Lin Ming-chang

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/9078697/publications.pdf

Version: 2024-02-01

221 papers	7,781 citations	46918 47 h-index	74018 75 g-index
221 all docs	221 docs citations	221 times ranked	6694 citing authors

#	Article	IF	Citations
1	Modification of the gaussianâ^'2 theoretical model: The use of coupledâ€cluster energies, densityâ€functional geometries, and frequencies. Journal of Chemical Physics, 1995, 103, 7414-7421.	1.2	468
2	Carbon-doped SnS2 nanostructure as a high-efficiency solar fuel catalyst under visible light. Nature Communications, 2018, 9, 169.	5.8	350
3	From Ni-YSZ to sulfur-tolerant anode materials for SOFCs: electrochemical behavior, in situ characterization, modeling, and future perspectives. Energy and Environmental Science, 2011, 4, 4380.	15.6	280
4	Ab Initio and RRKM Calculations for Multichannel Rate Constants of the C2H3+ O2Reaction. Journal of the American Chemical Society, 1996, 118, 9759-9771.	6.6	161
5	A Theoretical Study of Surface Reduction Mechanisms of CeO2(111) and (110) by H2. ChemPhysChem, 2007, 8, 849-855.	1.0	142
6	Oxygen Reduction on LaMnO3-Based Cathode Materials in Solid Oxide Fuel Cells. Chemistry of Materials, 2007, 19, 1690-1699.	3.2	126
7	Thermal decomposition of ethanol. I. Ab Initio molecular orbital/Riceâ€“Ramspergerâ€“Kasselâ€“Marcus prediction of rate constant and product branching ratios. Journal of Chemical Physics, 2002, 117, 3224-3231.	1.2	125
8	Extremely rapid self-reaction of the simplest Criegee intermediate CH2OO and its implications in atmospheric chemistry. Nature Chemistry, 2014, 6, 477-483.	6.6	125
9	Mechanism of Ethanol Reforming: Theoretical Foundations. Journal of Physical Chemistry C, 2009, 113, 6681-6688.	1.5	118
10	Niâ€Nanocluster Modified Black TiO₂ with Dual Active Sites for Selective Photocatalytic CO₂ Reduction. Small, 2018, 14, 1702928.	5.2	116
11	Vitalizing fuel cells with vitamins: pyrolyzed vitamin B12 as a non-precious catalyst for enhanced oxygen reduction reaction of polymer electrolyte fuel cells. Energy and Environmental Science, 2012, 5, 5305-5314.	15.6	115
12	Roaming-mediated isomerization in the photodissociation of nitrobenzene. Nature Chemistry, 2011, 3, 932-937.	6.6	110
13	A density functional study of the global potential energy surfaces of the [H,C,N,O] system in singlet and triplet states. Journal of Chemical Physics, 1996, 105, 6439-6454.	1.2	105
14	Computational Study on the Catalytic Mechanism of Oxygen Reduction on La_{0.5}Sr_{0.5}MnO₃ in Solid Oxide Fuel Cells. Angewandte Chemie - International Edition, 2007, 46, 7214-7219.	7.2	101
15	Experimental and reduced dimensionality quantum rate coefficients for H2(D2)+CNâ†'H(D)CN+H(D). Journal of Chemical Physics, 1990, 93, 4730-4739.	1.2	89
16	Kinetics and Mechanism of the OH + C6H6Reaction:Â A Detailed Analysis with First-Principles Calculations. Journal of Physical Chemistry A, 2002, 106, 11309-11326.	1.1	89
17	A simple pyrene based AIEE active schiff base probe for selective naked eye and fluoresence offâ€“on detection of trivalent cations with live cell application. Sensors and Actuators B: Chemical, 2016, 231, 18-29.	4.0	89
18	Abinitiomolecular orbital study of the HCO+O2reaction: Direct versus indirect abstraction channels. Journal of Chemical Physics, 1996, 105, 2346-2352.	1.2	82

