

Wen-Liang Wang

List of Publications by Year in descending order

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86
papers

1,232
citations

361413

20
h-index

454955

30
g-index

90
all docs

90
docs citations

90
times ranked

1204
citing authors

#	ARTICLE	IF	CITATIONS
1	Crystal morphology of 3,4-bis(3-nitrofurazan-4-yl)furoxan (DNTF) in a solvent system: molecular dynamics simulation and sensitivity study. <i>CrystEngComm</i> , 2016, 18, 2843-2851.	2.6	73
2	Single-layer assembly of pyrene end-capped terthiophene and its sensing performances to nitroaromatic explosives. <i>Journal of Materials Chemistry</i> , 2012, 22, 1069-1077.	6.7	69
3	Lateral substituent effects on UV stability of high-birefringence liquid crystals with the diaryl-diacetylene core: DFT/TD-DFT study. <i>Liquid Crystals</i> , 2017, 44, 1515-1524.	2.2	56
4	Exploring the Mechanism of Fluorescence Quenching and Aggregation-Induced Emission of a Phenylethylene Derivative by QM (CASSCF and TDDFT) and ONIOM (QM:MM) Calculations. <i>Journal of Physical Chemistry C</i> , 2016, 120, 21850-21857.	3.1	43
5	Water-catalyzed gas-phase hydrogen abstraction reactions of CH ₃ O ₂ and HO ₂ with HO ₂ : a computational investigation. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 20794.	2.8	42
6	First-Principles Determination of Active Sites of Ni Metal-Based Electrocatalysts for Hydrogen Evolution Reaction. <i>ACS Applied Materials & Interfaces</i> , 2018, 10, 39624-39630.	8.0	41
7	Theoretical Study on the Mechanism and Kinetics for the Self-Reaction of C ₂ H ₅ O ₂ Radicals. <i>Journal of Physical Chemistry A</i> , 2012, 116, 4610-4620.	2.5	36
8	Can a single water molecule really affect the HO ₂ + NO ₂ hydrogen abstraction reaction under tropospheric conditions?. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 15046-15055.	2.8	34
9	A study of solvent selectivity on the crystal morphology of FOX-7 via a modified attachment energy model. <i>RSC Advances</i> , 2016, 6, 59784-59793.	3.6	32
10	Defective h-BN sheet embedded atomic metals as highly active and selective electrocatalysts for NH ₃ fabrication <i>via</i> NO reduction. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 22627-22634.	2.8	32
11	Catalytic effect of a single water molecule on the atmospheric reaction of HO ₂ + OH: fact or fiction? A mechanistic and kinetic study. <i>RSC Advances</i> , 2013, 3, 7381.	3.6	30
12	Photochemistry of the Simplest Criegee Intermediate, CH ₂ OO: Photoisomerization Channel toward Dioxirane Revealed by CASPT2 Calculations and Trajectory Surface-Hopping Dynamics. <i>Journal of Physical Chemistry Letters</i> , 2018, 9, 978-981.	4.6	28
13	Theoretical investigation on electronic, optical, and charge transport properties of 7,8,15,16-tetraazaterrylene and its derivatives with electron-attracting substituents. <i>New Journal of Chemistry</i> , 2013, 37, 2925.	2.8	27
14	Water-catalyzed decomposition of the simplest Criegee intermediate CH ₂ OO. <i>Theoretical Chemistry Accounts</i> , 2016, 135, 1.	1.4	27
15	Direct dynamics study on the mechanism and the kinetics of the reaction of CH ₃ NH ₂ with OH. <i>International Journal of Quantum Chemistry</i> , 2009, 109, 1566-1575.	2.0	24
16	Formation mechanism of methanesulfonic acid and ammonia clusters: A kinetics simulation study. <i>Atmospheric Environment</i> , 2020, 222, 117161.	4.1	24
17	The catalytic effect of water, water dimers and water trimers on H ₂ S + ³ O ₂ formation by the HO ₂ + HS reaction under tropospheric conditions. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 17414-17427.	2.8	23
18	Mechanistic and kinetics investigations of oligomer formation from Criegee intermediate reactions with hydroxyalkyl hydroperoxides. <i>Atmospheric Chemistry and Physics</i> , 2019, 19, 4075-4091.	4.9	23

