WanZhen Liang

List of Publications by Year in descending order

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79	7,483	257101	66788
papers	citations	24 h-index	78 g-index

85	85	85	8678
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Advances in methods and algorithms in a modern quantum chemistry program package. Physical Chemistry Chemical Physics, 2006, 8, 3172-3191.	1.3	2,597
2	Advances in molecular quantum chemistry contained in the Q-Chem 4 program package. Molecular Physics, 2015, 113, 184-215.	0.8	2,561
3	Software for the frontiers of quantum chemistry: An overview of developments in the Q-Chem 5 package. Journal of Chemical Physics, 2021, 155, 084801.	1.2	518
4	Charge transfer in organic molecules for solar cells: theoretical perspective. Chemical Society Reviews, 2012, 41, 1075-1087.	18.7	150
5	Effect of Phase Junction Structure on the Photocatalytic Performance in Overall Water Splitting: Ga₂O₃ Photocatalyst as an Example. Journal of Physical Chemistry C, 2015, 119, 18221-18228.	1.5	101
6	The effect of moisture on the structures and properties of lead halide perovskites: a first-principles theoretical investigation. Physical Chemistry Chemical Physics, 2016, 18, 23174-23183.	1.3	89
7	How the Structures and Properties of Two-Dimensional Layered Perovskites MAPbI₃ and CsPbI₃ Vary with the Number of Layers. Journal of Physical Chemistry Letters, 2017, 8, 1517-1523.	2.1	89
8	Tuning the energy band-gap of crystalline gallium oxide to enhance photocatalytic water splitting: mixed-phase junctions. Journal of Materials Chemistry A, 2014, 2, 17005-17014.	5.2	84
9	Spectroscopic Signature of the Aggregation-Induced Emission Phenomena Caused by Restricted Nonradiative Decay: A Theoretical Proposal. Journal of Physical Chemistry C, 2015, 119, 5040-5047.	1.5	70
10	Vibronic Spectra of Perylene Bisimide Oligomers: Effects of Intermolecular Charge-Transfer Excitation and Conformational Flexibility. Journal of Physical Chemistry B, 2011, 115, 2699-2708.	1.2	56
11	Single-handed supramolecular double helix of homochiral bis(N-amidothiourea) supported by double crossed Câ˜IÂ·Â·Â·S halogen bonds. Nature Communications, 2019, 10, 3610.	5.8	55
12	Time-Dependent Approach to Resonance Raman Spectra Including Duschinsky Rotation and Herzbergâ€“Teller Effects: Formalism and Its Realistic Applications. Journal of Chemical Theory and Computation, 2012, 8, 4474-4482.	2.3	54
13	Real-Time Propagation of the Reduced One-Electron Density Matrix in Atom-Centered Orbitals: Application to Electron Injection Dynamics in Dye-Sensitized TiO₂ Clusters. Journal of Physical Chemistry C, 2008, 112, 16655-16662.	1.5	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. Physical Chemistry Chemical Physics, 2015, 17, 17679-17687.	1.3	43
15	Localized-Density-Matrix Method and Its Application to Carbon Nanotubes. Journal of Physical Chemistry A, 2000, 104, 2445-2453.	1.1	40
16	Generalized linear-scaling localized-density-matrix method. Journal of Chemical Physics, 1999, 110, 1844-1855.	1.2	37
17	Quantum Interference in Singlet Fission: J- and H-Aggregate Behavior. Journal of Physical Chemistry Letters, 2017, 8, 5105-5112.	2.1	37
18	Elucidating the Electronic Structure of a Delayed Fluorescence Emitter via Orbital Interactions, Excitation Energy Components, Charge-Transfer Numbers, and Vibrational Reorganization Energies. Journal of Physical Chemistry Letters, 2021, 12, 2712-2720.	2.1	35

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19	Electronic Excitation of Polyfluorenes:Â A Theoretical Study. Journal of Physical Chemistry B, 2006, 110, 9908-9915.	1.2	33