#	Article	IF	Citations
19	Composition of SiCN crystals consisting of a predominantly carbon-nitride network. Journal of Materials Research, 1997, 12, 322-325.	1.2	80
20	Ab Initio MO Study of the Unimolecular Decomposition of the Phenyl Radical. Journal of Physical Chemistry A, 1997, 101, 6790-6797.	1.1	77
21	Experimental and Theoretical Studies of the Reaction of the Phenyl Radical with Methane. Journal of Physical Chemistry A, 1999, 103, 3636-3645.	1.1	76
22	Unimolecular isomerization/decomposition of cyclopentadienyl and related bimolecular reverse process:ab initio MO/statistical theory study. Journal of Computational Chemistry, 2000, 21, 415-425.	1.5	74
23	Computational Study on the Kinetics and Mechanisms for the Unimolecular Decomposition of Formic and Oxalic Acidsâ€. Journal of Physical Chemistry A, 2007, 111, 6789-6797.	1.1	73
24	A Computational Study of the OH(OD) + CO Reactions:Â Effects of Pressure, Temperature, and Quantum-Mechanical Tunneling on Product Formation. Journal of Physical Chemistry A, 2001, 105, 11249-11259.	1.1	72
25	Novel pyrene containing monomeric and dimeric supramolecular AIEE active nano-probes utilized in selective â€œoffâ€“onâ€•trivalent metal and highly acidic pH sensing with live cell applications. Journal of Materials Chemistry C, 2016, 4, 2056-2071.	2.7	71
26	Nitromethaneâ^'Methyl Nitrite Rearrangement:Â A Persistent Discrepancy between Theory and Experiment. Journal of Physical Chemistry A, 2003, 107, 4286-4291.	1.1	70
27	Computational study on the reactions of H₂O₂ on TiO₂ anatase (101) and rutile (110) surfaces. Journal of Computational Chemistry, 2011, 32, 1065-1081.	1.5	64
28	Ab initiostudy of the CH3+O2 reaction: Kinetics, mechanism and product branching probabilities. Journal of Chemical Physics, 2001, 115, 195-203.	1.2	63
29	Density Functional Theory Study of the Adsorption and Reaction of H₂S on TiO₂ Rutile (110) and Anatase (101) Surfaces. Journal of Physical Chemistry C, 2009, 113, 20411-20420.	1.5	61
30	A shock tube study of the CH2O + NO2 reaction at high temperatures. International Journal of Chemical Kinetics, 1990, 22, 455-482.	1.0	60
31	Prediction of O2 Dissociation Kinetics on LaMnO3-Based Cathode Materials for Solid Oxide Fuel Cells. Journal of Physical Chemistry C, 2009, 113, 7290-7297.	1.5	57
32	Thermal decomposition of ethanol. II. A computational study of the kinetics and mechanism for the H+C2H5OH reaction. Journal of Chemical Physics, 2003, 118, 9990-9996.	1.2	56
33	Ab initio study of the OH + CH2O reaction: The effect of the OHÂ·Â·OCH2 complex on the H-abstraction kinetics. International Journal of Chemical Kinetics, 2006, 38, 322-326.	1.0	54
34	KSCN-induced Interfacial Dipole in Black TiO₂ for Enhanced Photocatalytic CO₂ Reduction. ACS Applied Materials & Interfaces, 2019, 11, 25186-25194.	4.0	54
35	Pyrene-Based AIEE Active Nanoprobe for Zn²⁺ and Tyrosine Detection Demonstrated by DFT, Bioimaging, and Organic Thin-Film Transistor. ACS Applied Materials & Interfaces, 2021, 13, 28610-28626.	4.0	53
36	Theoretical study of the thermal isomerization of fulvene to benzene. Journal of Physical Organic Chemistry, 1996, 9, 801-810.	0.9	52

#	Article	IF	Citations
37	Theoretical interpretation of the kinetics and mechanisms of the HNO + HNO and HNO + 2NO reactions with a unified model. International Journal of Chemical Kinetics, 1992, 24, 489-516.	1.0	51
38	Laserâ€assisted chemical vapor deposition of InN on Si(100). Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films, 1993, 11, 2931-2937.	0.9	51
39	Direct Synthesis of Zr-Doped Ceria Nanotubes. Journal of Physical Chemistry C, 2009, 113, 5031-5034.	1.5	51
40	Absolute rate constant for the reaction of Phenyl radical with Acetylene. International Journal of Chemical Kinetics, 1994, 26, 1095-1104.	1.0	50
41	Rate Constant of the HONO + HONO â†' H2O + NO + NO2 Reaction from ab Initio MO and TST Calculations. Journal of Physical Chemistry A, 1998, 102, 1803-1807.	1.1	50
42	Thermal decomposition of iso-propanol: First-principles prediction of total and product-branching rate constants. Journal of Chemical Physics, 2002, 117, 11188-11195.	1.2	50
43	Combined Quantum Chemical/RRKM-ME Computational Study of the Phenyl + Ethylene, Vinyl + Benzene, and H + Styrene Reactionsâ€. Journal of Physical Chemistry A, 2004, 108, 9697-9714.	1.1	50
44	Ab initio molecular orbital study of potential energy surface for the reaction of C2H3 with H2 and related reactions. Journal of Chemical Physics, 1995, 103, 3440-3449.	1.2	49
45	Direct Determination of Product Branching for the NH2+ NO Reaction at Temperatures between 302 and 1060 K. The Journal of Physical Chemistry, 1996, 100, 3317-3319.	2.9	49
46	Kinetics for the Recombination of Phenyl Radicals. Journal of Physical Chemistry A, 1997, 101, 14-18.	1.1	49
47	Experimental and Theoretical Studies of the C6H5+ C6H6Reaction. Journal of Physical Chemistry A, 1999, 103, 9036-9041.	1.1	49
48	Laser-Initiated NO Reduction by NH3:â€‰ Total Rate Constant and Product Branching Ratio Measurements for the NH2 + NO Reaction. Journal of Physical Chemistry A, 1997, 101, 5-13.	1.1	48
49	Potassium-Presenting Zinc Oxide Surfaces Induce Vertical Phase Separation in Fullerene-Free Organic Photovoltaics. Nano Letters, 2020, 20, 715-721.	4.5	48
50	Theoretical Rate Constants for the NH3+ NOxâ†' NH2+ HNOx(x= 1, 2) Reactions by ab Initio MO/VTST Calculations. The Journal of Physical Chemistry, 1996, 100, 7517-7525.	2.9	47
51	Acid/Base and H₂PO₄^{â€“} Controllable High-Contrast Optical Molecular Switches with a Novel BODIPY Functionalized [2]Rotaxane. ACS Applied Materials & Interfaces, 2015, 7, 26491-26503.	4.0	47
52	Novel rhodamine probe for colorimetric and fluorescent detection of Fe3+ ions in aqueous media with cellular imaging. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2020, 242, 118757.	2.0	47
53	A Mass Spectrometric Study of the NH2+ NO2Reaction. Journal of Physical Chemistry A, 1997, 101, 2643-2647.	1.1	45
54	Ab initiostudies of ClOx reactions. IV. Kinetics and mechanism for the self-reaction of ClO radicals. Journal of Chemical Physics, 2003, 118, 4094-4106.	1.2	45

