Wen-Liang Wang

List of Publications by Year
in descending order

86	1,232	361413	454955
papers	citations	20 h-index	30 g-index

90	90	90	1204
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Kinetic and Mechanistic Investigations of OH-Initiated Atmospheric Degradation of Methyl Butyl Ketone. Journal of Physical Chemistry A, 2022, 126, 2976-2988.	2.5	2
2	Atmospheric oxidation of 1-butene initiated by OH radical: Implications for ozone and nitrous acid formations. Atmospheric Environment, 2021, 244, 118010.	4.1	3
3	Atmospheric oxidation chemistry of hexafluoroisobutylene initiated by OH radical: Kinetics and mechanism. Computational and Theoretical Chemistry, 2021, 1197, 113137.	2.5	2
4	The catalytic effects of <scp>H₂O</scp>, basic and acidic catalysts on the gasâ€phase hydrolysis mechanism of carbonyl fluoride (<scp>CF₂O</scp>). International Journal of Quantum Chemistry, 2021, 121, e26657.	2.0	3
5	Performable enhancement of C220-based dyes via inserting auxiliary electron acceptors for dye-sensitized solar cells: a theoretical investigation. Journal of Computational Electronics, 2021, 20, 1277-1288.	2.5	2
6	The HO₄H â†' O₃â€‰+â€‰H₂O reaction catalysed by acidic, neutral and basic catalysts in the troposphere. Molecular Physics, 2020, 118, e1673912.	1.7	3
7	Enhanced photovoltaic performances of C219-based dye sensitisers by introducing electron-withdrawing substituents: a density functional theory study. Molecular Physics, 2020, 118, e1636151.	1.7	2
8	Atmospheric implications of hydration on the formation of methanesulfonic acid and methylamine clusters: A theoretical study. Chemosphere, 2020, 244, 125538.	8.2	18
9	Role of glycine on sulfuric acid-ammonia clusters formation: Transporter or participator. Journal of Environmental Sciences, 2020, 89, 125-135.	6.1	9
10	Formation mechanism of methanesulfonic acid and ammonia clusters: A kinetics simulation study. Atmospheric Environment, 2020, 222, 117161.	4.1	24
11	Resonance-assisted/impaired anionâ€“Ï€ interaction: towards the design of novel anion receptors. RSC Advances, 2020, 10, 36181-36191.	3.6	4
12	Atmospheric chemistry of CHF2CF2OCH2CF3: Reactions with Cl atoms, fate of CHF2CF2OCâ€¢HCF3 radical, formation of OH radical and Criegee Intermediate. Atmospheric Environment, 2020, 242, 117805.	4.1	13
13	Theoretical reinvestigation of the ozonolysis mechanism of allyl alcohol. International Journal of Quantum Chemistry, 2020, 120, e26387.	2.0	0
14	Defective h-BN sheet embedded atomic metals as highly active and selective electrocatalysts for NH₃ fabrication via NO reduction. Physical Chemistry Chemical Physics, 2020, 22, 22627-22634.	2.8	32
15	Atmospheric Chemistry of Enols: The Formation Mechanisms of Formic and Peroxyformic Acids in Ozonolysis of Vinyl Alcohol. Journal of Physical Chemistry A, 2020, 124, 4271-4279.	2.5	8
16	Hydrogen bond, ring tension and Ï€-conjugation effects: methyl and vinyl substitutions dramatically change the photodynamics of Criegee intermediates. Physical Chemistry Chemical Physics, 2020, 22, 15295-15302.	2.8	7
17	Atmospheric implication of synergy in methanesulfonic acidâ€“base trimers: a theoretical investigation. RSC Advances, 2020, 10, 5173-5182.	3.6	18
18	Photodynamics of methyl-vinyl Criegee intermediate: Different conical intersections govern the fates of syn/anti configurations. Chinese Journal of Chemical Physics, 2020, 33, 595-602.	1.3	2

