Lin Ming-chang

List of Publications by Citations

217 papers	6,465 citations	43 h-index	69 g-index
221 ext. papers	7,094 ext. citations	3.9 avg, IF	5.83 L-index

#	Paper	IF	Citations
217	Modification of the gaussian-2 theoretical model: The use of coupled-cluster energies, density-functional geometries, and frequencies. *Journal of Chemical Physics*, **1995**, 103, 7414-7421	3.9	437
216	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	35.4	232
215	Carbon-doped SnS nanostructure as a high-efficiency solar fuel catalyst under visible light. *Nature Communications*, **2018**, 9, 169	17.4	219
214	Ab Initio and RRKM Calculations for Multichannel Rate Constants of the C2H3 + O2 Reaction. *Journal of the American Chemical Society*, **1996**, 118, 9759-9771	16.4	150
213	A theoretical study of surface reduction mechanisms of CeO(2)(111) and (110) by H(2). *ChemPhysChem*, **2007**, 8, 849-55	3.2	128
212	Thermal decomposition of ethanol. I. Ab Initio molecular orbital/Rice-Ramsperger-Kassel-Marcus prediction of rate constant and product branching ratios. *Journal of Chemical Physics*, **2002**, 117, 3224-3231	3.9	111
211	Mechanism of Ethanol Reforming: Theoretical Foundations. *Journal of Physical Chemistry C*, **2009**, 113, 6681-6688	3.8	109
210	Oxygen Reduction on LaMnO3-Based Cathode Materials in Solid Oxide Fuel Cells. *Chemistry of Materials*, **2007**, 19, 1690-1699	9.6	109
209	Extremely rapid self-reaction of the simplest Criegee intermediate CH2OO and its implications in atmospheric chemistry. *Nature Chemistry*, **2014**, 6, 477-83	17.6	105
208	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	35.4	104
207	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	3.9	98
206	Roaming-mediated isomerization in the photodissociation of nitrobenzene. *Nature Chemistry*, **2011**, 3, 932-7	17.6	97
205	Computational study on the catalytic mechanism of oxygen reduction on La(0.5)Sr(0.5)MnO(3) in solid oxide fuel cells. *Angewandte Chemie - International Edition*, **2007**, 46, 7214-9	16.4	89
204	Kinetics and Mechanism of the OH + C6H6Reaction:A Detailed Analysis with First-Principles Calculations. *Journal of Physical Chemistry A*, **2002**, 106, 11309-11326	2.8	84
203	Experimental and reduced dimensionality quantum rate coefficients for H2(D2)+CN-H(D)CN+H(D). *Journal of Chemical Physics*, **1990**, 93, 4730-4739	3.9	84
202	Ni-Nanocluster Modified Black TiO with Dual Active Sites for Selective Photocatalytic CO Reduction. *Small*, **2018**, 14, 1702928	11	80
201	Ab initio molecular orbital study of the HCO+O2 reaction: Direct versus indirect abstraction channels. *Journal of Chemical Physics*, **1996**, 105, 2346-2352	3.9	78