#	Article	IF	Citations
55	Methylammonium Tin Tribromide Quantum Dots for Heavy Metal Ion Detection and Cellular Imaging. ACS Applied Nano Materials, 2022, 5, 2859-2874.	2.4	45
56	Ab initio study of the oxidation of NCN by O2. International Journal of Chemical Kinetics, 2005, 37, 593-598.	1.0	44
57	Adsorption Configurations and Reactions of Boric Acid on a TiO₂ Anatase (101) Surface. Journal of Physical Chemistry C, 2008, 112, 8276-8287.	1.5	44
58	Metal-free four-in-one modification of g-C3N4 for superior photocatalytic CO2 reduction and H2 evolution. Chemical Engineering Journal, 2022, 430, 132853.	6.6	44
59	Effect of Roaming Transition States upon Product Branching in the Thermal Decomposition of CH₃NO₂. Journal of Physical Chemistry A, 2013, 117, 7308-7313.	1.1	43
60	Ab Initio Kinetics for Decomposition/Isomerization Reactions of C₂H₅O Radicals. ChemPhysChem, 2009, 10, 972-982.	1.0	42
61	Implications of the HCN ? HNC process to high-temperature nitrogen-containing fuel chemistry. International Journal of Chemical Kinetics, 1992, 24, 1103-1107.	1.0	41
62	Ab Initio Study of the H + HONO Reaction:â€‰ Direct Abstraction versus Indirect Exchange Processes. Journal of Physical Chemistry A, 1997, 101, 60-66.	1.1	40
63	The NCO + NO Reaction Revisited:Â Ab Initio MO/VRRKM Calculations for Total Rate Constant and Product Branching Ratios. Journal of Physical Chemistry A, 2000, 104, 10807-10811.	1.1	40
64	Facile rhodamine-based colorimetric sensors for sequential detections of Cu(<scp>ii</scp>) ions and pyrophosphate (P₂O₇^{4â^'}) anions. RSC Advances, 2016, 6, 106631-106640.	1.7	40
65	Experimental and Theoretical Studies of the Unimolecular Decomposition of Nitrosobenzene:Â High-Pressure Rate Constants and the Câ^'N Bond Strength. Journal of Physical Chemistry A, 1997, 101, 6043-6047.	1.1	39
66	Ab initio study of the HO2+NO reaction: Prediction of the total rate constant and product branching ratios for the forward and reverse processes. Journal of Chemical Physics, 2003, 119, 10667-10677.	1.2	39
67	Sublimation of Ammonium Salts:â€‰ A Mechanism Revealed by a First-Principles Study of the NH₄Cl System. Journal of Physical Chemistry C, 2007, 111, 13831-13838.	1.5	38
68	An ab initio molecular orbital study of potential energy surface of the NH2+NO2 reaction. Journal of Chemical Physics, 1995, 103, 5640-5649.	1.2	37
69	Ab initio studies of ClOx reactions. VIII. Isomerization and decomposition of ClO2 radicals and related bimolecular processes. Journal of Chemical Physics, 2003, 119, 2075-2082.	1.2	37
70	Monomeric and aggregation emissions of tetraphenylethene in a photo-switchable polymer controlled by cyclization of diarylethene and solvent conditions. Journal of Materials Chemistry C, 2017, 5, 9952-9962.	2.7	37
71	Kinetics of the reaction of C6H5 with HBr. International Journal of Chemical Kinetics, 1993, 25, 875-880.	1.0	36
72	Computational Chemical Kinetics for the Reaction of Criegee Intermediate CH₂OO with HNO₃ and Its Catalytic Conversion to OH and HCO. Journal of Physical Chemistry A, 2017, 121, 3871-3878.	1.1	36

#	Article	IF	Citations
73	Quantum chemical elucidation of the mechanism for hydrogenation of TiO2 anatase crystals. Journal of Chemical Physics, 2013, 138, 154705.	1.2	35
74	A novel and facile decay path of Criegee intermediates by intramolecular insertion reactions via roaming transition states. Journal of Chemical Physics, 2015, 142, 124312.	1.2	35
75	Development of Hybrid Pseudohalide Tin Perovskites for Highly Stable Carbon-Electrode Solar Cells. ACS Applied Materials & Interfaces, 2020, 12, 21739-21747.	4.0	35
76	Ab initio molecular orbital study of potential energy surface for the NH+NO2 reaction. Journal of Chemical Physics, 1994, 101, 3916-3922.	1.2	34
77	Kinetics and Mechanism for the Reaction of Phenyl Radical with Formaldehyde. Journal of Physical Chemistry A, 2000, 104, 7030-7035.	1.1	34
78	Ab Initio Studies of ClOx Reactions: Prediction of the Rate Constants of ClO+NO for the Forward and Reverse Processes. ChemPhysChem, 2004, 5, 1864-1870.	1.0	34
79	Kinetics of CN reactions with N2O and CO2. International Journal of Chemical Kinetics, 1991, 23, 151-160.	1.0	33
80	A Comprehensive Kinetic Study of Thermal Reduction of NO2by H2. Journal of Physical Chemistry A, 1998, 102, 10099-10105.	1.1	33
81	Theoretical studies of nitroamino radical reactions: Rate constants for the unimolecular decomposition of HNNO2 and related bimolecular processes. Journal of Chemical Physics, 1998, 109, 8887-8896.	1.2	33
82	Computational Study of the HCCO + NO Reaction:Â ab Initio MO/vRRKM Calculations of the Total Rate Constant and Product Branching Ratios. Journal of Physical Chemistry A, 2003, 107, 1066-1076.	1.1	32
83	Ab Initio Chemical Kinetics for the Hydrolysis of N₂O₄ Isomers in the Gas Phase. Journal of Physical Chemistry A, 2012, 116, 4466-4472.	1.1	32
84	Ab initio studies of ClOx reactions. I. Kinetics and mechanism for the OH+ClO reaction. Journal of Chemical Physics, 2002, 116, 7452-7460.	1.2	31
85	Novel anthracene- and pyridine-containing Schiff base probe for selective â€œoffâ€“onâ€•fluorescent determination of Cu²⁺ ions towards live cell application. New Journal of Chemistry, 2016, 40, 6101-6108.	1.4	31
86	Novel Bimolecular Reactions between NH3 and HNO3 in the Gas Phase. Journal of Physical Chemistry A, 1998, 102, 1808-1814.	1.1	30
87	Computational Study on the Energetics of NCN Isomers and the Kinetics of the C + N2â‡„ N + CN Reaction. Journal of Physical Chemistry A, 2001, 105, 4156-4163.	1.1	30
88	Thermal unimolecular decomposition of 1,3,5-trioxane: Comparison of theory and experiment. International Journal of Chemical Kinetics, 1991, 23, 947-956.	1.0	29
89	Thermal reaction of HNCO with NO2 at moderate temperatures. International Journal of Chemical Kinetics, 1993, 25, 845-863.	1.0	29
90	Adsorption and Dissociation of H₂O on a W(111) Surface:â€‰ A Computational Study. Journal of Physical Chemistry C, 2007, 111, 17333-17339.	1.5	29

