Wei-Jie Chi

List of Publications by Year
in descending order

87 papers	3,086 citations	172207 29 h-index	174990 52 g-index
90 all docs	90 docs citations	90 times ranked	2481 citing authors

#	Article	IF	Citations
1	A Ï€-extended triphenylamine based dopant-free hole-transporting material for perovskite solar cells via heteroatom substitution. Physical Chemistry Chemical Physics, 2022, 24, 4635-4643.	1.3	9
2	A Descriptor for Accurate Predictions of Host Molecules Enabling Ultralong Roomâ€Temperature Phosphorescence in Guest Emitters. Angewandte Chemie - International Edition, 2022, 61, .	7.2	17
3	Revealing the Sole Impact of Acceptor's Molecular Conformation to Energy Loss and Device Performance of Organic Solar Cells through Positional Isomers. Advanced Science, 2022, 9, e2103428.	5.6	9
4	Overcoming Spectral Dependence: A General Strategy for Developing Farâ€Red and Nearâ€Infrared Ultraâ€Fluorogenic Tetrazine Bioorthogonal Probes. Angewandte Chemie - International Edition, 2022, 61, .	7.2	31
5	Overcoming Spectral Dependence: A General Strategy for Developing Farâ€Red and Nearâ€Infrared Ultraâ€Fluorogenic Tetrazine Bioorthogonal Probes. Angewandte Chemie, 2022, 134, .	1.6	3
6	A Systematic Study on the Relationship Between Viscosity Sensitivity and <scp>Temperature Dependency</scp> of <scp>BODIPY</scp> Rotors. Bulletin of the Korean Chemical Society, 2021, 42, 91-94.	1.0	5
7	A unified fluorescence quenching mechanism of tetrazine-based fluorogenic dyes: energy transfer to a dark state. Materials Chemistry Frontiers, 2021, 5, 7012-7021.	3.2	28
8	Boronâ€“nitrogen substituted planar cores: designing dopant-free hole-transporting materials for efficient perovskite solar cells. Nanoscale, 2021, 13, 4241-4248.	2.8	16
9	State-crossing from a Locally Excited to an Electron Transfer State(SLEET) Model Rationalizing the Aggregation-induced Emission Mechanism of (Bi)piperidylanthracenes. Chemical Research in Chinese Universities, 2021, 37, 157-161.	1.3	9
10	Pentadiamond: A Highly Efficient Electron Transport Layer for Perovskite Solar Cells. Journal of Physical Chemistry C, 2021, 125, 5372-5379.	1.5	18
11	Aggregation-induced emission or aggregation-caused quenching? Impact of covalent bridge between tetraphenylethene and naphthalimide. Chinese Chemical Letters, 2021, 32, 1790-1794.	4.8	54
12	Fluorescence umpolung enables light-up sensing of N-acetyltransferases and nerve agents. Nature Communications, 2021, 12, 3869.	5.8	51
13	Energy transfer followed by electron transfer (ETET) endows a TPE-NBD dyad with enhanced environmental sensitivity. Chinese Chemical Letters, 2021, 32, 1937-1941.	4.8	18
14	High carrier mobility and remarkable photovoltaic performance of two-dimensional Ruddlesdenâ€“Popper organicâ€“inorganic metal halides (PA)2(MA)2M3I10 for perovskite solar cell applications. Materials Today, 2021, 47, 45-52.	8.3	12
15	An Approach to Developing Cyanines with Simultaneous Intersystem Crossing Enhancement and Excited-State Lifetime Elongation for Photodynamic Antitumor Metastasis. Journal of the American Chemical Society, 2021, 143, 12345-12354.	6.6	80
16	Bio-orthogonal Red and Far-Red Fluorogenic Probes for Wash-Free Live-Cell and Super-resolution Microscopy. ACS Central Science, 2021, 7, 1561-1571.	5.3	57
17	Restriction of Twisted Intramolecular Charge Transfer Enables the Aggregation-Induced Emission of 1-(N,N-Dialkylamino)-naphthalene Derivatives. Journal of Physical Chemistry A, 2021, 125, 8397-8403.	1.1	19
18	Twisted intramolecular charge transfer (TICT) and twists beyond TICT: from mechanisms to rational designs of bright and sensitive fluorophores. Chemical Society Reviews, 2021, 50, 12656-12678.	18.7	221

