# Wei-Jie Chi

List of Publications by Year
in descending order



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|---|---|---|---|
| 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 | 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 |
| 2 | Achieving Amorphous Ultralong Room Temperature Phosphorescence by Coassembling Planar Small Organic Molecules with Polyvinyl Alcohol. Advanced Functional Materials, 2019, 29, 1807243. | 7.8 | 147 |
| 3 | Quaternary Piperazine-Substituted Rhodamines with Enhanced Brightness for Super-Resolution Imaging. Journal of the American Chemical Society, 2019, 141, 14491-14495. | 6.6 | 140 |
| 4 | 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 |
| 5 | 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 |
| 6 | 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 |
| 7 | 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 |
| 8 | 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 |
| 9 | 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 |
| 10 | Molecular Mechanism of Viscosity Sensitivity in BODIPY Rotors and Application to Motion-Based Fluorescent Sensors. ACS Sensors, 2020, 5, 731-739. | 4.0 | 80 |
| 11 | 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 |
| 12 | A Photoexcitationâ€Induced Twisted Intramolecular Charge Shuttle. Angewandte Chemie - International Edition, 2019, 58, 7073-7077. | 7.2 | 79 |
| 13 | 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 |
| 14 | De novo strategy with engineering anti-Kasha/Kasha fluorophores enables reliable ratiometric quantification of biomolecules. Nature Communications, 2020, 11, 793. | 5.8 | 74 |
| 15 | 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 |
| 16 | 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 |
| 17 | A strategy to improve the efficiency of hole transporting materials: introduction of a highly symmetrical core. Nanoscale, 2016, 8, 17752-17756. | 2.8 | 62 |
| 18 | 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 |

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|---|---|---|---|
| 19 | 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 |
| 20 | 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 |
| 21 | A Highly Reversible Mechanochromic Difluorobenzothiadiazole Dye with Nearâ€Infrared Emission. Chemistry - A European Journal, 2018, 24, 3671-3676. | 1.7 | 52 |
| 22 | Fluorescence umpolung enables light-up sensing of N-acetyltransferases and nerve agents. Nature Communications, 2021, 12, 3869. | 5.8 | 51 |
| 23 | 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 |
| 24 | Descriptor Î”G<sub>Câ€O</sub> 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 | 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 |
| 26 | 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 |
| 27 | Optimizing thienothiophene chain lengths of Dâ€“Î€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 |
| 28 | 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 |
| 29 | Emissive Nature and Molecular Behavior of Zero-Dimensional Organicâ€“Inorganic Metal Halides Bmpip<sub>2</sub>MX<sub>4</sub>. Journal of Physical Chemistry Letters, 2020, 11, 5234-5240. | 2.1 | 33 |
| 30 | 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 |
| 31 | Molecular design of Nâ€“NO<sub>2</sub>substituted cycloalkanes derivatives C<sub>m</sub>(Nâ€“NO<sub>2</sub>)<sub>m</sub>for energetic materials with high detonation performance and low impact sensitivity. RSC Advances, 2015, 5, 38048-38055. | 1.7 | 30 |
| 32 | Crystal Multiâ€Conformational Control Through Deformable Carbonâ€Sulfur Bond for Singletâ€Triplet Emissive Tuning. Angewandte Chemie, 2019, 131, 4372-4377. | 1.6 | 28 |
| 33 | 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 |
| 34 | Towards tetrazine-based near-infrared fluorogenic dyes: Is there a wavelength limit?. Dyes and Pigments, 2020, 177, 108313. | 2.0 | 25 |
| 35 | Revealing the switching mechanisms of an offâ€“onâ€“off fluorescent logic gate system. Physical Chemistry Chemical Physics, 2019, 21, 16798-16803. | 1.3 | 23 |
| 36 | Effects of water molecules on the chemical stability of MAGeI<sub>3</sub> perovskite explored from a theoretical viewpoint. Physical Chemistry Chemical Physics, 2016, 18, 24526-24536. | 1.3 | 22 |