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19	Effects of water, ammonia and formic acid on HO₂ + Cl reactions under atmospheric conditions: competition between a stepwise route and one elementary step. RSC Advances, 2019, 9, 21544-21556.	3.6	7
20	Reaction mechanism and kinetics of Criegee intermediate CH2OO with CH2â€¯=â€¯C(CH3)CHO. Computational and Theoretical Chemistry, 2019, 1170, 112644.	2.5	6
21	Theoretical Understanding of Electrocatalytic Hydrogen Production Performance by Low-Dimensional Metalâ€“Organic Frameworks on the Basis of Resonant Charge-Transfer Mechanisms. Journal of Physical Chemistry Letters, 2019, 10, 6955-6961.	4.6	15
22	Exploring the Mechanism of a Chiral Nâ€Alkyl Imineâ€Based Lightâ€Driven Molecular Rotary Motor at MSâ€CASPT2//CASSCF and MSâ€CASPT2//(TD) DFT Levels. Chemistry - A European Journal, 2019, 25, 4194-4201.	3.3	13
23	Mechanistic and kinetics investigations of oligomer formation from Criegee intermediate reactions with hydroxyalkyl hydroperoxides. Atmospheric Chemistry and Physics, 2019, 19, 4075-4091.	4.9	23
24	Atmospheric Chemistry of Enols: Vinyl Alcohol + OH + O₂ Reaction Revisited. Journal of Physical Chemistry A, 2019, 123, 3205-3213.	2.5	18
25	Atmospheric chemistry of the self-reaction of HO₂ radicals: stepwise mechanism versus one-step process in the presence of (H₂O)_n (n = 1â€“3) clusters. Physical Chemistry Chemical Physics, 2019, 21, 24042-24053.	2.8	18
26	Quantum chemical studies of the OH-initiated oxidation reactions of propenols in the presence of O2. Molecular Physics, 2019, 117, 682-692.	1.7	5
27	Impact of the acidic group on the hydrolysis of 2-dinitromethylene-5,5-dinitropyrimidine-4,6-dione. RSC Advances, 2018, 8, 13301-13309.	3.6	1
28	Photochemistry of the Simplest Criegee Intermediate, CH2OO: Photoisomerization Channel toward Dioxirane Revealed by CASPT2 Calculations and Trajectory Surface-Hopping Dynamics. Journal of Physical Chemistry Letters, 2018, 9, 978-981.	4.6	28
29	Modification on C217 by auxiliary acceptor toward efficient sensitiser for dye-sensitised solar cells: a theoretical study. Molecular Physics, 2018, 116, 536-545.	1.7	6
30	Triazacoronene Derivatives with Three periâ€Benzopyrano Extensions: Synthesis, Structure, and Properties. European Journal of Organic Chemistry, 2018, 2018, 869-873.	2.4	18
31	First-Principles Determination of Active Sites of Ni Metal-Based Electrocatalysts for Hydrogen Evolution Reaction. ACS Applied Materials & Interfaces, 2018, 10, 39624-39630.	8.0	41
32	Explicit Method To Evaluate the External Reorganization Energy of Charge-Transfer Reactions in Oligoacene Crystals Using the State-Specific Polarizable Force Field. Journal of Physical Chemistry A, 2018, 122, 8957-8964.	2.5	10
33	Reaction probability and defluorination mechanisms of a potent greenhouse gas SF₅CF₃ attacked by CH₃ radical: a theoretical study. Molecular Physics, 2018, 116, 2226-2238.	1.7	1
34	Theoretical estimation of the dissociation energy of CT states at the acenes/C60 interfaces using fragmental-based ALMO method. Computational and Theoretical Chemistry, 2018, 1140, 32-37.	2.5	2
35	Theoretical study on crystal morphologies of 1,1-diamino-2,2-dinitroethene in solvents: Modified attachment energy model and occupancy model. Journal of Molecular Graphics and Modelling, 2018, 85, 262-269.	2.4	16
36	Effect of oligomerization reactions of Criegee intermediate with organic acid/peroxy radical on secondary organic aerosol formation from isoprene ozonolysis. Atmospheric Environment, 2018, 187, 218-229.	4.1	17