#	Article	IF	Citations
91	Ab initio molecular orbital study of the O + C6H5O reaction. Journal of Physical Organic Chemistry, 1995, 8, 407-420.	0.9	28
92	Ab Initio Studies of ClOx Reactions:â€‰ VI. Theoretical Prediction of Total Rate Constant and Product Branching Probabilities for the HO2 + ClO Reaction. Journal of Physical Chemistry A, 2003, 107, 3841-3850.	1.1	28
93	Effects of nitric oxide on the thermal decomposition of methyl nitrite: Overall kinetics and rate constants for the HNO + HNO and HNO + 2NO reactions. International Journal of Chemical Kinetics, 1992, 24, 743-760.	1.0	27
94	Mechanism and Kinetics for Ammonium Perchlorate Sublimation: A First-principles Study. Journal of Physical Chemistry C, 2008, 112, 14481-14485.	1.5	27
95	Quantum Chemical Prediction of Pathways and Rate Constants for Reactions of CO and CO2 with Vacancy Defects on Graphite (0001) Surfaces. Journal of Physical Chemistry C, 2009, 113, 18772-18777.	1.5	27
96	FTIR and Mass-Spectrometric Measurements of the Rate Constant for the C6H5 + H2 Reaction. Journal of Physical Chemistry A, 1997, 101, 8839-8843.	1.1	26
97	Development of Novel Mixed Halide/Superhalide Tin-Based Perovskites for Mesoscopic Carbon-Based Solar Cells. Journal of Physical Chemistry Letters, 2020, 11, 2443-2448.	2.1	26
98	Thermal reduction of NO by H2: Kinetic measurement and computer modeling of the HNO + NO reaction. International Journal of Chemical Kinetics, 1995, 27, 867-881.	1.0	25
99	Product Branching Ratios in the NH2+ NO Reaction:Â A Re-Evaluation. Journal of Physical Chemistry A, 1999, 103, 8906-8907.	1.1	25
100	Kinetics of C6H5 Radical Reactions with Toluene and Xylenes by Cavity Ringdown Spectrometry. Journal of Physical Chemistry A, 1999, 103, 4002-4008.	1.1	25
101	Theoretical study of reactions of N2O with NO and OH radicals. International Journal of Chemical Kinetics, 1996, 28, 693-703.	1.0	24
102	Experimental and Computational Studies of the Phenyl Radical Reaction with Propyne. ChemPhysChem, 2005, 6, 2075-2085.	1.0	24
103	Experimental and theoretical investigation of rate coefficients of the reaction S(P3)+OCS in the temperature range of 298â€“985K. Journal of Chemical Physics, 2006, 125, 164329.	1.2	24
104	Kinetics of the reaction of C6H5 with HBr and DBr. International Journal of Chemical Kinetics, 1994, 26, 771-778.	1.0	23
105	Kinetics and mechanisms for reactions of HNO with CH3 and C6 H5 studied by quantum-chemical and statistical-theory calculations. International Journal of Chemical Kinetics, 2005, 37, 261-274.	1.0	23
106	Ab Initio Chemical Kinetics for the CH₃ + O(³P) Reaction and Related Isomerizationâ€“Decomposition of CH₃O and CH₂OH Radicals. Journal of Physical Chemistry A, 2015, 119, 7404-7417.	1.1	23
107	The thermal reaction of HNCO at moderate temperatures. International Journal of Chemical Kinetics, 1991, 23, 1129-1149.	1.0	22
108	Kinetics and mechanism for the CH2O + NO2 reaction: A computational study. International Journal of Chemical Kinetics, 2003, 35, 184-190.	1.0	22