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|---|---|---|---|
| 37 | 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 |
| 38 | 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 |
| 39 | Theoretical design of highly energetic poly-nitro cage compounds. RSC Advances, 2016, 6, 47607-47615. | 1.7 | 20 |
| 40 | 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 |
| 41 | Unusual intermolecular charge transfer enables supramolecular fluorescent viscosity sensors. Sensors and Actuators B: Chemical, 2018, 277, 55-61. | 4.0 | 19 |
| 42 | Molecular Origins of Photoinduced Backward Intramolecular Charge Transfer. Journal of Physical Chemistry C, 2020, 124, 16820-16826. | 1.5 | 19 |
| 43 | 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 |
| 44 | Ground-state conformers enable bright single-fluorophore ratiometric thermometers with positive temperature coefficients. Materials Chemistry Frontiers, 2017, 1, 2383-2390. | 3.2 | 18 |
| 45 | Descriptor Î”G<sub>Câ€Ō</sub> Enables the Quantitative Design of Spontaneously Blinking Rhodamines for Liveâ€Cell Superâ€Resolution Imaging. Angewandte Chemie, 2020, 132, 20390-20398. | 1.6 | 18 |
| 46 | Pentadiamond: A Highly Efficient Electron Transport Layer for Perovskite Solar Cells. Journal of Physical Chemistry C, 2021, 125, 5372-5379. | 1.5 | 18 |
| 47 | 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 |
| 48 | A Photoexcitationâ€Induced Twisted Intramolecular Charge Shuttle. Angewandte Chemie, 2019, 131, 7147-7151. | 1.6 | 17 |
| 49 | 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 |
| 50 | 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 |
| 51 | Looking for high energy density compounds among polynitraminecubanes. Journal of Molecular Modeling, 2013, 19, 571-580. | 0.8 | 16 |
| 52 | Boronâ€“nitrogen substituted planar cores: designing dopant-free hole-transporting materials for efficient perovskite solar cells. Nanoscale, 2021, 13, 4241-4248. | 2.8 | 16 |
| 53 | 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 |
| 54 | 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 |

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|---|---|---|---|
| 55 | 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 |
| 56 | Theoretical investigation on the heats of formation and detonation performance in polydinitroaminocubanes. Journal of Molecular Modeling, 2012, 18, 4217-4223. | 0.8 | 13 |
| 57 | 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 |
| 58 | Theoretical prediction of detonation performanceÂand stability for energetic polydinitroaminoprismanes. RSC Advances, 2015, 5, 7766-7772. | 1.7 | 13 |
| 59 | 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 |
| 60 | 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 |
| 61 | 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 |
| 62 | Density function theory study on energetic nitro-triaziridine derivatives. Structural Chemistry, 2013, 24, 375-381. | 1.0 | 10 |
| 63 | Looking for high energy density compounds among polynitraminepurines. Journal of Molecular Modeling, 2013, 19, 3491-3499. | 0.8 | 10 |
| 64 | 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 |
| 65 | 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 |
| 66 | 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 |
| 67 | 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 |
| 68 | Density functional study on the derivatives of purine. Journal of Molecular Modeling, 2012, 18, 3501-3506. | 0.8 | 8 |
| 69 | 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 |
| 70 | Theoretical investigation on detonation performances and thermodynamic stabilities of the prismane derivatives. Journal of Molecular Modeling, 2013, 19, 1049-1057. | 0.8 | 7 |
| 71 | 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 |
| 72 | 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 5 | 7.8 | 7 |

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|---|---|---|---|
| 73 | Computational studies on thermodynamic properties, detonation properties and bond dissociation energies for polydifluoroaminopurine compounds. Comptes Rendus Chimie, 2013, 16, 765-772. | 0.2 | 6 |
| 74 | A Descriptor for Accurate Predictions of Host Molecules Enabling Ultralong Roomâ€Temperature Phosphorescence in Guest Emitters. Angewandte Chemie, 0, , . | 1.6 | 6 |
| 75 | Computational studies on polynitropurines as potential high energy density materials. Journal of Molecular Modeling, 2013, 19, 2235-2242. | 0.8 | 5 |
| 76 | The photocatalytic mechanism of organic dithienophosphole derivatives as highly efficient photo-redox catalysts. Physical Chemistry Chemical Physics, 2020, 22, 20721-20731. | 1.3 | 5 |
| 77 | 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 |
| 78 | Density functional theory calculations on the thermodynamic properties of polynitrosoprismanes. Journal of Molecular Modeling, 2012, 18, 4557-4563. | 0.8 | 4 |
| 79 | 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 |
| 80 | Polymerization of phenylacetylenes by binuclear rhodium catalysts with different para-binucleating phenoxyiminato linkages. Polymer Chemistry, 2019, 10, 4163-4172. | 1.9 | 4 |
| 81 | New potential high energy density compounds: Oxadiaziridine derivatives. Russian Journal of Physical Chemistry A, 2014, 88, 1700-1705. | 0.1 | 3 |
| 82 | 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 |
| 83 | Visualizing Microglia with a Fluorescence Turnâ€On Ugt1a7c Substrate. Angewandte Chemie, 2019, 131, 8056-8060. | 1.6 | 2 |
| 84 | 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 |
| 85 | Is 1-nitro-1-triazene a high energy density material?. Journal of Molecular Modeling, 2014, 20, 2362. | 0.8 | 1 |
| 86 | 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 |
| 87 | Substituent effects on the properties related to detonation performance and stability for pentaprismane derivatives. Theoretical Chemistry Accounts, 2016, 135, 1. | 0.5 | 0 |