200	Composition of SiCN crystals consisting of a predominantly carbon-nitride network. *Journal of Materials Research*, **1997**, 12, 322-325	2.5	69
199	Ab Initio MO Study of the Unimolecular Decomposition of the Phenyl Radical. *Journal of Physical Chemistry A*, **1997**, 101, 6790-6797	2.8	69
198	Experimental and Theoretical Studies of the Reaction of the Phenyl Radical with Methane. *Journal of Physical Chemistry A*, **1999**, 103, 3636-3645	2.8	69
197	A Computational Study of the OH(OD) + CO Reactions: Effects of Pressure, Temperature, and Quantum-Mechanical Tunneling on Product Formation. *Journal of Physical Chemistry A*, **2001**, 105, 11249-11259	2.8	68
196	Nitromethane/Methyl Nitrite Rearrangement: A Persistent Discrepancy between Theory and Experiment. *Journal of Physical Chemistry A*, **2003**, 107, 4286-4291	2.8	67
195	Unimolecular isomerization/decomposition of cyclopentadienyl and related bimolecular reverse process: ab initio MO/statistical theory study. *Journal of Computational Chemistry*, **2000**, 21, 415-425	3.5	66
194	A simple pyrene based AIEE active schiff base probe for selective naked eye and fluoresence off–on detection of trivalent cations with live cell application. *Sensors and Actuators B: Chemical*, **2016**, 231, 18-29	8.5	64
193	Computational study on the kinetics and mechanisms for the unimolecular decomposition of formic and oxalic acids. *Journal of Physical Chemistry A*, **2007**, 111, 6789-97	2.8	63
192	Novel pyrene containing monomeric and dimeric supramolecular AIEE active nano-probes utilized in selective off–on trivalent metal and highly acidic pH sensing with live cell applications. *Journal of Materials Chemistry C*, **2016**, 4, 2056-2071	7.1	60
191	Prediction of O2 Dissociation Kinetics on LaMnO3-Based Cathode Materials for Solid Oxide Fuel Cells. *Journal of Physical Chemistry C*, **2009**, 113, 7290-7297	3.8	57
190	Ab initio study of the CH3+O2 reaction: Kinetics, mechanism and product branching probabilities. *Journal of Chemical Physics*, **2001**, 115, 195-203	3.9	56
189	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	3.8	54
188	Computational study on the reactions of H2O2 on TiO2 anatase (101) and rutile (110) surfaces. *Journal of Computational Chemistry*, **2011**, 32, 1065-81	3.5	53
187	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	3.9	50
186	Laser-assisted chemical vapor deposition of InN on Si(100). *Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films*, **1993**, 11, 2931-2937	2.9	49
185	A shock tube study of the CH2O + NO2 reaction at high temperatures. *International Journal of Chemical Kinetics*, **1990**, 22, 455-482	1.4	49
184	Direct Synthesis of Zr-Doped Ceria Nanotubes. *Journal of Physical Chemistry C*, **2009**, 113, 5031-5034	3.8	48
183	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	3.9	48

182	Thermal decomposition of iso-propanol: First-principles prediction of total and product-branching rate constants. *Journal of Chemical Physics*, **2002**, 117, 11188-11195	3.9	47
181	Theoretical study of the thermal isomerization of fulvene to benzene. *Journal of Physical Organic Chemistry*, **1996**, 9, 801-810	2.1	47
180	Absolute rate constant for the reaction of Phenyl radical with Acetylene. *International Journal of Chemical Kinetics*, **1994**, 26, 1095-1104	1.4	47
179	Experimental and Theoretical Studies of the C6H5 + C6H6 Reaction. *Journal of Physical Chemistry A*, **1999**, 103, 9036-9041	2.8	46
178	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	1.4	46
177	Kinetics for the Recombination of Phenyl Radicals. *Journal of Physical Chemistry A*, **1997**, 101, 14-18	2.8	45
176	Combined Quantum Chemical/RRKM-ME Computational Study of the Phenyl + Ethylene, Vinyl + Benzene, and H + Styrene Reactions *Journal of Physical Chemistry A*, **2004**, 108, 9697-9714	2.8	45
175	Ab initio studies of ClOx reactions. IV. Kinetics and mechanism for the self-reaction of ClO radicals. *Journal of Chemical Physics*, **2003**, 118, 4094-4106	3.9	44
174	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		43
173	Ab initio study of the OH + CH2O reaction: The effect of the OHOCH2 complex on the H-abstraction kinetics. *International Journal of Chemical Kinetics*, **2006**, 38, 322-326	1.4	42
172	A Mass Spectrometric Study of the NH2 + NO2 Reaction. *Journal of Physical Chemistry A*, **1997**, 101, 2643-2647	2.8	41
171	Laser-Initiated NO Reduction by NH3: Total Rate Constant and Product Branching Ratio Measurements for the NH2 + NO Reaction. *Journal of Physical Chemistry A*, **1997**, 101, 5-13	2.8	41
170	Rate Constant of the HONO + HONO -lH2O + NO + NO2 Reaction from ab Initio MO and TST Calculations. *Journal of Physical Chemistry A*, **1998**, 102, 1803-1807	2.8	41
169	Ab initio study of the oxidation of NCN by O2. *International Journal of Chemical Kinetics*, **2005**, 37, 593-598	1.4	40
168	Effect of roaming transition states upon product branching in the thermal decomposition of CH3NO2. *Journal of Physical Chemistry A*, **2013**, 117, 7308-13	2.8	39
167	Adsorption Configurations and Reactions of Boric Acid on a TiO2 Anatase (101) Surface. *Journal of Physical Chemistry C*, **2008**, 112, 8276-8287	3.8	39
166	Acid/Base and H2PO4(-) Controllable High-Contrast Optical Molecular Switches with a Novel BODIPY Functionalized [2]Rotaxane. *ACS Applied Materials & Interfaces*, **2015**, 7, 26491-503	9.5	38
165	Theoretical Rate Constants for the NH3 + NOx -lNH2 + HNOx (x = 1, 2) Reactions by ab Initio MO/VTST Calculations. *The Journal of Physical Chemistry*, **1996**, 100, 7517-7525		38