#	Article	IF	Citations
109	Low-Pressure Organometallic Chemical Vapor Deposition of Indium Nitride on Titanium Dioxide Nanoparticles. ChemPhysChem, 2004, 5, 1615-1618.	1.0	22
110	Mass-spectrometric determination of product branching probabilities for the NH2 + NO2 reaction at temperatures between 300 and 990 K. International Journal of Chemical Kinetics, 1996, 28, 879-883.	1.0	21
111	Adsorption and Thermal Decomposition of Acetaldehyde on Si(111)-7Ã—7. Journal of Physical Chemistry B, 1997, 101, 1872-1877.	1.2	21
112	Quantum chemical/vRRKM study on the thermal decomposition of cyclopentadiene. International Journal of Chemical Kinetics, 2004, 36, 139-151.	1.0	21
113	Ab Initio Chemical Kinetic Study for Reactions of H Atoms with SiH₄ and Si₂H₆: Comparison of Theory and Experiment. Journal of Physical Chemistry A, 2010, 114, 633-639.	1.1	21
114	Photodissociation Dynamics of Benzaldehyde (C₆H₅CHO) at 266, 248, and 193â€…nm. Chemistry - an Asian Journal, 2011, 6, 2961-2976.	1.7	21
115	A novel mechanism for the isomerization of N₂O₄ and its implication for the reaction with H₂O and acid rain formation. International Journal of Quantum Chemistry, 2018, 118, e25560.	1.0	21
116	Distinct Nanostructures and Organogel Driven by Reversible Molecular Switching of a Tetraphenylethene-Involved Calix[4]arene-Based Amphiphilic [2]Rotaxane. Chemistry of Materials, 2018, 30, 7221-7233.	3.2	21
117	The Reaction of C6H5with CO:Â Kinetic Measurement and Theoretical Correlation with the Reverse Process. Journal of Physical Chemistry A, 2000, 104, 1233-1239.	1.1	20
118	Adsorption Configurations and Reactions of Nitric Acid on TiO₂ Rutile (110) and Anatase (101) surfaces. Journal of Physical Chemistry C, 2009, 113, 6140-6149.	1.5	20
119	Rate constant for the NH3 + NO2 ? NH2 + HONO reaction: Comparison of kinetically modeled and predicted results. International Journal of Chemical Kinetics, 1997, 29, 245-251.	1.0	19
120	Experimental and Computational Studies of the Kinetics and Mechanisms for C6H5Reactions with Acetone-h6and -d6. Journal of Physical Chemistry A, 2003, 107, 7755-7761.	1.1	19
121	Ab Initio Studies of ClOxReactions. 3. Kinetics and Mechanism for the OH + OClO Reaction. Journal of Physical Chemistry A, 2003, 107, 1040-1049.	1.1	19
122	Ab initio Studies of ClOx Reactions: Prediction of the Rate Constants of ClO+NO2 for the Forward and Reverse Processes. ChemPhysChem, 2005, 6, 1514-1521.	1.0	19
123	Ab initio chemical kinetics for the NH₂ + HNO_x Reactions, Part I: Kinetics and Mechanism for NH₂ + HNO. International Journal of Chemical Kinetics, 2009, 41, 667-677.	1.0	19
124	Ab initio chemical kinetics for reactions of H atoms with SiH_x (x =) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 5 Chemistry, 2013, 113, 1735-1746.	1.0	19
125	Simultaneous Production and Surface Functionalization of Silver Nanoparticles for Label-free Colorimetric Detection of Copper Ion. Analytical Sciences, 2017, 33, 1115-1121.	0.8	19
126	Diversiform Nanostructures Constructed from Tetraphenylethene and Pyrene-Based Acid/Base Controllable Molecular Switching Amphiphilic [2]Rotaxanes with Tunable Aggregation-Induced Static Excimers. ACS Applied Materials & Interfaces, 2020, 12, 45222-45234.	4.0	19

#	Article	IF	Citations
127	Ab initio MO and TST calculations for the rate constant of the HNO+NO2?HONO+NO reaction. International Journal of Chemical Kinetics, 1998, 30, 729-736.	1.0	18
128	A Model Study of COâ^'CO Adsorbate Interaction on Si(100)-2Ã—1. Journal of Physical Chemistry B, 1999, 103, 7270-7276.	1.2	17
129	Kinetic Studies of Aromatic Radical Reactions by Cavity-Ringdown Spectroscopy. ACS Symposium Series, 1999, , 196-209.	0.5	17
130	Synergistic Effect of Hydrogenation and Thiocyanate Treatments on Ag-Loaded TiO₂ Nanoparticles for Solar-to-Hydrogen Conversion. Journal of Physical Chemistry C, 2017, 121, 9681-9690.	1.5	17
131	Novel supramolecular conjugated polyrotaxane as an acid-base controllable optical molecular switch. Sensors and Actuators B: Chemical, 2017, 243, 84-95.	4.0	17
132	Theoretical Study of the NH2+ C2H2Reaction. Journal of Physical Chemistry A, 1998, 102, 4687-4693.	1.1	16
133	Kinetics and mechanism for the H-for-X exchange process in the H + C6H5X reactions: A computational study. International Journal of Chemical Kinetics, 2001, 33, 633-653.	1.0	16
134	A computational study of the kinetics and mechanism for the reaction of HCO with HNO. International Journal of Chemical Kinetics, 2004, 36, 205-215.	1.0	16
135	A dihydrogen phosphate selective anion receptor based on acylhydrazone and pyrazole. New Journal of Chemistry, 2015, 39, 650-658.	1.4	16
136	A Theoretical and Experimental Study of the CN + NO Association Reaction. Journal of Physical Chemistry A, 1998, 102, 6973-6980.	1.1	15
137	Kinetic modeling of benzene decomposition near 1000 K: The effects of toluene impurity. International Journal of Chemical Kinetics, 1999, 31, 577-582.	1.0	15
138	Kinetics of C6H5 radical reactions with 2-methylpropane, 2,3-dimethylbutane and 2,3,4-trimethylpentane. International Journal of Chemical Kinetics, 1999, 31, 645-653.	1.0	15
139	Ab Initio Studies of ClOx Reactions. 2. Unimolecular Decomposition of s-ClO3 and the Bimolecular O + OClO Reaction. Journal of Physical Chemistry A, 2002, 106, 8386-8390.	1.1	15
140	Ab initiostudies of ClOx reactions. VII. Isomers of Cl2O3 and their roles in the ClO+OClO reaction. Journal of Chemical Physics, 2003, 118, 8645-8655.	1.2	15
141	Reaction Dynamics of O(¹D,³P) + OCS Studied with Time-Resolved Fourier Transform Infrared Spectroscopy and Quantum Chemical Calculations. Journal of Physical Chemistry A, 2009, 113, 13260-13272.	1.1	15
142	Ab Initio Chemical Kinetics for the Reaction of an H Atom with Si₃H₈. Journal of Physical Chemistry A, 2010, 114, 3642-3648.	1.1	15
143	Application of stimuli-responsive FRET behavior toward cyanide detection in a photo-switchable [2]pseudorotaxane polymer containing the BODIPY donor and the merocyanine acceptor. Journal of Materials Chemistry C, 2021, 9, 2321-2333.	2.7	15
144	KSCN-activation of hydrogenated NiO/TiO2 for enhanced photocatalytic hydrogen evolution. Applied Surface Science, 2020, 511, 145548.	3.1	15