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19	Role of water clusters in the reaction of the simplest Criegee intermediate CH ₂ OO with water vapour. <i>Theoretical Chemistry Accounts</i> , 2016, 135, 1.	1.4	22
20	Different conical intersections control nonadiabatic photochemistry of fluorene light-driven molecular rotary motor: A CASSCF and spin-flip DFT study. <i>Journal of Chemical Physics</i> , 2016, 145, 244311.	3.0	21
21	Competition between HO ₂ and H ₂ O ₂ Reactions with CH ₂ OO/ <i>anti</i> -CH ₃ CHO in the Oligomer Formation: A Theoretical Perspective. <i>Journal of Physical Chemistry A</i> , 2017, 121, 6981-6991.	2.5	21
22	Water effect on the formation of 3O ₂ from the self-reaction of two HO ₂ radicals in tropospheric conditions. <i>Computational and Theoretical Chemistry</i> , 2014, 1045, 135-144.	2.5	20
23	Electrostatic Polarization Energies of Charge Carriers in Organic Molecular Crystals: A Comparative Study with Explicit State-Specific Atomic Polarizability Based AMOEBA Force Field and Implicit Solvent Method. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 3728-3739.	5.3	20
24	Reactions between hydroxyl-substituted alkylperoxy radicals and Criegee intermediates: correlations of the electronic characteristics of methyl substituents and the reactivity. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 15073-15083.	2.8	18
25	Triazacoronene Derivatives with Three <i>peri</i> -Benzopyrano Extensions: Synthesis, Structure, and Properties. <i>European Journal of Organic Chemistry</i> , 2018, 2018, 869-873.	2.4	18
26	Atmospheric Chemistry of Enols: Vinyl Alcohol + OH + O ₂ Reaction Revisited. <i>Journal of Physical Chemistry A</i> , 2019, 123, 3205-3213.	2.5	18
27	Atmospheric chemistry of the self-reaction of HO ₂ radicals: stepwise mechanism <i>versus</i> one-step process in the presence of (H ₂ O) _n (<i>n</i> = 1-3) clusters. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 24042-24053.	2.8	18
28	Atmospheric implications of hydration on the formation of methanesulfonic acid and methylamine clusters: A theoretical study. <i>Chemosphere</i> , 2020, 244, 125538.	8.2	18
29	Atmospheric implication of synergy in methanesulfonic acid-base trimers: a theoretical investigation. <i>RSC Advances</i> , 2020, 10, 5173-5182.	3.6	18
30	Computational study on the reaction of CH ₃ SCH ₂ CH ₃ with OH radical: mechanism and enthalpy of formation. <i>Theoretical Chemistry Accounts</i> , 2011, 129, 771-780.	1.4	17
31	Effect of oligomerization reactions of Criegee intermediate with organic acid/peroxy radical on secondary organic aerosol formation from isoprene ozonolysis. <i>Atmospheric Environment</i> , 2018, 187, 218-229.	4.1	17
32	Effects of Protonation and C5 Methylation on the Electrophilic Addition Reaction of Cytosine: A Computational Study. <i>Journal of Physical Chemistry B</i> , 2013, 117, 3-12.	2.6	16
33	Theoretical study on crystal morphologies of 1,1-diamino-2,2-dinitroethene in solvents: Modified attachment energy model and occupancy model. <i>Journal of Molecular Graphics and Modelling</i> , 2018, 85, 262-269.	2.4	16
34	Theoretical Understanding of Electrocatalytic Hydrogen Production Performance by Low-Dimensional Metal-Organic Frameworks on the Basis of Resonant Charge-Transfer Mechanisms. <i>Journal of Physical Chemistry Letters</i> , 2019, 10, 6955-6961.	4.6	15
35	Computational study on the mechanism for the gas-phase reaction of dimethyl disulfide with OH. <i>International Journal of Quantum Chemistry</i> , 2011, 111, 644-651.	2.0	13
36	Direct dynamics study on mechanism and kinetics of the biradical self-reaction of HOO. <i>International Journal of Quantum Chemistry</i> , 2011, 111, 3029-3039.	2.0	13

