Pyrene-core Derivatives. Chinese Journal of Chemical Physics, 2010, 23, 664-668.	1.3	4
77	Electronic structures and spectral characteristics of the six C32 fullerene isomers. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2019, 212, 180-187.	3.9	4
78	Large Rectification Ratio of up to 106 for Conjugation-Group-Terminated Undecanethiolate Single-Molecule Diodes on Pt Electrodes. Journal of Physical Chemistry C, 2021, 125, 20783-20790.	3.1	4
79	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.	3.9	4
80	Distinguishing the six stable C₃₆ fullerene isomers by means of soft X-ray spectroscopies at DFT level. Molecular Physics, 2019, 117, 635-643.	1.7	3
81	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.	1.7	3
82	Highly efficient thermally activated delayed fluorescence emitters with suppressed energy loss and a fast reverse intersystem crossing process. Journal of Materials Chemistry C, 2022, 10, 3685-3690.	5.5	3
83	Simulations of inelastic electron tunneling spectroscopy of semifluorinated hexadecanethiol junctions. Frontiers of Physics in China, 2009, 4, 415-419.	1.0	2
84	Influence of Donor on the Sensing Performance of a Series of Throughâ€Bond Energy Transferâ€Based Twoâ€photon Fluorescent Cu²⁺ Probes. Photochemistry and Photobiology, 2016, 92, 528-536.	2.5	2
85	Solvent Effects on Two-Photon Absorption of Alkyne and Alkene Ï€-bridging Chromophores. Chinese Journal of Chemical Physics, 2017, 30, 63-70.	1.3	2
86	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.	3.9	2
87	Theoretical identification of buckyonion fullerene C20@C60 isomers by XPS and NEXAFS spectroscopy. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2020, 229, 117904.	3.9	2
88	Geometric and electronic structures of pyrazine molecule chemisorbed on Si(100) surface by XPS and NEXAFS spectroscopy. Chinese Journal of Chemical Physics, 2020, 33, 417-426.	1.3	2
89	Landscape of s-triazine molecule on Si(100) by a theoretical x-ray photoelectron spectroscopy and x-ray absorption near-edge structure spectra study. Chinese Physics B, 2018, 27, 113101.	1.4	1
90	Predicting and researching adsorption configurations of pyridazine on Si(100) surface by means of X-ray spectroscopies in theory. Molecular Physics, 2020, 118, e1679399.	1.7	0

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91	Structural recognition of three significant C88 isomers and its chlorinated derivatives by X-ray spectroscopy. Molecular Physics, 2020, 118, e1725670.	1.7	0
92	Electronic structures and spectral characteristics of five C28 fullerene and C30 fullerene isomers by XPS and NEXAFS spectra. Molecular Physics, 0, , e1921297.	1.7	0
93	Influence of halogen elements on the optical properties of two-photon fluorescent dyes. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2022, 267, 120493.	3.9	0
94	Adsorption configurations of furan molecule on Si(100)-2Ã—1 surface by X-ray photoelectron spectroscopy and near-edge X-ray absorption fine structure spectra. Molecular Physics, 2022, 120, .	1.7	0
95	Identification of C38 fullerene isomers by soft X-ray spectroscopy. Indian Journal of Physics, 0, , .	1.8	0