#	Article	IF	Citations
145	Theoretical Studies of Methyleneamino (CH2N) Radical Reactions. 1. Rate Constants and Product Branching Ratios for the CH2N + N2O Process by ab Initio Molecular Orbital/Statistical Theory Calculations. Journal of Physical Chemistry A, 1999, 103, 601-606.	1.1	14
146	Hydrogen-bonded effects on supramolecular blue phase liquid crystal dimeric complexes. RSC Advances, 2015, 5, 54629-54637.	1.7	14
147	Thermal decomposition of N₂O near 900 K studied by FTIR spectrometry: Comparison of experimental and theoretical O(³P) formation kinetics. International Journal of Chemical Kinetics, 2020, 52, 632-644.	1.0	14
148	Ab Initio Studies of ClOx Radical Reactions:â€‰ V. Evidence for a New Path in the Cl + ClOOCl Reaction. Journal of Physical Chemistry A, 2003, 107, 3836-3840.	1.1	13
149	Kinetics and Mechanism of the C6H5+ CH3CHO Reaction: Experimental Measurement and Theoretical Prediction of the Reactivity toward Four Molecular Sites. ChemPhysChem, 2004, 5, 661-668.	1.0	13
150	Homogeneous pyrolysis of acetylacetone at high temperatures in shock waves. International Journal of Chemical Kinetics, 1990, 22, 491-504.	1.0	12
151	Ab initio chemical kinetics for the NH₂ + HNO_x reactions, part II: Kinetics and mechanism for NH₂ + HONO. International Journal of Chemical Kinetics, 2009, 41, 678-688.	1.0	12
152	Kinetic Study of the C₁₀H₇ + O₂ Reaction. Journal of Physical Chemistry A, 2009, 113, 5348-5354.	1.1	12
153	Observation of Significant enhancement in the efficiency of a DSSC by InN nanoparticles over TiO2-nanoparticle films. Chemical Physics Letters, 2011, 510, 126-130.	1.2	12
154	Novel asymmetrical single- and double-chiral liquid crystal diads with wide blue phase ranges. RSC Advances, 2015, 5, 4615-4622.	1.7	12
155	Computational and experimental studies on the effect of hydrogenation of Ni-doped TiO₂ anatase nanoparticles for the application of water splitting. RSC Advances, 2015, 5, 81371-81377.	1.7	12
156	A Model Calculation for the Isomerization and Decomposition of Chemisorbed HCN on the Si(100)â€2Ã—1 Surface. Journal of the Chinese Chemical Society, 1999, 46, 395-402.	0.8	11
157	Computational study on the kinetics and mechanisms for the reactions of HCO with HONO and HNOH. International Journal of Chemical Kinetics, 2004, 36, 178-187.	1.0	11
158	Adsorption and Reaction of C2N2on Si(100)-2 Ã— 1:Â A Computational Study with Single- and Double-Dimer Cluster Models. Journal of Physical Chemistry B, 2004, 108, 9189-9197.	1.2	11
159	Adsorption Configurations and Decomposition Pathways of Boric Acid on TiO2 Rutile (110) Surface: A Computational Study. Journal of Physical Chemistry C, 2009, 113, 3751-3762.	1.5	11
160	Infrared Emission from Photodissociation of Methyl Formate [HC(O)OCH₃] at 248 and 193 nm: Absence of Roaming Signature. Journal of Physical Chemistry A, 2019, 123, 6130-6143.	1.1	11
161	Effective hydrogenation of TiO2 photocatalysts with CH3OH for enhanced water splitting: A computational and X-ray study. Applied Surface Science, 2019, 488, 546-554.	3.1	11
162	Kinetics of CN radical reactions with formaldehyde and 1,3,5-trioxane. International Journal of Chemical Kinetics, 1993, 25, 1053-1064.	1.0	10