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37	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. Journal of Chemical Theory and Computation, 2018, 14, 3728-3739.	5.3	20
38	Theoretical investigation on photovoltaic properties of PC₆₁BMâ€PDPP5T system as a promising polymerâ€based solar cell. Journal of Physical Organic Chemistry, 2017, 30, e3592.	1.9	1
39	Lateral substituent effects on UV stability of high-birefringence liquid crystals with the diaryl-diacetylene core: DFT/TD-DFT study. Liquid Crystals, 2017, 44, 1515-1524.	2.2	56
40	Facile Synthesis of Ï€â€Extended Viologens: Electronâ€Deficient Polycyclic Azaâ€aromatics. Chemistry - A European Journal, 2017, 23, 7409-7413.	3.3	12
41	Reactions between hydroxyl-substituted alkylperoxy radicals and Criegee intermediates: correlations of the electronic characteristics of methyl substituents and the reactivity. Physical Chemistry Chemical Physics, 2017, 19, 15073-15083.	2.8	18
42	Formic acid catalyzed isomerization of protonated cytosine: a lower barrier reaction for tautomer production of potential biological importance. Physical Chemistry Chemical Physics, 2017, 19, 13515-13523.	2.8	5
43	Evaluation of electronic polarization energy in oligoacene molecular crystals using the solvated supermolecular approach. Physical Chemistry Chemical Physics, 2017, 19, 14453-14461.	2.8	7
44	Combining the Advantages of Alkene and Azo Eâ€“Z Photoisomerizations: Mechanistic Insights into Ketoimine Photoswitches. Journal of Physical Chemistry A, 2017, 121, 2588-2596.	2.5	11
45	Competition between HO₂ and H₂O₂ Reactions with CH₂OO/anti-CH₃CHOO in the Oligomer Formation: A Theoretical Perspective. Journal of Physical Chemistry A, 2017, 121, 6981-6991.	2.5	21
46	Computational study on mechanisms of C2H5O2+OH reaction and properties of C2H5O3H complex. Chemical Research in Chinese Universities, 2017, 33, 623-630.	2.6	7
47	Oligomerization reactions for precursors to secondary organic aerosol: Comparison between two formation mechanisms for the oligomeric hydroxyalkyl hydroperoxides. Atmospheric Environment, 2017, 166, 1-8.	4.1	10
48	Theoretical kinetic investigation of thermal decomposition of nitropropane. Structural Chemistry, 2017, 28, 655-666.	2.0	12
49	Modeling Photovoltaic Performances of BTBPD-PC61BM System via Density Functional Theory Calculations. Chinese Journal of Chemical Physics, 2017, 30, 268-276.	1.3	2
50	Role of water clusters in the reaction of the simplest Criegee intermediate CH2OO with water vapour. Theoretical Chemistry Accounts, 2016, 135, 1.	1.4	22
51	Different conical intersections control nonadiabatic photochemistry of fluorene light-driven molecular rotary motor: A CASSCF and spin-flip DFT study. Journal of Chemical Physics, 2016, 145, 244311.	3.0	21
52	The catalytic effect of water, water dimers and water trimers on H₂S +³O₂formation by the HO₂+ HS reaction under tropospheric conditions. Physical Chemistry Chemical Physics, 2016, 18, 17414-17427.	2.8	23
53	Water-catalyzed decomposition of the simplest Criegee intermediate CH2OO. Theoretical Chemistry Accounts, 2016, 135, 1.	1.4	27
54	Exploring the Mechanism of Fluorescence Quenching and Aggregation-Induced Emission of a Phenylethylene Derivative by QM (CASSCF and TDDFT) and ONIOM (QM:MM) Calculations. Journal of Physical Chemistry C, 2016, 120, 21850-21857.	3.1	43

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55	Insight into the acidic group-induced nitration mechanism of 2-methyl-4,6-dihydroxypyrimidine (MDP) with nitronium. RSC Advances, 2016, 6, 80145-80157.	3.6	1
56	Theoretical investigation on exciton-dissociation and charge-recombination processes of PC61BM-PTDPPSe interface. Journal of Molecular Modeling, 2016, 22, 241.	1.8	2
57	Theoretical Prediction on Photovoltaic Properties of 4Clâ€BPPQ/PC₆₁BM System via Density Functional Theory Calculations. Chinese Journal of Chemistry, 2016, 34, 1143-1150.	4.9	8
58	A study of solvent selectivity on the crystal morphology of FOX-7 via a modified attachment energy model. RSC Advances, 2016, 6, 59784-59793.	3.6	32
59	The multi-channel reaction of the OH radical with 5-hydroxymethylcytosine: a computational study. RSC Advances, 2016, 6, 13349-13357.	3.6	1
60	Crystal morphology of 3,4-bis(3-nitrofurazan-4-yl)furoxan (DNTF) in a solvent system: molecular dynamics simulation and sensitivity study. CrystEngComm, 2016, 18, 2843-2851.	2.6	73
61	Density functional theory study on the reaction of triazol-3-one with nitronium: direct nitration versus acidic group-induced nitration. RSC Advances, 2015, 5, 25183-25191.	3.6	8
62	Theoretical study on the thermal decomposition and isomerization of 3-Me-1-heptyl radical. Computational and Theoretical Chemistry, 2015, 1063, 10-18.	2.5	2
63	Can a single water molecule really affect the HO2 + NO2 hydrogen abstraction reaction under tropospheric conditions?. Physical Chemistry Chemical Physics, 2015, 17, 15046-15055.	2.8	34
64	Effects of an acidâ€“alkaline environment on the reactivity of 5-carboxycytosine with hydroxyl radicals. RSC Advances, 2015, 5, 87364-87376.	3.6	2
65	Kinetic and mechanistic investigations of the thermal decomposition of methyl-substituted cycloalkyl radicals. RSC Advances, 2015, 5, 28044-28053.	3.6	1
66	A computational study on the mechanism and kinetics of the reaction between CH₃CH₂S and OH. RSC Advances, 2014, 4, 62835-62843.	3.6	2
67	Water effect on the formation of 3O2 from the self-reaction of two HO2 radicals in tropospheric conditions. Computational and Theoretical Chemistry, 2014, 1045, 135-144.	2.5	20
68	Thermal decomposition and isomerization of 1-heptyl radical: a computational investigation. Theoretical Chemistry Accounts, 2014, 133, 1.	1.4	3
69	Catalytic effect of a single water molecule on the atmospheric reaction of HO2 + OH: fact or fiction? A mechanistic and kinetic study. RSC Advances, 2013, 3, 7381.	3.6	30
70	Theoretical investigation on electronic, optical, and charge transport properties of 7,8,15,16-tetraazaterrylene and its derivatives with electron-attracting substituents. New Journal of Chemistry, 2013, 37, 2925.	2.8	27
71	Effects of Protonation and C5 Methylation on the Electrophilic Addition Reaction of Cytosine: A Computational Study. Journal of Physical Chemistry B, 2013, 117, 3-12.	2.6	16
72	Impact of Water Molecules on the Isomerization of CH₃S(OH)CH₂ to CH₃S(O)CH₃: A Computational Investigation. Chinese Journal of Chemistry, 2013, 31, 1341-1347.	4.9	0

