

Chuan-Kui Wang

List of Publications by Year in descending order

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#	ARTICLE	IF	CITATIONS
1	Influence of halogen elements on the optical properties of two-photon fluorescent dyes. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2022, 267, 120493.	3.9	0
2	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
3	Adsorption configurations of furan molecule on Si(100)-2 \times 1 surface by X-ray photoelectron spectroscopy and near-edge X-ray absorption fine structure spectra. <i>Molecular Physics</i> , 2022, 120, .	1.7	0
4	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
5	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
6	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
7	Design of multifunctional spin logic gates based on manganese porphyrin molecules connected to graphene electrodes. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 1849-1859.	2.8	6
8	A theoretical library of N1s core binding energies of polynitrogen molecules and ions in the gas phase. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 8196-8207.	2.8	15
9	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
10	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.	3.9	6
11	Stable Universal 1-and 2-input Single-Molecule Logic Gates. <i>Advanced Materials</i> , 2022, 34, e2202135.	21.0	10
12	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
13	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
14	An ultra-sensitive gas sensor based on a two-dimensional manganese porphyrin monolayer. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 11852-11862.	2.8	13
15	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
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.	4.6	48
17	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.	3.9	6
18	Large Rectification Ratio of up to 106 for Conjugation-Group-Terminated Undecanethiolate Single-Molecule Diodes on Pt Electrodes. <i>Journal of Physical Chemistry C</i> , 2021, 125, 20783-20790.	3.1	4

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19	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
20	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
21	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
22	Decoding Forming Processes of Different Contact Configurations in Au- and Ag-Electrode Single-Molecule Junctions. <i>Journal of Physical Chemistry C</i> , 2021, 125, 27290-27297.	3.1	5
23	Solvent effect on the photophysical properties of thermally activated delayed fluorescence molecules. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2020, 225, 117473.	3.9	7
24	Predicting and researching adsorption configurations of pyridazine on Si(100) surface by means of X-ray spectroscopies in theory. <i>Molecular Physics</i> , 2020, 118, e1679399.	1.7	0
25	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.	2.8	20
26	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.	5.5	27
27	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.	3.9	15
28	Effect of a Hydrogen Bond on Molecular Probing Properties in the Solvent. <i>Journal of Physical Chemistry A</i> , 2020, 124, 520-528.	2.5	7
29	Theoretical identification of buckyonion fullerene C20@C60 isomers by XPS and NEXAFS spectroscopy. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2020, 229, 117904.	3.9	2
30	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
31	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
32	Protonation control of spin transport properties in magnetic single-molecule junctions. <i>Journal of Materials Science</i> , 2020, 55, 16311-16322.	3.7	7
33	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.	2.5	14
34	Trapping effect and trajectory control of surface plasmon polaritons in a metal-dielectric-metal waveguide. <i>Physical Review A</i> , 2020, 102, .	2.5	6
35	Geometric and electronic structures of pyrazine molecule chemisorbed on Si(100) surface by XPS and NEXAFS spectroscopy. <i>Chinese Journal of Chemical Physics</i> , 2020, 33, 417-426.	1.3	2
36	Manipulating Current Spin Polarization in Magnetic Single-Molecule Junctions via Destructive Quantum Interference. <i>Journal of Physical Chemistry C</i> , 2020, 124, 12144-12152.	3.1	18

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37	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
38	Surface decoration of phosphorene nanoribbons with 4d transition metal atoms for spintronics. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 16063-16071.	2.8	9
39	Structural recognition of three significant C88 isomers and its chlorinated derivatives by X-ray spectroscopy. <i>Molecular Physics</i> , 2020, 118, e1725670.	1.7	0
40	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.	5.5	22
41	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
42	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
43	Multistate magnetoresistance in zigzag-edge trigonal graphene magnetic junctions. <i>Journal of Materials Science</i> , 2019, 54, 5551-5560.	3.7	5
44	Bias and molecular-length dependent odd-even effect of rectification in 4- ϵ^2 -methyl-2,2'-bipyridyl-terminated <i>n</i> -alkanethiolate single-molecule diodes. <i>Journal of Materials Chemistry C</i> , 2019, 7, 9000-9007.	5.5	7
45	Local structures of nitrogen-doped graphdiynes determined by computational X-ray spectroscopy. <i>Carbon</i> , 2019, 149, 672-678.	10.3	22
46	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
47	Monitoring Hydrogen/Deuterium Tautomerization in Transient Isomers of Single Porphine by Highly Localized Plasmonic Field. <i>Journal of Physical Chemistry C</i> , 2019, 123, 11081-11093.	3.1	9
48	Accurate K-edge X-ray photoelectron and absorption spectra of g-C ₃ N ₄ nanosheets by first-principles simulations and reinterpretations. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 22819-22830.	2.8	70
49	Controlling Rectification Performance by Tuning Molecule-Electrode Coupling Strength in Ferrocenyl-Undecanethiolate Molecular Diodes. <i>Journal of Physical Chemistry C</i> , 2019, 123, 1559-1565.	3.1	9
50	Electronic structures and spectral characteristics of the six C32 fullerene isomers. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2019, 212, 180-187.	3.9	4
51	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. <i>Molecular Physics</i> , 2019, 117, 672-680.	1.7	8
52	Theoretical study of nano onion-like fullerenes C20@C80 on XPS and NEXAFS spectra. <i>Molecular Physics</i> , 2019, 117, 794-803.	1.7	5
53	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
54	Distinguishing the six stable C ₃₆ fullerene isomers by means of soft X-ray spectroscopies at DFT level. <i>Molecular Physics</i> , 2019, 117, 635-643.	1.7	3