#	Article	IF	Citations
163	A computational study of the mechanism for the C6H5+CH2O reaction. Physical Chemistry Chemical Physics, 2000, 2, 5566-5570.	1.3	10
164	H2O-catalyzed formation of O3in the self-reaction of HO2: a computational study on the effect of nH2O (nâ€‰=â€‰1â€“3). PhysChemComm, 2003, 6, 51-54.	0.8	10
165	Ab initio studies of ClOx reactions. IX. Combination and disproportionation reactions of ClO and s-ClO3 radicals. Journal of Chemical Physics, 2003, 119, 8897-8904.	1.2	10
166	Density Functional Studies of the Adsorption and Dissociation of NO_x (x = 1,) Tj ETQq0 0 0 rgBT /Overlock 10	1.5	10
167	Ab Initio Chemical Kinetics for SiH₂ + Si₂H₆ and SiH₃ + Si₂H₅ Reactions and the Related Unimolecular Decomposition of Si₃H₈ under a-Si/H CVD Conditions. Journal of Physical Chemistry A, 2013, 117, 10811-10823.	1.1	10
168	Ab Initio Chemical Kinetics of Key Processes in the Hypergolic Ignition of Hydrazine and Nitrogen Tetroxide. Advances in Quantum Chemistry, 2014, 69, 253-301.	0.4	10
169	Multi-stimuli-responsive high contrast fluorescence molecular controls with a far-red emitting BODIPY-based [2]rotaxane. Sensors and Actuators B: Chemical, 2018, 270, 382-395.	4.0	10
170	Computational Study on the Mechanisms and Rate Constants for the O(³P,¹D) + OCS Reactions. Journal of Physical Chemistry A, 2019, 123, 8358-8364.	1.1	10
171	Acidâ€“base controllable nanostructures and the fluorescence detection of H₂PO₄^â by the molecular shuttling of tetraphenylethene-based [2]rotaxanes. Journal of Materials Chemistry C, 2021, 9, 3215-3228.	2.7	10
172	Synergistic Effects of Plasmonic Gold and Perovskite-Type SrTiO₃ for Enhanced Photocatalytic Performance of TiO₂ Nanotube Arrays. Journal of Physical Chemistry C, 2021, 125, 24340-24349.	1.5	10
173	Formation and Decomposition of Phenylvinylperoxy Radicals in the Reaction: C6H5C2H2+O2. ChemPhysChem, 2004, 5, 1231-1234.	1.0	9
174	Kinetics of phenyl radical reactions with propane,n-butane,n-hexane, andn-octane: Reactivity of C6H5 toward the secondary C?H bond of alkanes. International Journal of Chemical Kinetics, 2004, 36, 49-56.	1.0	9
175	Computational Study on the Mechanism and Rate Constant for the C6H5+ C6H5NO Reaction. Journal of Physical Chemistry A, 2005, 109, 9054-9060.	1.1	9
176	Synthesis of In(OH)3 and In2O3 nanomaterials incorporating Au. Journal of Materials Science, 2009, 44, 794-798.	1.7	9
177	Kinetic modeling of the CH3 + C2H2 reaction data with sensitivity analyses. International Journal of Chemical Kinetics, 1995, 27, 855-866.	1.0	8
178	Kinetics of phenyl radical reactions with ethane and neopentane: Reactivity of C6H5 toward the primary C-H bond of alkanes. International Journal of Chemical Kinetics, 2001, 33, 64-69.	1.0	8
179	Kinetics and Mechanisms for the Reactions of Phenyl Radical with Ketene and its Deuterated Isotopomer: An Experimental and Theoretical Study. ChemPhysChem, 2004, 5, 225-232.	1.0	8
180	Ab initio kinetic prediction of branching rate constants for reactions of H atoms with CH₃O and CH₂OH. Molecular Physics, 2007, 105, 2763-2776.	0.8	8

#	Article	IF	Citations
181	Ab Initio Chemical Kinetics for SiH₃ Reactions with Si_xH_{2x+2} (x = 1â"4). Journal of Physical Chemistry A, 2010, 114, 13353-13361.	1.1	8
182	Ab initio chemical kinetics for the HCCO + OH reaction. Chemical Physics Letters, 2014, 592, 175-181.	1.2	8
183	Isomerization of N2O4in Solid N2H4and Its Implication for the Explosion of N2O4â€"N2H4Solid Mixtures. Journal of Physical Chemistry C, 2018, 122, 23501-23505.	1.5	8
184	Effects of temperature and lithium on CH3 radical formation in the CH4 oxidative coupling reaction over MgO. International Journal of Chemical Kinetics, 1990, 22, 975-980.	1.0	7
185	The Adsorption and Thermal Decomposition of CH₂CO (CD₂CO) on Si(111)â€7 Ã— 7. Journal of the Chinese Chemical Society, 1995, 42, 309-316.	0.8	7
186	Quantum Chemical Prediction of Reaction Pathways and Rate Constants for Reactions of NO and NO₂ with Monovacancy Defects on Graphite (0001) Surfaces. Journal of Physical Chemistry C, 2010, 114, 8375-8382.	1.5	7
187	Reaction dynamics of O(1D) + HCOOD/DCOOH investigated with time-resolved Fourier-transform infrared emission spectroscopy. Journal of Chemical Physics, 2014, 141, 154313.	1.2	7
188	Ab initio chemical kinetics for the unimolecular decomposition of Si2 H5 radical and related reverse bimolecular reactions. International Journal of Quantum Chemistry, 2014, 114, 278-288.	1.0	6
189	Controlled Solâ€"Gel and Diversiform Nanostructure Transitions by Photoresponsive Molecular Switching of Tetraphenylethene- and Azobenzene-Functionalized Organogelators. ACS Applied Materials & Interfaces, 2020, 12, 29650-29660.	4.0	6
190	Investigation of Product Formation in the O(¹D, ³P) + N₂O Reactions: Comparison of Experimental and Theoretical Kinetics. Journal of Physical Chemistry A, 2022, 126, 1103-1113.	1.1	6
191	Ab initio study of ammonium perchlorate combustion initiation processes: unimolecular decomposition of perchloric acid and the related OHÂ+ÂClO3reaction. PhysChemComm, 2001, 4, 127-132.	0.8	5
192	Theoretical and experimental studies of the diketene system: Product branching decomposition rate constants and energetics of isomers. International Journal of Chemical Kinetics, 2007, 39, 580-590.	1.0	5
193	THE REACTIONS OF THE CN RADICAL WITH MOLECULES RELEVANT TO COMBUSTION AND ATMOSPHERIC CHEMISTRY. Advanced Series in Physical Chemistry, 1996, , 164-213.	1.5	5
194	Diels-Alder addition of some 6- and 5-member ring aromatic compounds on the Si(001)-2Ã—l surface: dependence of the binding energy on the resonance energy of the aromatic compounds. Science in China Series B: Chemistry, 2001, 44, 473-477.	0.8	4
195	An Experimental and Computational Study of the Thermal Oxidation of C6H5NO by NO2. Journal of Physical Chemistry A, 2002, 106, 2903-2907.	1.1	4
196	An ab initio chemical kinetic study on the reactions of H, OH, and Cl with HOClO₃. International Journal of Chemical Kinetics, 2010, 42, 253-261.	1.0	4
197	Photolytically and Thermally Initiated Reactions of NH3with NOx(XÂ=Â1,2). Combustion Science and Technology, 2010, 182, 365-379.	1.2	4
198	Quantum chemical investigation on the role of Li adsorbed on anatase (101) surface nano-materials on the storage of molecular hydrogen. Journal of Molecular Modeling, 2015, 21, 142.	0.8	4