164	KSCN-induced Interfacial Dipole in Black TiO for Enhanced Photocatalytic CO Reduction. *ACS Applied Materials & Interfaces*, **2019**, 11, 25186-25194	9.5	37
163	The NCO + NO Reaction Revisited: Ab Initio MO/VRRKM Calculations for Total Rate Constant and Product Branching Ratios. *Journal of Physical Chemistry A*, **2000**, 104, 10807-10811	2.8	37
162	Implications of the HCN -lHNC process to high-temperature nitrogen-containing fuel chemistry. *International Journal of Chemical Kinetics*, **1992**, 24, 1103-1107	1.4	36
161	Ab Initio Study of the H + HONO Reaction: Direct Abstraction versus Indirect Exchange Processes. *Journal of Physical Chemistry A*, **1997**, 101, 60-66	2.8	35
160	Potassium-Presenting Zinc Oxide Surfaces Induce Vertical Phase Separation in Fullerene-Free Organic Photovoltaics. *Nano Letters*, **2020**, 20, 715-721	11.5	34
159	Ab initio kinetics for decomposition/isomerization reactions of C2H5O radicals. *ChemPhysChem*, **2009**, 10, 972-82	3.2	33
158	An ab initio molecular orbital study of potential energy surface of the NH2+NO2 reaction. *Journal of Chemical Physics*, **1995**, 103, 5640-5649	3.9	33
157	A novel and facile decay path of Criegee intermediates by intramolecular insertion reactions via roaming transition states. *Journal of Chemical Physics*, **2015**, 142, 124312	3.9	32
156	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	3.9	32
155	Kinetics of the reaction of C6H5 with HBr. *International Journal of Chemical Kinetics*, **1993**, 25, 875-880	1.4	32
154	Experimental and Theoretical Studies of the Unimolecular Decomposition of Nitrosobenzene: High-Pressure Rate Constants and the C–N Bond Strength. *Journal of Physical Chemistry A*, **1997**, 101, 6043-6047	2.8	31
153	Ab initio studies of ClO, reactions: prediction of the rate constants of ClO + NO for the forward and reverse processes. *ChemPhysChem*, **2004**, 5, 1864-70	3.2	31
152	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	3.9	31
151	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	3.9	31
150	Quantum chemical elucidation of the mechanism for hydrogenation of TiO2 anatase crystals. *Journal of Chemical Physics*, **2013**, 138, 154705	3.9	30
149	Sublimation of Ammonium Salts: A Mechanism Revealed by a First-Principles Study of the NH4Cl System. *Journal of Physical Chemistry C*, **2007**, 111, 13831-13838	3.8	30
148	Computational Study of the HCCO + NO Reaction: ab Initio MO/vRRKM Calculations of the Total Rate Constant and Product Branching Ratios. *Journal of Physical Chemistry A*, **2003**, 107, 1066-1076	2.8	30
147	Ab initio studies of ClOx reactions. I. Kinetics and mechanism for the OH+ClO reaction. *Journal of Chemical Physics*, **2002**, 116, 7452-7460	3.9	30