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55	Theoretical studies on structures and spectral properties for two C ₈₆ isomers and their chlorinated derivatives. <i>Molecular Physics</i> , 2019, 117, 507-515.	1.7	5
56	Theoretical N K-edge NEXAFS spectroscopy study for configuration of a dipolar molecule on graphene. <i>Materials Chemistry and Physics</i> , 2018, 207, 309-314.	4.0	8
57	Designing molecular rectifiers and spin valves using metallocene-functionalized undecanethiolates: one transition metal atom matters. <i>Journal of Materials Chemistry C</i> , 2018, 6, 2105-2112.	5.5	36
58	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.	3.1	68
59	Theoretical Identification of the Six Stable C ₈₄ Isomers by IR, XPS, and NEXAFS Spectra. <i>Journal of Physical Chemistry A</i> , 2018, 122, 1019-1026.	2.5	8
60	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.	1.7	34
61	Landscape of s-triazine molecule on Si(100) by a theoretical x-ray photoelectron spectroscopy and x-ray absorption near-edge structure spectra study. <i>Chinese Physics B</i> , 2018, 27, 113101.	1.4	1
62	Isomerism and coordination mode effects on two-photon absorption of tris(picoly)amine-based fluorescent probes for zinc ions. <i>Chinese Physics B</i> , 2018, 27, 103301.	1.4	5
63	Fabricating Atom-Sized Gaps by Field-Aided Atom Migration in Nanoscale Junctions. <i>Physical Review Applied</i> , 2018, 9, .	3.8	31
64	Identification of Four C ₄₀ Isomers by Means of a Theoretical XPS/NEXAFS Spectra Study. <i>Journal of Physical Chemistry A</i> , 2018, 122, 4750-4755.	2.5	7
65	Electroluminescent Mechanism of Thermally Activated Delayed Fluorescence Emitters: Conformational Effect. <i>Journal of Physical Chemistry C</i> , 2018, 122, 19953-19961.	3.1	22
66	Obvious modulation of rectifying performance by conjugation breaking of the bridging fragment in donor-bridge-acceptor molecular diodes. <i>RSC Advances</i> , 2017, 7, 14200-14205.	3.6	6
67	Effect of H ₂ O Adsorption on Negative Differential Conductance Behavior of Single Junction. <i>Scientific Reports</i> , 2017, 7, 4195.	3.3	8
68	Towards Rectifying Performance at the Molecular Scale. <i>Topics in Current Chemistry</i> , 2017, 375, 85.	5.8	9
69	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.	3.6	18
70	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.	5.5	91
71	Solvent Effects on Two-Photon Absorption of Alkyne and Alkene π -bridging Chromophores. <i>Chinese Journal of Chemical Physics</i> , 2017, 30, 63-70.	1.3	2
72	Theoretical identification of seven C ₈₀ fullerene isomers by XPS and NEXAFS spectroscopy. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 32647-32654.	2.8	12

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73	Spin Polarization at Organic-Ferromagnetic Interface: Effect of Contact Configuration. Chinese Journal of Chemical Physics, 2016, 29, 344-348.	1.3	11
74	Influence of Donor on the Sensing Performance of a Series of Through-Bond Energy Transfer-Based Two-photon Fluorescent Cu ²⁺ Probes. Photochemistry and Photobiology, 2016, 92, 528-536.	2.5	2
75	Theoretical Identification of Three C ₆₆ 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
76	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
77	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
78	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
79	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
80	Theoretical Isomer Identification of Three C ₅₆ Fullerenes and Their Chlorinated Derivatives by XPS and NEXAFS Spectra. Journal of Physical Chemistry C, 2016, 120, 13779-13786.	3.1	21
81	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
82	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
83	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
84	Theoretical Studies on Protonation-Induced Inversion of the Rectifying Direction in Dipyrimidinyl-Diphenyl Diblock Molecular Junctions. Journal of Physical Chemistry C, 2012, 116, 3773-3778.	3.1	36
85	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
86	Assignments of Inelastic Electron Tunneling Spectra of Semifluorinated Alkanethiol Molecular Junctions. Journal of Physical Chemistry C, 2011, 115, 20301-20306.	3.1	5
87	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
88	Rotational Doppler effect in x-ray photoionization. Physical Review A, 2010, 82, .	2.5	30
89	Two-photon-induced x-ray emission in neon atoms. Physical Review A, 2010, 82, .	2.5	6
90	Auger effect in the presence of strong x-ray pulses. Physical Review A, 2010, 81, .	2.5	38

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91	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
92	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
93	Simulations of inelastic electron tunneling spectroscopy of semifluorinated hexadecanethiol junctions. Frontiers of Physics in China, 2009, 4, 415-419.	1.0	2
94	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
95	Identification of C38 fullerene isomers by soft X-ray spectroscopy. Indian Journal of Physics, 0, , .	1.8	0