20	Nature of Low-Lying Excited States in H-Aggregated Perylene Bisimide Dyes: Results of TD-LRC-DFT and the Mixed Exciton Model. Journal of Physical Chemistry B, 2009, 113, 14581-14587.	1.2	33
21	Aggregation-Induced Emission Mechanism of Dimethoxy-Tetraphenylethylene in Water Solution: Molecular Dynamics and QM/MM Investigations. Journal of Chemical Theory and Computation, 2015, 11, 2257-2267.	2.3	32
22	Effects of Charge Transfer State and Exciton Migration on Singlet Fission Dynamics in Organic Aggregates. Journal of Physical Chemistry C, 2016, 120, 13351-13359.	1.5	31
23	Non-Condon effect on charge transport in dithiophene-tetrathiafulvalene crystal. Journal of Chemical Physics, 2010, 133, 024501.	1.2	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. Physical Chemistry Chemical Physics, 2015, 17, 16835-16845.	1.3	28
25	Analytic energy gradient of excited electronic state within TDDFT/MMpol framework: Benchmark tests and parallel implementation. Journal of Chemical Physics, 2015, 143, 134104.	1.2	25
26	Vibronic Coupling Effect on the Vibrationally Resolved Electronic Spectra and Intersystem Crossing Rates of a TADF Emitter: 7-PhQAD. Journal of Physical Chemistry A, 2022, 126, 239-248.	1.1	25
27	Generalized timeâ€dependent approaches to vibrationally resolved electronic and Raman spectra: Theory and applications. International Journal of Quantum Chemistry, 2015, 115, 550-563.	1.0	24
28	Lead-free low-dimensional tin halide perovskites with functional organic spacers: breaking the charge-transport bottleneck. Journal of Materials Chemistry A, 2019, 7, 16742-16747.	5.2	24
29	Harmonic generation of open-ended and capped carbon nanotubes investigated by time-dependent Hartree-Fock theory. Physical Review B, 2007, 75, .	1.1	20
30	Energy relaxation and separation of a hot electron-hole pair in organic aggregates from a time-dependent wavepacket diffusion method. Journal of Chemical Physics, 2014, 140, 214107.	1.2	20
31	Assessment of mode-mixing and Herzberg-Teller effects on two-photon absorption and resonance hyper-Raman spectra from a time-dependent approach. Journal of Chemical Physics, 2014, 140, 094107.	1.2	20
32	An efficient approach for self-consistent-field energy and energy second derivatives in the atomic-orbital basis. Journal of Chemical Physics, 2005, 123, 194106.	1.2	19
33	Theoretical investigation of resonance Raman scattering of dye molecules absorbed on semiconductor surfaces. Journal of Chemical Physics, 2011, 135, 044108.	1.2	19
34	Size-Dependent Optical Properties of Aluminum Nanoparticles: From Classical to Quantum Description. Journal of Physical Chemistry C, 2018, 122, 10545-10551.	1.5	19
35	H-Type-like Aggregation-Accelerated Singlet Fission Process in Dipyrrolonaphthyridinedione Thin Film: The Role of Charge Transfer/Excimer Mixed Intermediate State. Journal of Physical Chemistry Letters, 2021, 12, 12276-12282.	2.1	19
36	Theoretical studies of vibrationally resolved absorption and emission spectra: From a single chromophore to multichromophoric oligomers/aggregates. Science China Chemistry, 2010, 53, 297-309.	4.2	18

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37	Spectral Characteristics of Chemical Enhancement on SERS of Benzene-like Derivatives: Franckâ€“Condon and Herzbergâ€“Teller Contributions. Journal of Physical Chemistry C, 2015, 119, 27609-27619.	1.5	18
38	Effect of charge-transfer states on the vibrationally resolved absorption spectra and exciton dynamics in ZnPc aggregates: Simulations from a non-Makovian stochastic SchrÃ¶dinger equation. Journal of Chemical Physics, 2020, 153, 034116.	1.2	18