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37	Exploring the Mechanism of a Chiral <i>N</i> -Alkyl Imine-Based Light-Driven Molecular Rotary Motor at MS-CASPT2//CASSCF and MS-CASPT2//TD DFT Levels. <i>Chemistry - A European Journal</i> , 2019, 25, 4194-4201.	3.3	13
38	Atmospheric chemistry of CHF ₂ CF ₂ OCH ₂ CF ₃ : Reactions with Cl atoms, fate of CHF ₂ CF ₂ OĊHCF ₃ radical, formation of OH radical and Criegee Intermediate. <i>Atmospheric Environment</i> , 2020, 242, 117805.	4.1	13
39	Facile Synthesis of ĩ-Extended Viologens: Electron-Deficient Polycyclic Azaaromatics. <i>Chemistry - A European Journal</i> , 2017, 23, 7409-7413.	3.3	12
40	Theoretical kinetic investigation of thermal decomposition of nitropropane. <i>Structural Chemistry</i> , 2017, 28, 655-666.	2.0	12
41	Theoretical studies on atmospheric reactions of CH ₂ FO ₂ with HO ₂ and HO ₂ ...H ₂ O complex. <i>Computational and Theoretical Chemistry</i> , 2012, 991, 13-21.	2.5	11
42	Combining the Advantages of Alkene and Azo <i>E</i> / <i>Z</i> Photoisomerizations: Mechanistic Insights into Ketoimine Photoswitches. <i>Journal of Physical Chemistry A</i> , 2017, 121, 2588-2596.	2.5	11
43	Oligomerization reactions for precursors to secondary organic aerosol: Comparison between two formation mechanisms for the oligomeric hydroxyalkyl hydroperoxides. <i>Atmospheric Environment</i> , 2017, 166, 1-8.	4.1	10
44	Explicit Method To Evaluate the External Reorganization Energy of Charge-Transfer Reactions in Oligoacene Crystals Using the State-Specific Polarizable Force Field. <i>Journal of Physical Chemistry A</i> , 2018, 122, 8957-8964.	2.5	10
45	Role of glycine on sulfuric acid-ammonia clusters formation: Transporter or participator. <i>Journal of Environmental Sciences</i> , 2020, 89, 125-135.	6.1	9
46	Density functional theory study on the reaction of triazol-3-one with nitronium: direct nitration versus acidic group-induced nitration. <i>RSC Advances</i> , 2015, 5, 25183-25191.	3.6	8
47	Theoretical Prediction on Photovoltaic Properties of 4Cl-BPPQ/PC ₆₁ BM System via Density Functional Theory Calculations. <i>Chinese Journal of Chemistry</i> , 2016, 34, 1143-1150.	4.9	8
48	Atmospheric Chemistry of Enols: The Formation Mechanisms of Formic and Peroxyformic Acids in Ozonolysis of Vinyl Alcohol. <i>Journal of Physical Chemistry A</i> , 2020, 124, 4271-4279.	2.5	8
49	Evaluation of electronic polarization energy in oligoacene molecular crystals using the solvated supermolecular approach. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 14453-14461.	2.8	7
50	Computational study on mechanisms of C ₂ H ₅ O ₂ +OH reaction and properties of C ₂ H ₅ O ₃ H complex. <i>Chemical Research in Chinese Universities</i> , 2017, 33, 623-630.	2.6	7
51	Effects of water, ammonia and formic acid on HO ₂ + Cl reactions under atmospheric conditions: competition between a stepwise route and one elementary step. <i>RSC Advances</i> , 2019, 9, 21544-21556.	3.6	7
52	Hydrogen bond, ring tension and ĩ-conjugation effects: methyl and vinyl substitutions dramatically change the photodynamics of Criegee intermediates. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 15295-15302.	2.8	7
53	Modification on C217 by auxiliary acceptor toward efficient sensitiser for dye-sensitised solar cells: a theoretical study. <i>Molecular Physics</i> , 2018, 116, 536-545.	1.7	6
54	Reaction mechanism and kinetics of Criegee intermediate CH ₂ OO with CH ₂ =ĊC(CH ₃)CHO. <i>Computational and Theoretical Chemistry</i> , 2019, 1170, 112644.	2.5	6