146	Ab initio molecular orbital study of potential energy surface for the NH+NO2 reaction. *Journal of Chemical Physics*, **1994**, 101, 3916-3922	3.9	30
145	Kinetics of CN reactions with N2O and CO2. *International Journal of Chemical Kinetics*, **1991**, 23, 151-160	1.4	30
144	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	7.1	29
143	Kinetics and Mechanism for the Reaction of Phenyl Radical with Formaldehyde. *Journal of Physical Chemistry A*, **2000**, 104, 7030-7035	2.8	28
142	Novel Bimolecular Reactions between NH3 and HNO3 in the Gas Phase. *Journal of Physical Chemistry A*, **1998**, 102, 1808-1814	2.8	28
141	A Comprehensive Kinetic Study of Thermal Reduction of NO2by H2. *Journal of Physical Chemistry A*, **1998**, 102, 10099-10105	2.8	27
140	Thermal reaction of HNCO with NO2 at moderate temperatures. *International Journal of Chemical Kinetics*, **1993**, 25, 845-863	1.4	27
139	Ab initio chemical kinetics for the hydrolysis of N2O4 isomers in the gas phase. *Journal of Physical Chemistry A*, **2012**, 116, 4466-72	2.8	26
138	Ab Initio Studies of ClOx Reactions: 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	2.8	26
137	Ab initio molecular orbital study of the O + C6H5O reaction. *Journal of Physical Organic Chemistry*, **1995**, 8, 407-420	2.1	26
136	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	3.8	25
135	Adsorption and Dissociation of H2O on a W(111) Surface: A Computational Study. *Journal of Physical Chemistry C*, **2007**, 111, 17333-17339	3.8	25
134	Thermal unimolecular decomposition of 1,3,5-trioxane: Comparison of theory and experiment. *International Journal of Chemical Kinetics*, **1991**, 23, 947-956	1.4	25
133	Novel rhodamine probe for colorimetric and fluorescent detection of Fe ions in aqueous media with cellular imaging. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2020**, 242, 118757	4.4	24
132	Computational Chemical Kinetics for the Reaction of Criegee Intermediate CHOO with HNO and Its Catalytic Conversion to OH and HCO. *Journal of Physical Chemistry A*, **2017**, 121, 3871-3878	2.8	23
131	Mechanism and Kinetics for Ammonium Perchlorate Sublimation: A First-principles Study. *Journal of Physical Chemistry C*, **2008**, 112, 14481-14485	3.8	23
130	Computational Study on the Energetics of NCN Isomers and the Kinetics of the C + N2? N + CN Reaction. *Journal of Physical Chemistry A*, **2001**, 105, 4156-4163	2.8	23
129	Facile rhodamine-based colorimetric sensors for sequential detections of Cu(II) ions and pyrophosphate ($P_2O_7^{4-}$) anions. *RSC Advances*, **2016**, 6, 106631-106640	3.7	22

128	FTIR and Mass-Spectrometric Measurements of the Rate Constant for the C6H5 + H2 Reaction. *Journal of Physical Chemistry A*, **1997**, 101, 8839-8843	2.8	22
127	Experimental and computational studies of the phenyl radical reaction with propyne. *ChemPhysChem*, **2005**, 6, 2075-85	3.2	22
126	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	1.4	22
125	Experimental and theoretical investigation of rate coefficients of the reaction S(3P)+OCS in the temperature range of 298-985 K. *Journal of Chemical Physics*, **2006**, 125, 164329	3.9	21
124	Low-pressure organometallic chemical vapor deposition of indium nitride on titanium dioxide nanoparticles. *ChemPhysChem*, **2004**, 5, 1615-8	3.2	21
123	Product Branching Ratios in the NH2 + NO Reaction: A Re-Evaluation. *Journal of Physical Chemistry A*, **1999**, 103, 8906-8907	2.8	21
122	The thermal reaction of HNCO at moderate temperatures. *International Journal of Chemical Kinetics* , **1991**, 23, 1129-1149	1.4	21
121	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	1.4	21
120	Kinetics of C6H5 Radical Reactions with Toluene and Xylenes by Cavity Ringdown Spectrometry. *Journal of Physical Chemistry A*, **1999**, 103, 4002-4008	2.8	20
119	Kinetics of the reaction of C6H5 with HBr and DBr. *International Journal of Chemical Kinetics*, **1994**, 26, 771-778	1.4	20
118	Ab initio chemical kinetic study for reactions of H atoms with SiH(4) and Si(2)H(6): comparison of theory and experiment. *Journal of Physical Chemistry A*, **2010**, 114, 633-9	2.8	19
117	Adsorption and Thermal Decomposition of Acetaldehyde on Si(111)-7⍰. *Journal of Physical Chemistry B*, **1997**, 101, 1872-1877	3.4	19
116	Kinetics and mechanisms for reactions of HNO with CH3 and C6H5 studied by quantum-chemical and statistical-theory calculations. *International Journal of Chemical Kinetics*, **2005**, 37, 261-274	1.4	19
115	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	1.4	19
114	Photodissociation dynamics of benzaldehyde (C6H5CHO) at 266, 248, and 193 nm. *Chemistry - an Asian Journal*, **2011**, 6, 2961-76	4.5	18
113	Rate constant for the NH3 + NO2 -lNH2 + HONO reaction: Comparison of kinetically modeled and predicted results. *International Journal of Chemical Kinetics*, **1997**, 29, 245-251	1.4	18
112	Quantum chemical/vRRKM study on the thermal decomposition of cyclopentadiene. *International Journal of Chemical Kinetics*, **2004**, 36, 139-151	1.4	18
111	Ab Initio Studies of ClOx Reactions. 3. Kinetics and Mechanism for the OH + OClO Reaction. *Journal of Physical Chemistry A*, **2003**, 107, 1040-1049	2.8	18

