# Lin Ming-chang

## List of Publications by Year in Descending Order



| | | | |
|---|---|---|---|
| 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 | 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 |
| 216 | 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 | 9.5 | 7 |
| 215 | 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 |
| 214 | Acid–base controllable nanostructures and the fluorescence detection of $H_2PO_4^-$ by the molecular shuttling of tetraphenylethene-based [2]rotaxanes. *Journal of Materials Chemistry C*, **2021**, 9, 3215-3228 | 7.1 | 2 |
| 213 | Experimental and theoretical studies on the reaction of H atom with C3H6. *International Journal of Chemical Kinetics*, **2021**, 53, 646-659 | 1.4 | 1 |
| 212 | 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 |
| 211 | 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 |
| 210 | 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 |
| 209 | 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 |
| 208 | On the Reduction of O2 on Cathode Surfaces of Co–Corrin and Co–Porphyrin: 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 |
| 207 | KSCN-activation of hydrogenated NiO/TiO2 for enhanced photocatalytic hydrogen evolution. *Applied Surface Science*, **2020**, 511, 145548 | 6.7 | 7 |
| 206 | Potassium-Presenting Zinc Oxide Surfaces Induce Vertical Phase Separation in Fullerene-Free Organic Photovoltaics. *Nano Letters*, **2020**, 20, 715-721 | 11.5 | 34 |
| 205 | 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 |
| 204 | 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 |
| 203 | Hydrogenation engineering of bimetallic Ag–Cu-modified-titania photocatalysts for production of hydrogen. *Catalysis Today*, **2020**, 388-389, 79-79 | 5.3 | 2 |
| 202 | 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 |
| 201 | Development of Hybrid Pseudohalide Tin Perovskites for Highly Stable Carbon-Electrode Solar Cells. *ACS Applied Materials & Interfaces*, **2020**, 12, 21739-21747 | 9.5 | 18 |

| | | | |
|---|---|---|---|
| 200 | 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 |
| 199 | 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 |
| 198 | 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 |
| 197 | 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 |
| 196 | Ab Initio Chemical Kinetics for the Thermal Decomposition of SiH2+ and SiH3+ Ions and Related Reverse Ion□Molecule Reactions of Interest to PECVD of □Si:H Films. *Plasma Chemistry and Plasma Processing*, **2019**, 39, 1559-1573 | 3.6 | 0 |
| 195 | KSCN-induced Interfacial Dipole in Black TiO for Enhanced Photocatalytic CO Reduction. *ACS Applied Materials & Interfaces*, **2019**, 11, 25186-25194 | 9.5 | 37 |
| 194 | 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 |
| 193 | Carbon-doped SnS nanostructure as a high-efficiency solar fuel catalyst under visible light. *Nature Communications*, **2018**, 9, 169 | 17.4 | 219 |
| 192 | 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 |
| 191 | Ni-Nanocluster Modified Black TiO with Dual Active Sites for Selective Photocatalytic CO Reduction. *Small*, **2018**, 14, 1702928 | 11 | 80 |
| 190 | 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 |
| 189 | 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 |
| 188 | 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 |
| 187 | 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 |
| 186 | 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 |
| 185 | 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 |
| 184 | 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 |
| 183 | Novel supramolecular conjugated polyrotaxane as an acid-base controllable optical molecular switch. *Sensors and Actuators B: Chemical*, **2017**, 243, 84-95 | 8.5 | 14 |

| | | | |
|---|---|---|---|
| 182 | 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 |
| 181 | A Hydrogen Pyrophosphate Selective Anion Receptor Based on Thiosemicarbazone. *Bulletin of the Korean Chemical Society*, **2017**, 38, 1435-1442 | 1.2 | 2 |
| 180 | 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 |
| 179 | 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 |
| 178 | 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 |
| 177 | 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 |
| 176 | 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 |
| 175 | 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 |
| 174 | Ab Initio Chemical Kinetics for the HCCO + H Reaction. *Combustion Science and Technology*, **2016**, 188, 1095-1114 | 1.5 | 2 |
| 173 | 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 |
| 172 | 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 |
| 171 | Novel anthracene- and pyridine-containing Schiff base probe for selective □off□on□fluorescent determination of Cu2+ ions towards live cell application. *New Journal of Chemistry*, **2016**, 40, 6101-6108 | 3.6 | 16 |
| 170 | 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 |
| 169 | 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 |
| 168 | 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 |
| 167 | A dihydrogen phosphate selective anion receptor based on acylhydrazone and pyrazole. *New Journal of Chemistry*, **2015**, 39, 650-658 | 3.6 | 13 |
| 166 | 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 |
| 165 | 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 |