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55	Formic acid catalyzed isomerization of protonated cytosine: a lower barrier reaction for tautomer production of potential biological importance. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 13515-13523.	2.8	5
56	Quantum chemical studies of the OH-initiated oxidation reactions of propenols in the presence of O ₂ . <i>Molecular Physics</i> , 2019, 117, 682-692.	1.7	5
57	Resonance-assisted/impaired anion-π interaction: towards the design of novel anion receptors. <i>RSC Advances</i> , 2020, 10, 36181-36191.	3.6	4
58	A 3D interpenetrating supramolecular compound based on Cu-π-N weak coordination: synthesis, crystal structure and DFT investigation. <i>Journal of Coordination Chemistry</i> , 2008, 61, 2916-2925.	2.2	3
59	Theoretical Studies on the Electronic Structures and Optical Properties of Triaryl Endcapped Terthiophene Derivatives. <i>Chinese Journal of Chemistry</i> , 2010, 28, 1907-1914.	4.9	3
60	Thermal decomposition and isomerization of 1-heptyl radical: a computational investigation. <i>Theoretical Chemistry Accounts</i> , 2014, 133, 1.	1.4	3
61	Oligomerization Reactions of Criegee Intermediates with Hydroxyalkyl Hydroperoxides: Mechanism, Kinetics, and Structure-Reactivity Relationship. <i>Atmospheric Chemistry and Physics Discussions</i> , 0, 1-35.	1.0	3
62	The HO ₄ H ⁺ O ₃ +H ₂ O reaction catalysed by acidic, neutral and basic catalysts in the troposphere. <i>Molecular Physics</i> , 2020, 118, e1673912.	1.7	3
63	Atmospheric oxidation of 1-butene initiated by OH radical: Implications for ozone and nitrous acid formations. <i>Atmospheric Environment</i> , 2021, 244, 118010.	4.1	3
64	The catalytic effects of H ₂ O, basic and acidic catalysts on the gas-phase hydrolysis mechanism of carbonyl fluoride (CF ₂ O). <i>International Journal of Quantum Chemistry</i> , 2021, 121, e26657.	2.0	3
65	Theoretical Investigation into Electronic Structures and Charge Transfer Properties of π-Conjugated System with Different Combinations of Thiophene and Vinyl/Butadiene. <i>Chinese Journal of Chemistry</i> , 2012, 30, 2501-2508.	4.9	2
66	A computational study on the mechanism and kinetics of the reaction between CH ₃ CH ₂ S and OH. <i>RSC Advances</i> , 2014, 4, 62835-62843.	3.6	2
67	Theoretical study on the thermal decomposition and isomerization of 3-Me-1-heptyl radical. <i>Computational and Theoretical Chemistry</i> , 2015, 1063, 10-18.	2.5	2
68	Effects of an acidic-alkaline environment on the reactivity of 5-carboxycytosine with hydroxyl radicals. <i>RSC Advances</i> , 2015, 5, 87364-87376.	3.6	2
69	Theoretical investigation on exciton-dissociation and charge-recombination processes of PC61BM-PTDPPSe interface. <i>Journal of Molecular Modeling</i> , 2016, 22, 241.	1.8	2
70	Modeling Photovoltaic Performances of BTBPD-PC61BM System via Density Functional Theory Calculations. <i>Chinese Journal of Chemical Physics</i> , 2017, 30, 268-276.	1.3	2
71	Theoretical estimation of the dissociation energy of CT states at the acenes/C60 interfaces using fragmental-based ALMO method. <i>Computational and Theoretical Chemistry</i> , 2018, 1140, 32-37.	2.5	2
72	Enhanced photovoltaic performances of C219-based dye sensitizers by introducing electron-withdrawing substituents: a density functional theory study. <i>Molecular Physics</i> , 2020, 118, e1636151.	1.7	2