110	Development of Hybrid Pseudohalide Tin Perovskites for Highly Stable Carbon-Electrode Solar Cells. *ACS Applied Materials & Interfaces*, **2020**, 12, 21739-21747	9.5	18
109	Adsorption Configurations and Reactions of Nitric Acid on TiO2 Rutile (110) and Anatase (101) surfaces. *Journal of Physical Chemistry C*, **2009**, 113, 6140-6149	3.8	17
108	Kinetics and mechanism for the CH2O + NO2 reaction: A computational study. *International Journal of Chemical Kinetics*, **2003**, 35, 184-190	1.4	17
107	Ab initio studies of ClO(x) reactions: prediction of the rate constants of ClO+NO2 for the forward and reverse processes. *ChemPhysChem*, **2005**, 6, 1514-21	3.2	17
106	Theoretical study of reactions of N2O with NO and OH radicals. *International Journal of Chemical Kinetics*, **1996**, 28, 693-703	1.4	17
105	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	9.6	17
104	Ab Initio Chemical Kinetics for the CH3 + O((3)P) Reaction and Related Isomerization-Decomposition of CH3O and CH2OH Radicals. *Journal of Physical Chemistry A*, **2015**, 119, 7404-17	2.8	16
103	Experimental and Computational Studies of the Kinetics and Mechanisms for C6H5 Reactions with Acetone-h6 and -d6. *Journal of Physical Chemistry A*, **2003**, 107, 7755-7761	2.8	16
102	The Reaction of C6H5 with CO: Kinetic Measurement and Theoretical Correlation with the Reverse Process. *Journal of Physical Chemistry A*, **2000**, 104, 1233-1239	2.8	16
101	Theoretical Study of the NH2 + C2H2 Reaction. *Journal of Physical Chemistry A*, **1998**, 102, 4687-4693	2.8	16
100	Novel anthracene- and pyridine-containing Schiff base probe for selective □ff□n□ fluorescent determination of Cu2+ ions towards live cell application. *New Journal of Chemistry*, **2016**, 40, 6101-6108	3.6	16
99	Ab initio chemical kinetics for reactions of H atoms with SiHx (x = 1□) radicals and related unimolecular decomposition processes. *International Journal of Quantum Chemistry*, **2013**, 113, 1735-1746	2.1	15
98	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	1.4	15
97	A Model Study of CO□□O Adsorbate Interaction on Si(100)-2□1. *Journal of Physical Chemistry B*, **1999**, 103, 7270-7276	3.4	15
96	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	3.8	14
95	Novel supramolecular conjugated polyrotaxane as an acid-base controllable optical molecular switch. *Sensors and Actuators B: Chemical*, **2017**, 243, 84-95	8.5	14
94	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	1.4	14
93	A computational study of the kinetics and mechanism for the reaction of HCO with HNO. *International Journal of Chemical Kinetics*, **2004**, 36, 205-215	1.4	14

