

WanZhen Liang

List of Publications by Year in descending order

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79
papers

7,483
citations

258631

24
h-index

67222

78
g-index

85
all docs

85
docs citations

85
times ranked

8678
citing authors

#	ARTICLE	IF	CITATIONS
1	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
2	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
3	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.	3.1	518
4	Charge transfer in organic molecules for solar cells: theoretical perspective. <i>Chemical Society Reviews</i> , 2012, 41, 1075-1087.	39.2	150
5	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.	3.2	101
6	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
7	How the Structures and Properties of Two-Dimensional Layered Perovskites MAPb ₃ and CsPb ₃ Vary with the Number of Layers. <i>Journal of Physical Chemistry Letters</i> , 2017, 8, 1517-1523.	4.7	89
8	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.	10.4	84
9	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.	3.2	70
10	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.	2.7	56
11	Single-handed supramolecular double helix of homochiral bis(N-amidothiourea) supported by double crossed C ⁺ ⋯A⋯S halogen bonds. <i>Nature Communications</i> , 2019, 10, 3610.	13.0	55
12	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.	5.4	54
13	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.	3.2	47
14	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
15	Localized-Density-Matrix Method and Its Application to Carbon Nanotubes. <i>Journal of Physical Chemistry A</i> , 2000, 104, 2445-2453.	2.5	40
16	Generalized linear-scaling localized-density-matrix method. <i>Journal of Chemical Physics</i> , 1999, 110, 1844-1855.	3.1	37
17	Quantum Interference in Singlet Fission: J- and H-Aggregate Behavior. <i>Journal of Physical Chemistry Letters</i> , 2017, 8, 5105-5112.	4.7	37
18	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.	4.7	35

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19	Electronic Excitation of Polyfluorenes: A Theoretical Study. <i>Journal of Physical Chemistry B</i> , 2006, 110, 9908-9915.	2.7	33
20	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.	2.7	33
21	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.	5.4	32
22	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.	3.2	31
23	Non-Condon effect on charge transport in dithiophene-tetrathiafulvalene crystal. <i>Journal of Chemical Physics</i> , 2010, 133, 024501.	3.1	30
24	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
25	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.	3.1	25
26	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
27	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
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.	10.4	24
29	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
30	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.	3.1	20
31	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.	3.1	20
32	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.	3.1	19
33	Theoretical investigation of resonance Raman scattering of dye molecules absorbed on semiconductor surfaces. <i>Journal of Chemical Physics</i> , 2011, 135, 044108.	3.1	19
34	Size-Dependent Optical Properties of Aluminum Nanoparticles: From Classical to Quantum Description. <i>Journal of Physical Chemistry C</i> , 2018, 122, 10545-10551.	3.2	19
35	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.	4.7	19
36	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.	8.4	18