39	Theoretical study of the low-lying electronic excited states for molecular aggregates. Science China Chemistry, 2013, 56, 1258-1262.	4.2	16
40	Analytical derivative techniques for TDDFT excited-state properties: Theory and application. Science China Chemistry, 2014, 57, 48-57.	4.2	16
41	Electronic Couplings for Photoinduced Charge Transfer and Excitation Energy Transfer Based on Fragment Particleâ€“Hole Densities. Journal of Physical Chemistry Letters, 2021, 12, 1032-1039.	2.1	15
42	Joint Effects of Excitonâ€“Exciton and Excitonâ€“Photon Couplings on the Singlet Fission Dynamics in Organic Aggregates. Journal of Physical Chemistry C, 2021, 125, 1654-1664.	1.5	15
43	Atomically Thin pâ€“n/pâ€“n Nanodevices by Surface Charge Transfer Doping of Arsenene/Antimonene Heterostructures. ACS Applied Materials & Interfaces, 2018, 10, 23851-23857.	4.0	14
44	Analysis and visualization of energy densities. II. Insights from linear-response time-dependent density functional theory calculations. Physical Chemistry Chemical Physics, 2020, 22, 26852-26864.	1.3	12
45	Molecular Design Strategy for Practical Singlet Fission Materials: The Charm of Donor/Acceptor Decorated Quinoidal Structure. CCS Chemistry, 2022, 4, 2748-2756.	4.6	12
46	Plasmon Resonance of Isolated Gold Hollow Nanoparticles and Nanoparticle Pairs: Insights from Electronic Structure Calculations. Journal of Physical Chemistry C, 2012, 116, 1755-1763.	1.5	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. Journal of Chemical Physics, 2014, 140, 18A506.	1.2	11
48	Vibrationally Resolved Absorption Spectra and Exciton Dynamics in Zinc Phthalocyanine Aggregates: Effects of Aggregation Lengths and Remote Exciton Transfer. Journal of Physical Chemistry A, 2021, 125, 2932-2943.	1.1	11
49	Influence of intrinsic defects on the structure and dynamics of the mixed Pbâ€“Sn perovskite: first-principles DFT and NAMD simulations. Journal of Materials Chemistry A, 2021, 10, 234-244.	5.2	11
50	Theoretical studies on electronic spectroscopy and dynamics with the real-time time-dependent density functional theory. Frontiers of Chemistry in China: Selected Publications From Chinese Universities, 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. Journal of Chemical Physics, 2015, 143, 154105.	1.2	10
52	Structural characteristics and photoinduced carrier behaviors of the mixed-phase BiVO4: a first-principles theoretical study. Theoretical Chemistry Accounts, 2016, 135, 1.	0.5	10
53	Charge Carrier Mobilities and Singlet Fission Dynamics in Thienoquinoidal Compounds. Journal of Physical Chemistry C, 2017, 121, 22587-22596.	1.5	10
54	Why Hybrid Tin-Based Perovskites Simultaneously Improve the Structural Stability and Charge Carriersâ€™ Lifetime: Ab Initio Quantum Dynamics. ACS Applied Materials & Interfaces, 2021, 13, 16567-16575.	4.0	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. Journal of Chemical Physics, 2022, 156, .	1.2	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. Journal of Physical Chemistry A, 2008, 112, 10442-10447.	1.1	9
57	NB-Type Electronic Asymmetric Compounds as Potential Blue-Color TADF Emitters: Steric Hindrance, Substitution Effect, and Electronic Characteristics. ACS Omega, 2017, 2, 3098-3109.	1.6	9
58	Benzazasiline combined with triphenylborane-based cores for constructing deep-blue donor-acceptor-donor TADF emitters. Organic Electronics, 2018, 57, 74-81.	1.4	9
59	Analysis and visualization of energy densities. I. Insights from real-time time-dependent density functional theory simulations. Physical Chemistry Chemical Physics, 2020, 22, 26838-26851.	1.3	9