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19	Accelerating evaluation of the mobility of ionic liquid-modulated PEDOT flexible electronics using machine learning. Journal of Materials Chemistry A, 2021, 9, 25547-25557.	5.2	11
20	Emerging Design Principle of Nearâ€Infrared Upconversion Sensitizer Based on Mitochondriaâ€Targeted Organic Dye for Enhanced Photodynamic Therapy. Chemistry - A European Journal, 2021, 27, 16707-16715.	1.7	2
21	Positional Effect of the Triphenylamine Group on the Optical and Chargeâ€Transfer Properties of Thiopheneâ€Based Holeâ€Transporting Materials. Chemistry - an Asian Journal, 2020, 15, 287-293.	1.7	15
22	Molecular Origins of Heteroatom Engineering on the Emission Wavelength Tuning, Quantum Yield Variations and Fluorogenicity of NBDâ€like SCOTfluors. Chemistry - an Asian Journal, 2020, 15, 4082-4086.	1.7	8
23	Molecular Origins of Photoinduced Backward Intramolecular Charge Transfer. Journal of Physical Chemistry C, 2020, 124, 16820-16826.	1.5	19
24	Descriptor Î”G_{Câ€O} Enables the Quantitative Design of Spontaneously Blinking Rhodamines for Liveâ€Cell Superâ€Resolution Imaging. Angewandte Chemie - International Edition, 2020, 59, 20215-20223.	7.2	50
25	The photocatalytic mechanism of organic dithienophosphole derivatives as highly efficient photo-redox catalysts. Physical Chemistry Chemical Physics, 2020, 22, 20721-20731.	1.3	5
26	Descriptor Î”G_{Câ€O} Enables the Quantitative Design of Spontaneously Blinking Rhodamines for Liveâ€Cell Superâ€Resolution Imaging. Angewandte Chemie, 2020, 132, 20390-20398.	1.6	18
27	Emissive Nature and Molecular Behavior of Zero-Dimensional Organicâ€“Inorganic Metal Halides Bmpip₂MX₄. Journal of Physical Chemistry Letters, 2020, 11, 5234-5240.	2.1	33
28	A General Descriptor Î”E Enables the Quantitative Development of Luminescent Materials Based on Photoinduced Electron Transfer. Journal of the American Chemical Society, 2020, 142, 6777-6785.	6.6	115
29	De novo strategy with engineering anti-Kasha/Kasha fluorophores enables reliable ratiometric quantification of biomolecules. Nature Communications, 2020, 11, 793.	5.8	74
30	Molecular Mechanism of Viscosity Sensitivity in BODIPY Rotors and Application to Motion-Based Fluorescent Sensors. ACS Sensors, 2020, 5, 731-739.	4.0	80
31	Towards tetrazine-based near-infrared fluorogenic dyes: Is there a wavelength limit?. Dyes and Pigments, 2020, 177, 108313.	2.0	25
32	Non-fullerene electron acceptors constructed by simple electron-withdrawing core: Distinct effect of bithiazole vs thiazolothiazole core on photovoltaic properties. Dyes and Pigments, 2020, 177, 108319.	2.0	11
33	A Unified Pushâ€“Pull Model for Understanding the Ring-Opening Mechanism of Rhodamine Dyes. Journal of Physical Chemistry C, 2020, 124, 3793-3801.	1.5	58
34	Controlling Metallophilic Interactions in Chiral Gold(I) Double Salts towards Excitation Wavelengthâ€Tunable Circularly Polarized Luminescence. Angewandte Chemie - International Edition, 2020, 59, 6915-6922.	7.2	71
35	Quantitative Design of Bright Fluorophores and AIEgens by the Accurate Prediction of Twisted Intramolecular Charge Transfer (TICT). Angewandte Chemie, 2020, 132, 10246-10258.	1.6	36
36	Quantitative Design of Bright Fluorophores and AIEgens by the Accurate Prediction of Twisted Intramolecular Charge Transfer (TICT). Angewandte Chemie - International Edition, 2020, 59, 10160-10172.	7.2	131