#	Article	IF	Citations
199	A computational study on the adsorption configurations and reactions of SiHx(x = 1-4) on clean and H-covered Si(100) surfaces. Applied Surface Science, 2016, 387, 546-556.	3.1	4
200	Ab Initio Chemical Kinetics for SiH_xReactions with Si₂H_y(x= 1,2,3,4;y= 6,5,4,3;x+y= 7) under a-Si:H CVD Condition. International Journal of Chemical Kinetics, 2017, 49, 197-208.	1.0	4
201	Quantum-chemical prediction of the effects of Ni-loading on the hydrogenation and water-splitting efficiency of TiO2 nanoparticles with an experimental test. Chemical Physics Letters, 2017, 667, 278-283.	1.2	4
202	Hydrogenation engineering of bimetallic Agâ€“Cu-modified-titania photocatalysts for production of hydrogen. Catalysis Today, 2022, 388-389, 79-86.	2.2	4
203	On the Reduction of O₂ on Cathode Surfaces of Coâ€“Corrin and Coâ€“Porphyrin: A Computational and Experimental Study on Their Relative Efficiencies in H₂O/H₂O₂ Formation. Journal of Physical Chemistry C, 2020, 124, 4652-4659.	1.5	4
204	LPCVD of InN on GaAs(110) Using HN3 and TMIn: Comparison with Si(100) Results. Materials Research Society Symposia Proceedings, 1993, 335, 21.	0.1	3
205	Does CH3 addition to C6H6 occur as reported?. International Journal of Chemical Kinetics, 2001, 33, 803-807.	1.0	3
206	Ab initio chemical kinetics for the NH₂ + HNO_x reactions, part III: Kinetics and mechanism for NH₂ + HONO₂. International Journal of Chemical Kinetics, 2010, 42, 69-78.	1.0	3
207	Lateral fluoro-substitution and chiral effects on supramolecular liquid crystals containing rod-like and H-bonded bent-core mesogens. RSC Advances, 2016, 6, 110482-110492.	1.7	3
208	Ab Initio Chemical Kinetics for the HCCO + H Reaction. Combustion Science and Technology, 2016, 188, 1095-1114.	1.2	3
209	Capturing H and H2by SiHx+(xâ‰ 4) ions: Comparison between Langevin and quantum statistical models. Japanese Journal of Applied Physics, 2017, 56, 026101.	0.8	3
210	Artificial Photosynthesis: Niâ€Nanocluster Modified Black TiO₂ with Dual Active Sites for Selective Photocatalytic CO₂ Reduction (Small 2/2018). Small, 2018, 14, 1870008.	5.2	3
211	A Computational Study on the Redox Reactions of Ammonia and Methylamine with Nitrogen Tetroxide. Journal of Physical Chemistry A, 2020, 124, 9923-9932.	1.1	3
212	KINETIC MODELING OF HYPERGOLIC IGNITION OF N2H4-NTO MIXTURES AT LOW TEMPERATURES AND THE SAWYER-GLASSMAN EXPERIMENT ON REACTIONS OF N2H4 WITH NOx (x = 1, 2) AT HIGH TEMPERATURES. International Journal of Energetic Materials and Chemical Propulsion, 2015, 14, 357-379.	0.2	3
213	Blue/near UV light emission from hybrid InN/TiO2 nanoparticle films. Journal of Materials Chemistry, 2011, 21, 8540.	6.7	2
214	A Hydrogen Pyrophosphate Selective Anion Receptor Based on Thiosemicarbazone. Bulletin of the Korean Chemical Society, 2017, 38, 1435-1442.	1.0	2
215	Ab Initio Chemical Kinetics for the Thermal Decomposition of SiH4 + Ion and Related Reverse Ionâ€“Molecule Reactions of Interest to PECVD of a-Si:H Films. Plasma Chemistry and Plasma Processing, 2017, 37, 1249-1264.	1.1	2
216	A model study on the mechanism and kinetics for the dissociation of water anion. International Journal of Chemical Kinetics, 2019, 51, 610-617.	1.0	2

#	Article	IF	Citations
217	Ab Initio Chemical Kinetics for Nitrogen Tetroxide Reactions with 1,1â€•and 1,2â€Dimethylhydrazines. Propellants, Explosives, Pyrotechnics, 2020, 45, 1478-1486.	1.0	2
218	Experimental and theoretical studies on the reaction of H atom with C 3 H 6. International Journal of Chemical Kinetics, 2021, 53, 646-659.	1.0	2
219	Low Pressure Chemical Vapor Deposition of III/Vâ€Nitrides Using Organometallics and Hydrazoic Acid Precursors. Journal of the Chinese Chemical Society, 1995, 42, 423-432.	0.8	1
220	Ab Initio Chemical Kinetics for the Thermal Decomposition of SiH2+ and SiH3+ Ions and Related Reverse Ionâ€“Molecule Reactions of Interest to PECVD of Î±-Si:H Films. Plasma Chemistry and Plasma Processing, 2019, 39, 1559-1573.	1.1	1
221	Theoretical study of the thermal isomerization of fulvene to benzene. Journal of Physical Organic Chemistry, 1996, 9, 801-810.	0.9	1