60	Theory and algorithms for the excited states of large molecules and molecular aggregates. Science China Chemistry, 2013, 56, 1267-1270.	4.2	8
61	Characterizing the Structures, Spectra, and Energy Landscapes Involved in the Excited-State Proton Transfer Process of Red Fluorescent Protein LSSmKate1. Journal of Physical Chemistry B, 2016, 120, 9833-9842.	1.2	8
62	Vibrationally resolved absorption spectra and ultrafast exciton dynamics in Î±-phase and Î²-phase zinc phthalocyanine aggregates. Physical Chemistry Chemical Physics, 2022, 24, 2974-2987.	1.3	8
63	Localized-density-matrix method and nonlinear optical response. Journal of Chemical Physics, 2000, 113, 1403-1408.	1.2	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. Journal of Chemical Physics, 2020, 152, 014102.	1.2	7
65	Understanding the mechanism of plasmon-driven water splitting: hot electron injection and a near field enhancement effect. Physical Chemistry Chemical Physics, 2021, 23, 25629-25636.	1.3	7
66	Singlet/triplet exciton dissociation and charge recombination in donorâ€acceptor ThQsâ€€ 60 /PDIxCN 2 complexes. Journal of Computational Chemistry, 2019, 40, 997-1004.	1.5	6
67	How the Structures and Properties of Pristine and Anion Vacancy Defective Organicâ€“Inorganic Hybrid Double Perovskites MA₂AgIn(Br_xI_{1â€“x})₆ Vary with Br Content x. Journal of Physical Chemistry Letters, 2020, 11, 10315-10322.	2.1	6
68	Potassium doping-induced variations in the structures and photoelectric properties of a MAPbI₃ perovskite and a MAPbI₃/TiO₂ junction. Physical Chemistry Chemical Physics, 2020, 22, 20553-20561.	1.3	6
69	Nonlinear features of Fano resonance: a QM/EM study. Physical Chemistry Chemical Physics, 2021, 23, 15994-16004.	1.3	6
70	Gold-Based Double Perovskite-Related Polymorphs: Low Dimensional with an Ultranarrow Bandgap. Chemistry of Materials, 2022, 34, 1544-1553.	3.2	6
71	Collaborative effect of plasmon-induced resonance energy and electron transfer on the interfacial electron injection dynamics of dye-sensitized solar cell. Journal of Chemical Physics, 2019, 151, 044702.	1.2	5
72	Structure and property tunability in monolayer halide lead-free double hybrid perovskites: effects of Rashba and biaxial strain. Journal of Materials Chemistry A, 2019, 7, 11487-11496.	5.2	5

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73	Plasmon-driven high harmonic generation of benzene: effect of spatial inhomogenity of near field. Electronic Structure, 2019, 1, 044001.	1.0	4
74	Plasmon-enhanced high order harmonic generation of open-ended finite-sized carbon nanotubes: The effects of incident fieldâ€™s intensity and frequency and the interference between the incident and scattered fields. Journal of Chemical Physics, 2020, 152, 224708.	1.2	4
75	Localized-density-matrix method and its application to nanomaterials. Pure and Applied Chemistry, 2000, 72, 281-291.	0.9	3
76	One- and two-photon absorption spectra of the yellow fluorescent protein citrine: effects of intramolecular electron-vibrational coupling and intermolecular interactions. Molecular Physics, 2018, 116, 885-897.	0.8	3
77	Constructing spinâ€adiabatic states for the modeling of spinâ€crossing reactions. I. A sharedâ€orbital implementation. International Journal of Quantum Chemistry, 2020, 120, e26123.	1.0	3
78	Theoretical investigation of the non-Condon effect on electron transfer: Application to organic semiconductor. Science China Chemistry, 2011, 54, 707-714.	4.2	1
79	Unveiling the effect of electron tunneling on the plasmonic resonance of closely spaced gold particles. Physical Chemistry Chemical Physics, 2020, 22, 1747-1755.	1.3	1