

WanZhen Liang

List of Publications by Year in descending order

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79
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257450

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8678
citing authors

#	ARTICLE	IF	CITATIONS
1	Molecular Design Strategy for Practical Singlet Fission Materials: The Charm of Donor/Acceptor Decorated Quinoidal Structure. <i>CCS Chemistry</i> , 2022, 4, 2748-2756.	7.8	12
2	Vibronic Coupling Effect on the Vibrationally Resolved Electronic Spectra and Intersystem Crossing Rates of a TADF Emitter: 7-PhQAD. <i>Journal of Physical Chemistry A</i> , 2022, 126, 239-248.	2.5	25
3	Vibrationally resolved absorption spectra and ultrafast exciton dynamics in $\hat{1}\pm$ -phase and $\hat{1}^2$ -phase zinc phthalocyanine aggregates. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 2974-2987.	2.8	8
4	Gold-Based Double Perovskite-Related Polymorphs: Low Dimensional with an Ultranarrow Bandgap. <i>Chemistry of Materials</i> , 2022, 34, 1544-1553.	6.7	6
5	Evaluation of molecular photophysical and photochemical properties using linear response time-dependent density functional theory with classical embedding: Successes and challenges. <i>Journal of Chemical Physics</i> , 2022, 156, .	3.0	10
6	Nonlinear features of Fano resonance: a QM/EM study. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 15994-16004.	2.8	6
7	Electronic Couplings for Photoinduced Charge Transfer and Excitation Energy Transfer Based on Fragment Particleâ€”Hole Densities. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 1032-1039.	4.6	15
8	Joint Effects of Excitonâ€”Exciton and Excitonâ€”Photon Couplings on the Singlet Fission Dynamics in Organic Aggregates. <i>Journal of Physical Chemistry C</i> , 2021, 125, 1654-1664.	3.1	15
9	Elucidating the Electronic Structure of a Delayed Fluorescence Emitter via Orbital Interactions, Excitation Energy Components, Charge-Transfer Numbers, and Vibrational Reorganization Energies. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 2712-2720.	4.6	35
10	Why Hybrid Tin-Based Perovskites Simultaneously Improve the Structural Stability and Charge Carriersâ€™ Lifetime: Ab Initio Quantum Dynamics. <i>ACS Applied Materials & Interfaces</i> , 2021, 13, 16567-16575.	8.0	10
11	Vibrationally Resolved Absorption Spectra and Exciton Dynamics in Zinc Phthalocyanine Aggregates: Effects of Aggregation Lengths and Remote Exciton Transfer. <i>Journal of Physical Chemistry A</i> , 2021, 125, 2932-2943.	2.5	11
12	Software for the frontiers of quantum chemistry: An overview of developments in the Q-Chem 5 package. <i>Journal of Chemical Physics</i> , 2021, 155, 084801.	3.0	518
13	Understanding the mechanism of plasmon-driven water splitting: hot electron injection and a near field enhancement effect. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 25629-25636.	2.8	7
14	Influence of intrinsic defects on the structure and dynamics of the mixed Pbâ€”Sn perovskite: first-principles DFT and NAMD simulations. <i>Journal of Materials Chemistry A</i> , 2021, 10, 234-244.	10.3	11
15	H-Type-like Aggregation-Accelerated Singlet Fission Process in Dipyrrolonaphthyridinedione Thin Film: The Role of Charge Transfer/Excimer Mixed Intermediate State. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 12276-12282.	4.6	19
16	Unveiling the effect of electron tunneling on the plasmonic resonance of closely spaced gold particles. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 1747-1755.	2.8	1
17	Constructing spinâ€”adiabatic states for the modeling of spinâ€”crossing reactions. I. A sharedâ€”orbital implementation. <i>International Journal of Quantum Chemistry</i> , 2020, 120, e26123.	2.0	3
18	Effect of charge-transfer states on the vibrationally resolved absorption spectra and exciton dynamics in ZnPc aggregates: Simulations from a non-Markovian stochastic Schrâ”odinger equation. <i>Journal of Chemical Physics</i> , 2020, 153, 034116.	3.0	18