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37	Revealing the switching mechanisms of an offâ€“onâ€“off fluorescent logic gate system. Physical Chemistry Chemical Physics, 2019, 21, 16798-16803.	1.3	23
38	Structural Engineering of Luminogens with High Emission Efficiency Both in Solution and in the Solid State. Angewandte Chemie, 2019, 131, 11541-11545.	1.6	21
39	Polymerization of phenylacetylenes by binuclear rhodium catalysts with different para-binucleating phenoxyiminato linkages. Polymer Chemistry, 2019, 10, 4163-4172.	1.9	4
40	Quaternary Piperazine-Substituted Rhodamines with Enhanced Brightness for Super-Resolution Imaging. Journal of the American Chemical Society, 2019, 141, 14491-14495.	6.6	140
41	Crystal Multiâ€Conformational Control Through Deformable Carbonâ€Sulfur Bond for Singletâ€Triplet Emissive Tuning. Angewandte Chemie - International Edition, 2019, 58, 4328-4333.	7.2	82
42	Structural Engineering of Luminogens with High Emission Efficiency Both in Solution and in the Solid State. Angewandte Chemie - International Edition, 2019, 58, 11419-11423.	7.2	133
43	Regulation of aggregation-induced emission behaviours and mechanofluorochromism of tetraphenylethene through different oxidation states of sulphur moieties. Journal of Materials Chemistry C, 2019, 7, 8244-8249.	2.7	21
44	Visualizing Microglia with a Fluorescence Turnâ€On Ugt1a7c Substrate. Angewandte Chemie, 2019, 131, 8056-8060.	1.6	2
45	Crystal Multiâ€Conformational Control Through Deformable Carbonâ€Sulfur Bond for Singletâ€Triplet Emissive Tuning. Angewandte Chemie, 2019, 131, 4372-4377.	1.6	28
46	Room Temperature Phosphorescence: Achieving Amorphous Ultralong Room Temperature Phosphorescence by Coassembling Planar Small Organic Molecules with Polyvinyl Alcohol (Adv.) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 3	7.8	
47	A Photoexcitationâ€Induced Twisted Intramolecular Charge Shuttle. Angewandte Chemie - International Edition, 2019, 58, 7073-7077.	7.2	79
48	A Photoexcitationâ€Induced Twisted Intramolecular Charge Shuttle. Angewandte Chemie, 2019, 131, 7147-7151.	1.6	17
49	A H-bond strategy to develop acid-resistant photoswitchable rhodamine spirolactams for super-resolution single-molecule localization microscopy. Chemical Science, 2019, 10, 4914-4922.	3.7	72
50	Simple-Structured NIR-Absorbing Small-Molecule Acceptors with a Thiazolothiazole Core: Multiple Noncovalent Conformational Locks and Dâ€“A Effect for Efficient OSCs. ACS Applied Materials & Interfaces, 2019, 11, 48128-48133.	4.0	50
51	How to stabilize the HOMO levels and to improve the charge transport properties of hole-transporting materials? Introducing a symmetrical core unit. Synthetic Metals, 2019, 247, 157-162.	2.1	17
52	Strong Ï€-Ï€ stacking interactions led to the mis-assignment of dimer emissions to the monomers of 1-acetylpyrene. Chinese Chemical Letters, 2019, 30, 601-604.	4.8	10
53	Achieving Amorphous Ultralong Room Temperature Phosphorescence by Coassembling Planar Small Organic Molecules with Polyvinyl Alcohol. Advanced Functional Materials, 2019, 29, 1807243.	7.8	147
54	A Highly Reversible Mechanochromic Difluorobenzothiadiazole Dye with Nearâ€Infrared Emission. Chemistry - A European Journal, 2018, 24, 3671-3676.	1.7	52