| | | | |
|---|---|---|---|
| 164 | Hydrogen-bonded effects on supramolecular blue phase liquid crystal dimeric complexes. *RSC Advances*, **2015**, 5, 54629-54637 | 3.7 | 13 |
| 163 | Novel asymmetrical single- and double-chiral liquid crystal diads with wide blue phase ranges. *RSC Advances*, **2015**, 5, 4615-4622 | 3.7 | 12 |
| 162 | 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 |
| 161 | Ab initio chemical kinetics for the HCCO + OH reaction. *Chemical Physics Letters*, **2014**, 592, 175-181 | 2.5 | 5 |
| 160 | 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 |
| 159 | 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 |
| 158 | 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 |
| 157 | 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 |
| 156 | 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 |
| 155 | Quantum chemical elucidation of the mechanism for hydrogenation of TiO2 anatase crystals. *Journal of Chemical Physics*, **2013**, 138, 154705 | 3.9 | 30 |
| 154 | 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 |
| 153 | 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 |
| 152 | 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 |
| 151 | Roaming-mediated isomerization in the photodissociation of nitrobenzene. *Nature Chemistry*, **2011**, 3, 932-7 | 17.6 | 97 |
| 150 | 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 |
| 149 | Photodissociation dynamics of benzaldehyde (C6H5CHO) at 266, 248, and 193 nm. *Chemistry - an Asian Journal*, **2011**, 6, 2961-76 | 4.5 | 18 |
| 148 | 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 |
| 147 | Blue/near UV light emission from hybrid InN/TiO2 nanoparticle films. *Journal of Materials Chemistry*, **2011**, 21, 8540 | | 2 |

| | | | |
|---|---|---|---|
| 146 | 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 |
| 145 | Photolytically and Thermally Initiated Reactions of NH3 with NOx (X = 1,2). *Combustion Science and Technology*, **2010**, 182, 365-379 | 1.5 | 3 |
| 144 | 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 |
| 143 | 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 |
| 142 | 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 |
| 141 | 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 |
| 140 | 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 |
| 139 | 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 |
| 138 | Ab initio kinetics for decomposition/isomerization reactions of C2H5O radicals. *ChemPhysChem*, **2009**, 10, 972-82 | 3.2 | 33 |
| 137 | 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 |
| 136 | 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 |
| 135 | Synthesis of In(OH)3 and In2O3 nanomaterials incorporating Au. *Journal of Materials Science*, **2009**, 44, 794-798 | 4.3 | 8 |
| 134 | Mechanism of Ethanol Reforming: Theoretical Foundations. *Journal of Physical Chemistry C*, **2009**, 113, 6681-6688 | 3.8 | 109 |
| 133 | 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 |
| 132 | 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 |
| 131 | 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 |
| 130 | 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 |
| 129 | Kinetic study of the C(10)H(7) + O(2) reaction. *Journal of Physical Chemistry A*, **2009**, 113, 5348-54 | 2.8 | 11 |

| | | | |
|---|---|---|---|
| 128 | 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 |
| 127 | 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 |
| 126 | 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 |
| 125 | Direct Synthesis of Zr-Doped Ceria Nanotubes. *Journal of Physical Chemistry C*, **2009**, 113, 5031-5034 | 3.8 | 48 |
| 124 | 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 |
| 123 | Mechanism and Kinetics for Ammonium Perchlorate Sublimation: A First-principles Study. *Journal of Physical Chemistry C*, **2008**, 112, 14481-14485 | 3.8 | 23 |
| 122 | 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 |
| 121 | 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 |
| 120 | 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 |
| 119 | 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 |
| 118 | A theoretical study of surface reduction mechanisms of CeO(2)(111) and (110) by H(2). *ChemPhysChem*, **2007**, 8, 849-55 | 3.2 | 128 |
| 117 | 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 |
| 116 | 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 |
| 115 | Oxygen Reduction on LaMnO3-Based Cathode Materials in Solid Oxide Fuel Cells. *Chemistry of Materials*, **2007**, 19, 1690-1699 | 9.6 | 109 |
| 114 | Ab initio study of the OH + CH2O reaction: The effect of the OH□□OCH2 complex on the H-abstraction kinetics. *International Journal of Chemical Kinetics*, **2006**, 38, 322-326 | 1.4 | 42 |
| 113 | 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 |
| 112 | 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 |
| 111 | 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 |

| | | | |
|---|---|---|---|
| 110 | Experimental and computational studies of the phenyl radical reaction with propyne. *ChemPhysChem*, **2005**, 6, 2075-85 | 3.2 | 22 |
| 109 | Ab initio study of the oxidation of NCN by O2. *International Journal of Chemical Kinetics*, **2005**, 37, 593-598 | 1.4 | 40 |
| 108 | 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 |
| 107 | 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 |
| 106 | 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 |
| 105 | Formation and decomposition of phenylvinylperoxy radicals in the reaction: C6H5C2H2 + O2. *ChemPhysChem*, **2004**, 5, 1231-4 | 3.2 | 8 |
| 104 | Low-pressure organometallic chemical vapor deposition of indium nitride on titanium dioxide nanoparticles. *ChemPhysChem*, **2004**, 5, 1615-8 | 3.2 | 21 |
| 103 | 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 |
| 102 | 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 |
| 101 | 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 |
| 100 | Quantum chemical/vRRKM study on the thermal decomposition of cyclopentadiene. *International Journal of Chemical Kinetics*, **2004**, 36, 139-151 | 1.4 | 18 |
| 99 | 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 |
| 98 | 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 |
| 97 | 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 |
| 96 | Kinetics and mechanism for the CH2O + NO2 reaction: A computational study. *International Journal of Chemical Kinetics*, **2003**, 35, 184-190 | 1.4 | 17 |
| 95 | 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 |
| 94 | 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 |
| 93 | Nitromethane□Methyl Nitrite Rearrangement:  A Persistent Discrepancy between Theory and Experiment. *Journal of Physical Chemistry A*, **2003**, 107, 4286-4291 | 2.8 | 67 |