92	Ab initio studies of ClOx reactions. VII. Isomers of Cl2O3 and their roles in the ClO+OClO reaction. *Journal of Chemical Physics*, **2003**, 118, 8645-8655	3.9	14
91	Kinetic modeling of benzene decomposition near 1000 K: The effects of toluene impurity. *International Journal of Chemical Kinetics*, **1999**, 31, 577-582	1.4	14
90	Kinetic Studies of Aromatic Radical Reactions by Cavity-Ringdown Spectroscopy. *ACS Symposium Series*, **1999**, 196-209	0.4	14
89	A dihydrogen phosphate selective anion receptor based on acylhydrazone and pyrazole. *New Journal of Chemistry*, **2015**, 39, 650-658	3.6	13
88	Simultaneous Production and Surface Functionalization of Silver Nanoparticles for Label-free Colorimetric Detection of Copper Ion. *Analytical Sciences*, **2017**, 33, 1115-1121	1.7	13
87	Hydrogen-bonded effects on supramolecular blue phase liquid crystal dimeric complexes. *RSC Advances*, **2015**, 5, 54629-54637	3.7	13
86	Ab initio chemical kinetics for the reaction of an H atom with Si3H8. *Journal of Physical Chemistry A*, **2010**, 114, 3642-8	2.8	13
85	Ab initio chemical kinetics for the NH2 + HNOx Reactions, Part I: Kinetics and Mechanism for NH2 + HNO. *International Journal of Chemical Kinetics*, **2009**, 41, 667-677	1.4	13
84	Reaction dynamics of O((1)D,(3)P) + OCS studied with time-resolved Fourier transform infrared spectroscopy and quantum chemical calculations. *Journal of Physical Chemistry A*, **2009**, 113, 13260-72	2.8	13
83	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	2.8	13
82	A Theoretical and Experimental Study of the CN + NO Association Reaction. *Journal of Physical Chemistry A*, **1998**, 102, 6973-6980	2.8	13
81	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	2.8	13
80	Development of Novel Mixed Halide/Superhalide Tin-Based Perovskites for Mesoscopic Carbon-Based Solar Cells. *Journal of Physical Chemistry Letters*, **2020**, 11, 2443-2448	6.4	12
79	Novel asymmetrical single- and double-chiral liquid crystal diads with wide blue phase ranges. *RSC Advances*, **2015**, 5, 4615-4622	3.7	12
78	Kinetics and mechanism of the C6H5 + CH3CHO reaction: experimental measurement and theoretical prediction of the reactivity toward four molecular sites. *ChemPhysChem*, **2004**, 5, 661-8	3.2	12
77	Ab Initio Studies of ClOx Radical Reactions: V. Evidence for a New Path in the Cl + ClOOCl Reaction. *Journal of Physical Chemistry A*, **2003**, 107, 3836-3840	2.8	12
76	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	2.1	12
75	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	3.7	11

74	Kinetic study of the C(10)H(7) + O(2) reaction. *Journal of Physical Chemistry A*, **2009**, 113, 5348-54	2.8	11
73	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	3.8	11
72	Observation of Significant enhancement in the efficiency of a DSSC by InN nanoparticles over TiO2-nanoparticle films. *Chemical Physics Letters*, **2011**, 510, 126-130	2.5	11
71	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	1.4	11
70	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	1.4	10
69	Adsorption and Reaction of C2N2 on Si(100)-2 □1: A Computational Study with Single- and Double-Dimer Cluster Models. *Journal of Physical Chemistry B*, **2004**, 108, 9189-9197	3.4	10
68	A Model Calculation for the Isomerization and Decomposition of Chemisorbed HCN on the Si(100)-2□1 Surface. *Journal of the Chinese Chemical Society*, **1999**, 46, 395-402	1.5	10
67	Homogeneous pyrolysis of acetylacetone at high temperatures in shock waves. *International Journal of Chemical Kinetics*, **1990**, 22, 491-504	1.4	10
66	Density Functional Studies of the Adsorption and Dissociation of NOx (x = 1, 2) Molecules on the W(111) Surface. *Journal of Physical Chemistry C*, **2009**, 113, 5300-5307	3.8	9
65	Kinetics of phenyl radical reactions with propane, n-butane, n-hexane, and n-octane: Reactivity of C6H5 toward the secondary C?H bond of alkanes. *International Journal of Chemical Kinetics*, **2004**, 36, 49-56	1.4	9
64	A computational study of the mechanism for the C6H5+ CH2O reaction. *Physical Chemistry Chemical Physics*, **2000**, 2, 5566-5570	3.6	9
63	Kinetics of CN radical reactions with formaldehyde and 1,3,5-trioxane. *International Journal of Chemical Kinetics*, **1993**, 25, 1053-1064	1.4	9
62	Effective hydrogenation of TiO2 photocatalysts with CH3OH for enhanced water splitting: A computational and X-ray study. *Applied Surface Science*, **2019**, 488, 546-554	6.7	8
61	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	1.4	8
60	Infrared Emission from Photodissociation of Methyl Formate [HC(O)OCH] at 248 and 193 nm: Absence of Roaming Signature. *Journal of Physical Chemistry A*, **2019**, 123, 6130-6143	2.8	8
59	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, 10811-23	2.8	8
58	Ab Initio Chemical Kinetics of Key Processes in the Hypergolic Ignition of Hydrazine and Nitrogen Tetroxide. *Advances in Quantum Chemistry*, **2014**, 69, 253-301	1.4	8
57	Ab initio chemical kinetics for SiH3 reactions with Si(x)H2x+2 (x = 1-4). *Journal of Physical Chemistry A*, **2010**, 114, 13353-61	2.8	8