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19	Analysis and visualization of energy densities. I. Insights from real-time time-dependent density functional theory simulations. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 26838-26851.	2.8	9
20	Analysis and visualization of energy densities. II. Insights from linear-response time-dependent density functional theory calculations. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 26852-26864.	2.8	12
21	How the Structures and Properties of Pristine and Anion Vacancy Defective Organic-Inorganic Hybrid Double Perovskites $\text{MA}_2\text{AgIn}(\text{Br}_x\text{I}_{1-x})_6$ Vary with Br Content. <i>Journal of Physical Chemistry Letters</i> , 2020, 11, 10315-10322.	4.6	6
22	Potassium doping-induced variations in the structures and photoelectric properties of a MAPbI_3 perovskite and a $\text{MAPbI}_3/\text{TiO}_2$ junction. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 20553-20561.	2.8	6
23	Plasmon-enhanced high order harmonic generation of open-ended finite-sized carbon nanotubes: The effects of incident field's intensity and frequency and the interference between the incident and scattered fields. <i>Journal of Chemical Physics</i> , 2020, 152, 224708.	3.0	4
24	The vibronic absorption spectra and exciton dynamics of plasmon-exciton hybrid systems in the regimes ranged from Fano antiresonance to Rabi-like splitting. <i>Journal of Chemical Physics</i> , 2020, 152, 014102.	3.0	7
25	Single-handed supramolecular double helix of homochiral bis(N-amidothiourea) supported by double crossed $\text{C}^{\sim}\text{I}^{\sim}\text{S}$ halogen bonds. <i>Nature Communications</i> , 2019, 10, 3610.	12.8	55
26	Collaborative effect of plasmon-induced resonance energy and electron transfer on the interfacial electron injection dynamics of dye-sensitized solar cell. <i>Journal of Chemical Physics</i> , 2019, 151, 044702.	3.0	5
27	Plasmon-driven high harmonic generation of benzene: effect of spatial inhomogeneity of near field. <i>Electronic Structure</i> , 2019, 1, 044001.	2.8	4
28	Lead-free low-dimensional tin halide perovskites with functional organic spacers: breaking the charge-transport bottleneck. <i>Journal of Materials Chemistry A</i> , 2019, 7, 16742-16747.	10.3	24
29	Structure and property tunability in monolayer halide lead-free double hybrid perovskites: effects of Rashba and biaxial strain. <i>Journal of Materials Chemistry A</i> , 2019, 7, 11487-11496.	10.3	5
30	Singlet/triplet exciton dissociation and charge recombination in donor-acceptor $\text{ThQs}^{\sim}60/\text{PDI}^{\sim}\text{CN}^{\sim}2$ complexes. <i>Journal of Computational Chemistry</i> , 2019, 40, 997-1004.	3.3	6
31	Benzazasiline combined with triphenylborane-based cores for constructing deep-blue donor-acceptor-donor TADF emitters. <i>Organic Electronics</i> , 2018, 57, 74-81.	2.6	9
32	Size-Dependent Optical Properties of Aluminum Nanoparticles: From Classical to Quantum Description. <i>Journal of Physical Chemistry C</i> , 2018, 122, 10545-10551.	3.1	19
33	One- and two-photon absorption spectra of the yellow fluorescent protein citrine: effects of intramolecular electron-vibrational coupling and intermolecular interactions. <i>Molecular Physics</i> , 2018, 116, 885-897.	1.7	3
34	Atomically Thin n/n Nanodevices by Surface Charge Transfer Doping of Arsenene/Antimonene Heterostructures. <i>ACS Applied Materials & Interfaces</i> , 2018, 10, 23851-23857.	8.0	14
35	How the Structures and Properties of Two-Dimensional Layered Perovskites MAPbI_3 and CsPbI_3 Vary with the Number of Layers. <i>Journal of Physical Chemistry Letters</i> , 2017, 8, 1517-1523.	4.6	89
36	Quantum Interference in Singlet Fission: J- and H-Aggregate Behavior. <i>Journal of Physical Chemistry Letters</i> , 2017, 8, 5105-5112.	4.6	37