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73	Atmospheric oxidation chemistry of hexafluoroisobutylene initiated by OH radical: Kinetics and mechanism. <i>Computational and Theoretical Chemistry</i> , 2021, 1197, 113137.	2.5	2
74	Performable enhancement of C220-based dyes via inserting auxiliary electron acceptors for dye-sensitized solar cells: a theoretical investigation. <i>Journal of Computational Electronics</i> , 2021, 20, 1277-1288.	2.5	2
75	Photodynamics of methyl-vinyl Criegee intermediate: Different conical intersections govern the fates of <i>syn/anti</i> configurations. <i>Chinese Journal of Chemical Physics</i> , 2020, 33, 595-602.	1.3	2
76	Kinetic and Mechanistic Investigations of OH-Initiated Atmospheric Degradation of Methyl Butyl Ketone. <i>Journal of Physical Chemistry A</i> , 2022, 126, 2976-2988.	2.5	2
77	Kinetic and mechanistic investigations of the thermal decomposition of methyl-substituted cycloalkyl radicals. <i>RSC Advances</i> , 2015, 5, 28044-28053.	3.6	1
78	Insight into the acidic group-induced nitration mechanism of 2-methyl-4,6-dihydropyrimidine (MDP) with nitronium. <i>RSC Advances</i> , 2016, 6, 80145-80157.	3.6	1
79	The multi-channel reaction of the OH radical with 5-hydroxymethylcytosine: a computational study. <i>RSC Advances</i> , 2016, 6, 13349-13357.	3.6	1
80	Theoretical investigation on photovoltaic properties of PC ₆₁ BM/PPDPP5T system as a promising polymer-based solar cell. <i>Journal of Physical Organic Chemistry</i> , 2017, 30, e3592.	1.9	1
81	Impact of the acidic group on the hydrolysis of 2-dinitromethylene-5,5-dinitropyrimidine-4,6-dione. <i>RSC Advances</i> , 2018, 8, 13301-13309.	3.6	1
82	Reaction probability and defluorination mechanisms of a potent greenhouse gas SF ₅ CF ₃ attacked by CH ₃ radical: a theoretical study. <i>Molecular Physics</i> , 2018, 116, 2226-2238.	1.7	1
83	Efficient improvement of W05-based dyes by inserting auxiliary electron acceptors for dye-sensitized solar cells: A theoretical investigation. <i>Journal of Physical Organic Chemistry</i> , 0, , e4290.	1.9	1
84	Impact of Water Molecules on the Isomerization of CH ₃ S(OH)CH ₂ to CH ₃ S(O)CH ₃ : A Computational Investigation. <i>Chinese Journal of Chemistry</i> , 2013, 31, 1341-1347.	4.9	0
85	Theoretical reinvestigation of the ozonolysis mechanism of allyl alcohol. <i>International Journal of Quantum Chemistry</i> , 2020, 120, e26387.	2.0	0
86	Effect of methyl hydrogen sulfate on the formation of sulfuric acid-ammonia clusters: A theoretical study. <i>Journal of the Chinese Chemical Society</i> , 0, , .	1.4	0