56	Synthesis of In(OH)3 and In2O3 nanomaterials incorporating Au. *Journal of Materials Science*, **2009**, 44, 794-798	4.3	8
55	Computational study on the mechanism and rate constant for the C6H5 + C6H5NO reaction. *Journal of Physical Chemistry A*, **2005**, 109, 9054-60	2.8	8
54	Formation and decomposition of phenylvinylperoxy radicals in the reaction: C6H5C2H2 + O2. *ChemPhysChem*, **2004**, 5, 1231-4	3.2	8
53	H2O-catalyzed formation of O3 in the self-reaction of HO2: a computational study on the effect of nH2O (n = 1□3). *PhysChemComm*, **2003**, 6, 51-54		8
52	Kinetic modeling of the CH3 + C2H2 reaction data with sensitivity analyses. *International Journal of Chemical Kinetics*, **1995**, 27, 855-866	1.4	8
51	Computational Study on the Mechanisms and Rate Constants for the O(P,D) + OCS Reactions. *Journal of Physical Chemistry A*, **2019**, 123, 8358-8364	2.8	7
50	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	3.8	7
49	Ab initio chemical kinetics for the NH2 + HNOx reactions, part II: Kinetics and mechanism for NH2 + HONO. *International Journal of Chemical Kinetics*, **2009**, 41, 678-688	1.4	7
48	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	3.9	7
47	Metal-free four-in-one modification of g-C3N4 for superior photocatalytic CO2 reduction and H2 evolution. *Chemical Engineering Journal*, **2022**, 430, 132853	14.7	7
46	KSCN-activation of hydrogenated NiO/TiO2 for enhanced photocatalytic hydrogen evolution. *Applied Surface Science*, **2020**, 511, 145548	6.7	7
45	Pyrene-Based AIEE Active Nanoprobe for Zn and Tyrosine Detection Demonstrated by DFT, Bioimaging, and Organic Thin-Film Transistor. *ACS Applied Materials & Interfaces*, **2021**, 13, 28610-28626	8.5	7
44	Ab initio chemical kinetics for the unimolecular decomposition of Si2H5 radical and related reverse bimolecular reactions. *International Journal of Quantum Chemistry*, **2014**, 114, 278-288	2.1	6
43	Reaction dynamics of O(□D) + HCOOD/DCOOH investigated with time-resolved Fourier-transform infrared emission spectroscopy. *Journal of Chemical Physics*, **2014**, 141, 154313	3.9	6
42	Kinetics and mechanisms for the reactions of phenyl radical with ketene and its deuterated isotopomer: an experimental and theoretical study. *ChemPhysChem*, **2004**, 5, 225-32	3.2	6
41	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	1.4	6
40	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	1.4	6
39	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	7.1	6

38	Isomerization of N2O4 in Solid N2H4 and Its Implication for the Explosion of N2O4/N2H4 Solid Mixtures. *Journal of Physical Chemistry C*, **2018**, 122, 23501-23505	3.8	6
37	Ab initio chemical kinetics for the HCCO + OH reaction. *Chemical Physics Letters*, **2014**, 592, 175-181	2.5	5
36	Ab initio kinetic prediction of branching rate constants for reactions of H atoms with CH3O and CH2OH. *Molecular Physics*, **2007**, 105, 2763-2776	1.7	5
35	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	9.5	5
34	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	8.5	5
33	Controlled Sol-Gel and Diversiform Nanostructure Transitions by Photoresponsive Molecular Switching of Tetraphenylethene- and Azobenzene-Functionalized Organogelators. *ACS Applied Materials & Interfaces*, **2020**, 12, 29650-29660	9.5	4
32	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	1.4	4
31	The Adsorption and Thermal Decomposition of CH2CO (CD2CO) on Si(111)-7 ×7. *Journal of the Chinese Chemical Society*, **1995**, 42, 309-316	1.5	4
30	Ab Initio Chemical Kinetics for SiHx Reactions with Si2Hy (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	1.4	3
29	Capturing H and H2by SiHx+(x≤4) ions: Comparison between Langevin and quantum statistical models. *Japanese Journal of Applied Physics*, **2017**, 56, 026101	1.4	3
28	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	3.7	3
27	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	2.5	3
26	Photolytically and Thermally Initiated Reactions of NH3 with NOx (X = 1,2). *Combustion Science and Technology*, **2010**, 182, 365-379	1.5	3
25	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	1.4	3
24	Ab initio chemical kinetics for the NH2 + HNOx reactions, part III: Kinetics and mechanism for NH2 + HONO2. *International Journal of Chemical Kinetics*, **2010**, 42, 69-78	1.4	3
23	Diels-Alder addition of some 6- and 5-member ring aromatic compounds on the Si(001)-2×1 surface: dependence of the binding energy on the resonance energy of the aromatic compounds. *Science in China Series B: Chemistry*, **2001**, 44, 473-477		3
22	An Experimental and Computational Study of the Thermal Oxidation of C6H5NO by NO2. *Journal of Physical Chemistry A*, **2002**, 106, 2903-2907	2.8	3
21	Ab initio study of ammonium perchlorate combustion initiation processes: unimolecular decomposition of perchloric acid and the related OH + ClO3 reaction. *PhysChemComm*, **2001**, 4, 127-132		3