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37	Charge Carrier Mobilities and Singlet Fission Dynamics in Thienoquinoidal Compounds. <i>Journal of Physical Chemistry C</i> , 2017, 121, 22587-22596.	3.1	10
38	NB-Type Electronic Asymmetric Compounds as Potential Blue-Color TADF Emitters: Steric Hindrance, Substitution Effect, and Electronic Characteristics. <i>ACS Omega</i> , 2017, 2, 3098-3109.	3.5	9
39	Structural characteristics and photoinduced carrier behaviors of the mixed-phase BiVO ₄ : a first-principles theoretical study. <i>Theoretical Chemistry Accounts</i> , 2016, 135, 1.	1.4	10
40	Characterizing the Structures, Spectra, and Energy Landscapes Involved in the Excited-State Proton Transfer Process of Red Fluorescent Protein LSSmKate1. <i>Journal of Physical Chemistry B</i> , 2016, 120, 9833-9842.	2.6	8
41	The effect of moisture on the structures and properties of lead halide perovskites: a first-principles theoretical investigation. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 23174-23183.	2.8	89
42	Effects of Charge Transfer State and Exciton Migration on Singlet Fission Dynamics in Organic Aggregates. <i>Journal of Physical Chemistry C</i> , 2016, 120, 13351-13359.	3.1	31
43	Resonance Raman spectra of organic molecules absorbed on inorganic semiconducting surfaces: Contribution from both localized intramolecular excitation and intermolecular charge transfer excitation. <i>Journal of Chemical Physics</i> , 2015, 143, 154105.	3.0	10
44	Analytic energy gradient of excited electronic state within TDDFT/MMpol framework: Benchmark tests and parallel implementation. <i>Journal of Chemical Physics</i> , 2015, 143, 134104.	3.0	25
45	A computational view of the change in the geometric and electronic properties of perovskites caused by the partial substitution of Pb by Sn. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 17679-17687.	2.8	43
46	How does the plasmonic enhancement of molecular absorption depend on the energy gap between molecular excitation and plasmon modes: a mixed TDDFT/FDTD investigation. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 16835-16845.	2.8	28
47	Spectroscopic Signature of the Aggregation-Induced Emission Phenomena Caused by Restricted Nonradiative Decay: A Theoretical Proposal. <i>Journal of Physical Chemistry C</i> , 2015, 119, 5040-5047.	3.1	70
48	Effect of Phase Junction Structure on the Photocatalytic Performance in Overall Water Splitting: Ga ₂ O ₃ Photocatalyst as an Example. <i>Journal of Physical Chemistry C</i> , 2015, 119, 18221-18228.	3.1	101
49	Aggregation-Induced Emission Mechanism of Dimethoxy-Tetraphenylethylene in Water Solution: Molecular Dynamics and QM/MM Investigations. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 2257-2267.	5.3	32
50	Generalized time-dependent approaches to vibrationally resolved electronic and Raman spectra: Theory and applications. <i>International Journal of Quantum Chemistry</i> , 2015, 115, 550-563.	2.0	24
51	Spectral Characteristics of Chemical Enhancement on SERS of Benzene-like Derivatives: Franck-Condon and Herzberg-Teller Contributions. <i>Journal of Physical Chemistry C</i> , 2015, 119, 27609-27619.	3.1	18
52	Advances in molecular quantum chemistry contained in the Q-Chem 4 program package. <i>Molecular Physics</i> , 2015, 113, 184-215.	1.7	2,561
53	Energy relaxation and separation of a hot electron-hole pair in organic aggregates from a time-dependent wavepacket diffusion method. <i>Journal of Chemical Physics</i> , 2014, 140, 214107.	3.0	20
54	Assessment of mode-mixing and Herzberg-Teller effects on two-photon absorption and resonance hyper-Raman spectra from a time-dependent approach. <i>Journal of Chemical Physics</i> , 2014, 140, 094107.	3.0	20