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73	Theoretical Study on the Mechanism and Kinetics for the Self-Reaction of C2H5O2 Radicals. Journal of Physical Chemistry A, 2012, 116, 4610-4620.	2.5	36
74	Theoretical studies on atmospheric reactions of CH2FO2 with HO2 and HO2â‹…H2O complex. Computational and Theoretical Chemistry, 2012, 991, 13-21.	2.5	11
75	Theoretical Investigation into Electronic Structures and Charge Transfer Properties of Ï€â€Conjugated System with Different Combinations of Thiophene and Vinyl/Butadiene. Chinese Journal of Chemistry, 2012, 30, 2501-2508.	4.9	2
76	Single-layer assembly of pyrene end-capped terthiophene and its sensing performances to nitroaromatic explosives. Journal of Materials Chemistry, 2012, 22, 1069-1077.	6.7	69
77	Water-catalyzed gas-phase hydrogen abstraction reactions of CH3O2 and HO2 with HO2: a computational investigation. Physical Chemistry Chemical Physics, 2011, 13, 20794.	2.8	42
78	Computational study on the reaction of CH3SCH2CH3 with OH radical: mechanism and enthalpy of formation. Theoretical Chemistry Accounts, 2011, 129, 771-780.	1.4	17
79	Computational study on the mechanism for the gasâ€phase reaction of dimethyl disulfide with OH. International Journal of Quantum Chemistry, 2011, 111, 644-651.	2.0	13
80	Direct dynamics study on mechanism and kinetics of the biradical selfâ€reaction of HOO. International Journal of Quantum Chemistry, 2011, 111, 3029-3039.	2.0	13
81	Theoretical Studies on the Electronic Structures and Optical Properties of Triâ€aryl Endâ€capped Terthiophene Derivatives. Chinese Journal of Chemistry, 2010, 28, 1907-1914.	4.9	3
82	Direct dynamics study on the mechanism and the kinetics of the reaction of CH₃NH₂ with OH. International Journal of Quantum Chemistry, 2009, 109, 1566-1575.	2.0	24
83	A 3D interpenetrating supramolecular compound based on Cu Â·Â·Â· N weak coordination: synthesis, crystal structure and DFT investigation. Journal of Coordination Chemistry, 2008, 61, 2916-2925.	2.2	3
84	Oligomerization Reactions of Criegee Intermediates with Hydroxyalkyl Hydroperoxides: Mechanism, Kinetics, and Structure-Reactivity Relationship. Atmospheric Chemistry and Physics Discussions, 0, , 1-35.	1.0	3
85	Efficient improvement of W05â€based dyes by inserting auxiliary electron acceptors for dyeâ€sensitized solar cells: A theoretical investigation. Journal of Physical Organic Chemistry, 0, , e4290.	1.9	1
86	Effect of methyl hydrogen sulfate on the formation of sulfuric acidâ€ammonia clusters: A theoretical study. Journal of the Chinese Chemical Society, 0, , .	1.4	0