20	LPCVD of InN on GaAs(110) Using HN3 and TMIn: Comparison with Si(100) Results. *Materials Research Society Symposia Proceedings*, **1993**, 335, 21		3
19	THE REACTIONS OF THE CN RADICAL WITH MOLECULES RELEVANT TO COMBUSTION AND ATMOSPHERIC CHEMISTRY. *Advanced Series in Physical Chemistry*, **1996**, 164-213		3
18	A model study on the mechanism and kinetics for the dissociation of water anion. *International Journal of Chemical Kinetics*, **2019**, 51, 610-617	1.4	2
17	On the Reduction of O2 on Cathode Surfaces of Co□orrin and Co□orphyrin: A Computational and Experimental Study on Their Relative Efficiencies in H2O/H2O2 Formation. *Journal of Physical Chemistry C*, **2020**, 124, 4652-4659	3.8	2
16	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	6.7	2
15	Ab Initio Chemical Kinetics for the HCCO + H Reaction. *Combustion Science and Technology*, **2016**, 188, 1095-1114	1.5	2
14	A Hydrogen Pyrophosphate Selective Anion Receptor Based on Thiosemicarbazone. *Bulletin of the Korean Chemical Society*, **2017**, 38, 1435-1442	1.2	2
13	Ab Initio Chemical Kinetics for the Thermal Decomposition of SiH4 + Ion and Related Reverse Ion□Molecule Reactions of Interest to PECVD of a-Si:H Films. *Plasma Chemistry and Plasma Processing*, **2017**, 37, 1249-1264	3.6	2
12	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	2	2
11	Blue/near UV light emission from hybrid InN/TiO2 nanoparticle films. *Journal of Materials Chemistry* , **2011**, 21, 8540		2
10	Does CH3 addition to C6H6 occur as reported?. *International Journal of Chemical Kinetics*, **2001**, 33, 803-807	1.4	2
9	Hydrogenation engineering of bimetallic Ag□u-modified-titania photocatalysts for production of hydrogen. *Catalysis Today*, **2020**, 388-389, 79-79	5.3	2
8	Acid□ase controllable nanostructures and the fluorescence detection of H2PO4□by the molecular shuttling of tetraphenylethene-based [2]rotaxanes. *Journal of Materials Chemistry C*, **2021**, 9, 3215-3228	7.1	2
7	Ab Initio Chemical Kinetics for Nitrogen Tetroxide Reactions with 1,1- and 1,2-Dimethylhydrazines. *Propellants, Explosives, Pyrotechnics*, **2020**, 45, 1478-1486	1.7	1
6	Artificial Photosynthesis: Ni-Nanocluster Modified Black TiO2 with Dual Active Sites for Selective Photocatalytic CO2 Reduction (Small 2/2018). *Small*, **2018**, 14, 1870008	11	1
5	Low Pressure Chemical Vapor Deposition of III/V-Nitrides Using Organometallics and Hydrazoic Acid Precursors. *Journal of the Chinese Chemical Society*, **1995**, 42, 423-432	1.5	1
4	A Computational Study on the Redox Reactions of Ammonia and Methylamine with Nitrogen Tetroxide. *Journal of Physical Chemistry A*, **2020**, 124, 9923-9932	2.8	1
3	Theoretical study of the thermal isomerization of fulvene to benzene **1996**, 9, 801		1

2	Experimental and theoretical studies on the reaction of H atom with C3H6. *International Journal of Chemical Kinetics*, **2021**, 53, 646-659	1.4	1
1	Ab Initio Chemical Kinetics for the Thermal Decomposition of SiH2+ and SiH3+ Ions and Related Reverse Ion–Molecule Reactions of Interest to PECVD of a-Si:H Films. *Plasma Chemistry and Plasma Processing*, **2019**, 39, 1559-1573	3.6	0