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55	Analytical derivative techniques for TDDFT excited-state properties: Theory and application. <i>Science China Chemistry</i> , 2014, 57, 48-57.	8.2	16
56	Tuning the energy band-gap of crystalline gallium oxide to enhance photocatalytic water splitting: mixed-phase junctions. <i>Journal of Materials Chemistry A</i> , 2014, 2, 17005-17014.	10.3	84
57	Molecular properties of excited electronic state: Formalism, implementation, and applications of analytical second energy derivatives within the framework of the time-dependent density functional theory/molecular mechanics. <i>Journal of Chemical Physics</i> , 2014, 140, 18A506.	3.0	11
58	Theoretical study of the low-lying electronic excited states for molecular aggregates. <i>Science China Chemistry</i> , 2013, 56, 1258-1262.	8.2	16
59	Theory and algorithms for the excited states of large molecules and molecular aggregates. <i>Science China Chemistry</i> , 2013, 56, 1267-1270.	8.2	8
60	Time-Dependent Approach to Resonance Raman Spectra Including Duschinsky Rotation and Herzberg-Teller Effects: Formalism and Its Realistic Applications. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 4474-4482.	5.3	54
61	Plasmon Resonance of Isolated Gold Hollow Nanoparticles and Nanoparticle Pairs: Insights from Electronic Structure Calculations. <i>Journal of Physical Chemistry C</i> , 2012, 116, 1755-1763.	3.1	11
62	Charge transfer in organic molecules for solar cells: theoretical perspective. <i>Chemical Society Reviews</i> , 2012, 41, 1075-1087.	38.1	150
63	Vibronic Spectra of Perylene Bisimide Oligomers: Effects of Intermolecular Charge-Transfer Excitation and Conformational Flexibility. <i>Journal of Physical Chemistry B</i> , 2011, 115, 2699-2708.	2.6	56
64	Theoretical investigation of the non-Condon effect on electron transfer: Application to organic semiconductor. <i>Science China Chemistry</i> , 2011, 54, 707-714.	8.2	1
65	Theoretical investigation of resonance Raman scattering of dye molecules absorbed on semiconductor surfaces. <i>Journal of Chemical Physics</i> , 2011, 135, 044108.	3.0	19
66	Theoretical studies of vibrationally resolved absorption and emission spectra: From a single chromophore to multichromophoric oligomers/aggregates. <i>Science China Chemistry</i> , 2010, 53, 297-309.	8.2	18
67	Theoretical studies on electronic spectroscopy and dynamics with the real-time time-dependent density functional theory. <i>Frontiers of Chemistry in China: Selected Publications From Chinese Universities</i> , 2010, 5, 11-28.	0.4	10
68	Non-Condon effect on charge transport in dithiophene-tetrathiafulvalene crystal. <i>Journal of Chemical Physics</i> , 2010, 133, 024501.	3.0	30
69	Nature of Low-Lying Excited States in H-Aggregated Perylene Bisimide Dyes: Results of TD-LRC-DFT and the Mixed Exciton Model. <i>Journal of Physical Chemistry B</i> , 2009, 113, 14581-14587.	2.6	33
70	Real-Time Propagation of the Reduced One-Electron Density Matrix in Atom-Centered Orbitals: Application to Multielectron Dynamics of Carbon Clusters C_n in the Strong Laser Pulses. <i>Journal of Physical Chemistry A</i> , 2008, 112, 10442-10447.	2.5	9
71	Real-Time Propagation of the Reduced One-Electron Density Matrix in Atom-Centered Orbitals: Application to Electron Injection Dynamics in Dye-Sensitized TiO_2 Clusters. <i>Journal of Physical Chemistry C</i> , 2008, 112, 16655-16662.	3.1	47
72	Harmonic generation of open-ended and capped carbon nanotubes investigated by time-dependent Hartree-Fock theory. <i>Physical Review B</i> , 2007, 75, .	3.2	20

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73	Electronic Excitation of Polyfluorenes: A Theoretical Study. <i>Journal of Physical Chemistry B</i> , 2006, 110, 9908-9915.	2.6	33
74	Advances in methods and algorithms in a modern quantum chemistry program package. <i>Physical Chemistry Chemical Physics</i> , 2006, 8, 3172-3191.	2.8	2,597
75	An efficient approach for self-consistent-field energy and energy second derivatives in the atomic-orbital basis. <i>Journal of Chemical Physics</i> , 2005, 123, 194106.	3.0	19
76	Localized-density-matrix method and its application to nanomaterials. <i>Pure and Applied Chemistry</i> , 2000, 72, 281-291.	1.9	3
77	Localized-density-matrix method and nonlinear optical response. <i>Journal of Chemical Physics</i> , 2000, 113, 1403-1408.	3.0	7
78	Localized-Density-Matrix Method and Its Application to Carbon Nanotubes. <i>Journal of Physical Chemistry A</i> , 2000, 104, 2445-2453.	2.5	40
79	Generalized linear-scaling localized-density-matrix method. <i>Journal of Chemical Physics</i> , 1999, 110, 1844-1855.	3.0	37