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37	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.	3.2	18
38	Effect of charge-transfer states on the vibrationally resolved absorption spectra and exciton dynamics in ZnPc aggregates: Simulations from a non-Markovian stochastic Schrödinger equation. <i>Journal of Chemical Physics</i> , 2020, 153, 034116.	3.1	18
39	Theoretical study of the low-lying electronic excited states for molecular aggregates. <i>Science China Chemistry</i> , 2013, 56, 1258-1262.	8.4	16
40	Analytical derivative techniques for TDDFT excited-state properties: Theory and application. <i>Science China Chemistry</i> , 2014, 57, 48-57.	8.4	16
41	Electronic Couplings for Photoinduced Charge Transfer and Excitation Energy Transfer Based on Fragment Particle-Hole Densities. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 1032-1039.	4.7	15
42	Joint Effects of Exciton-Exciton and Exciton-Photon Couplings on the Singlet Fission Dynamics in Organic Aggregates. <i>Journal of Physical Chemistry C</i> , 2021, 125, 1654-1664.	3.2	15
43	Atomically Thin n/n Nanodevices by Surface Charge Transfer Doping of Arsenene/Antimonene Heterostructures. <i>ACS Applied Materials & Interfaces</i> , 2018, 10, 23851-23857.	8.2	14
44	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
45	Molecular Design Strategy for Practical Singlet Fission Materials: The Charm of Donor/Acceptor Decorated Quinoidal Structure. <i>CCS Chemistry</i> , 2022, 4, 2748-2756.	8.0	12
46	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.	3.2	11
47	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.	3.1	11
48	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
49	Influence of intrinsic defects on the structure and dynamics of the mixed Pb-Sn perovskite: first-principles DFT and NAMD simulations. <i>Journal of Materials Chemistry A</i> , 2021, 10, 234-244.	10.4	11
50	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
51	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.	3.1	10
52	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
53	Charge Carrier Mobilities and Singlet Fission Dynamics in Thienoquinoidal Compounds. <i>Journal of Physical Chemistry C</i> , 2017, 121, 22587-22596.	3.2	10
54	Why Hybrid Tin-Based Perovskites Simultaneously Improve the Structural Stability and Charge Carriers' Lifetime: Ab Initio Quantum Dynamics. <i>ACS Applied Materials & Interfaces</i> , 2021, 13, 16567-16575.	8.2	10

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55	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, .	3.1	10
56	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
57	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.	3.6	9
58	Benzazasiline combined with triphenylborane-based cores for constructing deep-blue donor-acceptor-donor TADF emitters. <i>Organic Electronics</i> , 2018, 57, 74-81.	2.7	9
59	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
60	Theory and algorithms for the excited states of large molecules and molecular aggregates. <i>Science China Chemistry</i> , 2013, 56, 1267-1270.	8.4	8
61	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.	2.7	8
62	Vibrationally resolved absorption spectra and ultrafast exciton dynamics in \hat{I}^{\pm} -phase and \hat{I}^2 -phase zinc phthalocyanine aggregates. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 2974-2987.	2.8	8
63	Localized-density-matrix method and nonlinear optical response. <i>Journal of Chemical Physics</i> , 2000, 113, 1403-1408.	3.1	7
64	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.	3.1	7
65	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
66	Singlet/triplet exciton dissociation and charge recombination in donor-acceptor ThQs-60/PDIxCN 2 complexes. <i>Journal of Computational Chemistry</i> , 2019, 40, 997-1004.	3.4	6
67	How the Structures and Properties of Pristine and Anion Vacancy Defective Organic-Inorganic Hybrid Double Perovskites $MA_2AgIn(Br_xI_{1-x})_6$ Vary with Br Content x . <i>Journal of Physical Chemistry Letters</i> , 2020, 11, 10315-10322.	4.7	6
68	Potassium doping-induced variations in the structures and photoelectric properties of a $MAPbI_3$ perovskite and a $MAPbI_3/TiO_2$ junction. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 20553-20561.	2.8	6
69	Nonlinear features of Fano resonance: a QM/EM study. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 15994-16004.	2.8	6
70	Gold-Based Double Perovskite-Related Polymorphs: Low Dimensional with an Ultranarrow Bandgap. <i>Chemistry of Materials</i> , 2022, 34, 1544-1553.	6.9	6
71	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.	3.1	5
72	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.	10.4	5

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73	Plasmon-driven high harmonic generation of benzene: effect of spatial inhomogeneity of near field. <i>Electronic Structure</i> , 2019, 1, 044001.	2.9	4
74	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.	3.1	4
75	Localized-density-matrix method and its application to nanomaterials. <i>Pure and Applied Chemistry</i> , 2000, 72, 281-291.	1.9	3
76	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
77	Constructing spin-adiabatic states for the modeling of spin-crossing reactions. I. A shared-orbital implementation. <i>International Journal of Quantum Chemistry</i> , 2020, 120, e26123.	2.0	3
78	Theoretical investigation of the non-Condon effect on electron transfer: Application to organic semiconductor. <i>Science China Chemistry</i> , 2011, 54, 707-714.	8.4	1
79	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