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55	Simple-structured small molecule acceptors constructed by a weakly electron-deficient thiazolothiazole core for high-efficiency non-fullerene organic solar cells. Journal of Materials Chemistry A, 2018, 6, 24267-24276.	5.2	78
56	Unusual intermolecular charge transfer enables supramolecular fluorescent viscosity sensors. Sensors and Actuators B: Chemical, 2018, 277, 55-61.	4.0	19
57	Strategy for designing stable and powerful nitrogen-rich high-energy materials by introducing boron atoms. Journal of Molecular Modeling, 2017, 23, 191.	0.8	4
58	Strategy of improving the stability and detonation performance for energetic material by introducing the boron atoms. Journal of Physical Organic Chemistry, 2017, 30, e3699.	0.9	7
59	Ground-state conformers enable bright single-fluorophore ratiometric thermometers with positive temperature coefficients. Materials Chemistry Frontiers, 2017, 1, 2383-2390.	3.2	18
60	Optimizing thienothiophene chain lengths of Dâ€“Ï€â€“D hole transport materials in perovskite solar cells for improving energy levels and hole mobility. Journal of Materials Chemistry C, 2017, 5, 10055-10060.	2.7	37
61	Effect of Nitrogen-Doping on Detonation and Stability Properties of CL-20 Derivatives from a Theoretical Viewpoint. Propellants, Explosives, Pyrotechnics, 2017, 42, 1044-1050.	1.0	1
62	How to regulate energy levels and hole mobility of spiro-type hole transport materials in perovskite solar cells. Physical Chemistry Chemical Physics, 2016, 18, 27073-27077.	1.3	45
63	Theoretical design of highly energetic poly-nitro cage compounds. RSC Advances, 2016, 6, 47607-47615.	1.7	20
64	A strategy to improve the efficiency of hole transporting materials: introduction of a highly symmetrical core. Nanoscale, 2016, 8, 17752-17756.	2.8	62
65	Effects of water molecules on the chemical stability of MAGeI₃ perovskite explored from a theoretical viewpoint. Physical Chemistry Chemical Physics, 2016, 18, 24526-24536.	1.3	22
66	Substituent effects on the properties related to detonation performance and stability for pentaprismane derivatives. Theoretical Chemistry Accounts, 2016, 135, 1.	0.5	0
67	Effect of thiophene chain lengths on the optical and hole transport properties for perovskite solar cells. Synthetic Metals, 2016, 211, 107-114.	2.1	20
68	Exploring the electrochemical properties of hole transport materials with spiro-cores for efficient perovskite solar cells from first-principles. Nanoscale, 2016, 8, 6146-6154.	2.8	124
69	The theoretical investigation on the 4-(4-phenyl-4-Î±-naphthylbutadieny)-triphenylamine derivatives as hole transporting materials for perovskite-type solar cells. Physical Chemistry Chemical Physics, 2015, 17, 5991-5998.	1.3	84
70	Molecular design of Nâ€“NO₂substituted cycloalkanes derivatives C_m(Nâ€“NO₂)_mfor energetic materials with high detonation performance and low impact sensitivity. RSC Advances, 2015, 5, 38048-38055.	1.7	30
71	Effects of Molecular Configuration on Charge Diffusion Kinetics within Hole-Transporting Materials for Perovskites Solar Cells. Journal of Physical Chemistry C, 2015, 119, 8584-8590.	1.5	40
72	Molecular design of prismane-based potential energetic materials with high detonation performance and low impact sensitivity. Comptes Rendus Chimie, 2015, 18, 1270-1276.	0.2	14

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73	Theoretical prediction of detonation performanceÂand stability for energetic polydinitroaminoprismanes. RSC Advances, 2015, 5, 7766-7772.	1.7	13
74	Is 1-nitro-1-triazene a high energy density material?. Journal of Molecular Modeling, 2014, 20, 2362.	0.8	1
75	New potential high energy density compounds: Oxadiaziridine derivatives. Russian Journal of Physical Chemistry A, 2014, 88, 1700-1705.	0.1	3
76	Density function theory study on energetic nitro-triaziridine derivatives. Structural Chemistry, 2013, 24, 375-381.	1.0	10
77	Looking for high energy density compounds among polynitraminepurines. Journal of Molecular Modeling, 2013, 19, 3491-3499.	0.8	10
78	Looking for high energy density compounds among polynitraminecubanes. Journal of Molecular Modeling, 2013, 19, 571-580.	0.8	16
79	Computational studies on thermodynamic properties, detonation properties and bond dissociation energies for polydifluoroaminopurine compounds. Comptes Rendus Chimie, 2013, 16, 765-772.	0.2	6
80	Theoretical investigation on detonation performances and thermodynamic stabilities of the prismane derivatives. Journal of Molecular Modeling, 2013, 19, 1049-1057.	0.8	7
81	Computational studies on polynitropurines as potential high energy density materials. Journal of Molecular Modeling, 2013, 19, 2235-2242.	0.8	5
82	Density functional study on the derivatives of purine. Journal of Molecular Modeling, 2012, 18, 3501-3506.	0.8	8
83	Theoretical investigation on the heats of formation and detonation performance in polydinitroaminocubanes. Journal of Molecular Modeling, 2012, 18, 4217-4223.	0.8	13
84	Density functional theory calculations on the thermodynamic properties of polynitrosoprismanes. Journal of Molecular Modeling, 2012, 18, 4557-4563.	0.8	4
85	Density functional calculation on a high energy density compound having the formula C2OH4â^'n (NO2) n. Structural Chemistry, 2012, 23, 1837-1841.	1.0	13
86	Density functional calculations for a high energy density compound of formula C6H6â^'n (NO2) n. Journal of Molecular Modeling, 2012, 18, 3695-3704.	0.8	15
87	A Descriptor for Accurate Predictions of Host Molecules Enabling Ultralong Roomâ€Temperature Phosphorescence in Guest Emitters. Angewandte Chemie, 0, , .	1.6	6