| | | | |
|---|---|---|---|
| 92 | 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 |
| 91 | 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 |
| 90 | 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 |
| 89 | 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 |
| 88 | 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 |
| 87 | 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 |
| 86 | 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 |
| 85 | 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 |
| 84 | 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 |
| 83 | 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 |
| 82 | 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 |
| 81 | 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 |
| 80 | 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 |
| 79 | 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 |
| 78 | 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 |
| 77 | 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 |
| 76 | Diels-Alder addition of some 6- and 5-member ring aromatic compounds on the Si(001)-2□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 |
| 75 | Does CH3 addition to C6H6 occur as reported?. *International Journal of Chemical Kinetics*, **2001**, 33, 803-807 | 1.4 | 2 |

| | | | |
|---|---|---|---|
| 74 | 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 |
| 73 | 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 |
| 72 | 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 |
| 71 | 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 |
| 70 | 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 |
| 69 | 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 |
| 68 | 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 |
| 67 | Kinetics and Mechanism for the Reaction of Phenyl Radical with Formaldehyde. *Journal of Physical Chemistry A*, **2000**, 104, 7030-7035 | 2.8 | 28 |
| 66 | A computational study of the mechanism for the C6H5+ CH2O reaction. *Physical Chemistry Chemical Physics*, **2000**, 2, 5566-5570 | 3.6 | 9 |
| 65 | 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 |
| 64 | 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 |
| 63 | 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 |
| 62 | 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 |
| 61 | 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 |
| 60 | 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 |
| 59 | Product Branching Ratios in the NH2 + NO Reaction: A Re-Evaluation. *Journal of Physical Chemistry A*, **1999**, 103, 8906-8907 | 2.8 | 21 |
| 58 | 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 |
| 57 | Experimental and Theoretical Studies of the C6H5 + C6H6 Reaction. *Journal of Physical Chemistry A*, **1999**, 103, 9036-9041 | 2.8 | 46 |

| | | | |
|---|---|---|---|
| 56 | A Model Study of CO□O Adsorbate Interaction on Si(100)-2□. *Journal of Physical Chemistry B*, **1999**, 103, 7270-7276 | 3.4 | 15 |
| 55 | Kinetic Studies of Aromatic Radical Reactions by Cavity-Ringdown Spectroscopy. *ACS Symposium Series*, **1999**, 196-209 | 0.4 | 14 |
| 54 | A Model Calculation for the Isomerization and Decomposition of Chemisorbed HCN on the Si(100)-2□ Surface. *Journal of the Chinese Chemical Society*, **1999**, 46, 395-402 | 1.5 | 10 |
| 53 | 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 |
| 52 | 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 |
| 51 | Novel Bimolecular Reactions between NH3 and HNO3 in the Gas Phase. *Journal of Physical Chemistry A*, **1998**, 102, 1808-1814 | 2.8 | 28 |
| 50 | A Comprehensive Kinetic Study of Thermal Reduction of NO2by H2. *Journal of Physical Chemistry A*, **1998**, 102, 10099-10105 | 2.8 | 27 |
| 49 | Theoretical Study of the NH2 + C2H2 Reaction. *Journal of Physical Chemistry A*, **1998**, 102, 4687-4693 | 2.8 | 16 |
| 48 | A Theoretical and Experimental Study of the CN + NO Association Reaction. *Journal of Physical Chemistry A*, **1998**, 102, 6973-6980 | 2.8 | 13 |
| 47 | 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 |
| 46 | Composition of SiCN crystals consisting of a predominantly carbon-nitride network. *Journal of Materials Research*, **1997**, 12, 322-325 | 2.5 | 69 |
| 45 | 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 |
| 44 | A Mass Spectrometric Study of the NH2 + NO2 Reaction. *Journal of Physical Chemistry A*, **1997**, 101, 2643-2647 | 2.8 | 41 |
| 43 | Kinetics for the Recombination of Phenyl Radicals. *Journal of Physical Chemistry A*, **1997**, 101, 14-18 | 2.8 | 45 |
| 42 | Ab Initio MO Study of the Unimolecular Decomposition of the Phenyl Radical. *Journal of Physical Chemistry A*, **1997**, 101, 6790-6797 | 2.8 | 69 |
| 41 | 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 |
| 40 | Adsorption and Thermal Decomposition of Acetaldehyde on Si(111)-7□. *Journal of Physical Chemistry B*, **1997**, 101, 1872-1877 | 3.4 | 19 |
| 39 | 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 |

| | | | |
|---|---|---|---|
| 38 | 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 |
| 37 | 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 |
| 36 | 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 |
| 35 | 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 |
| 34 | 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 |
| 33 | Theoretical study of the thermal isomerization of fulvene to benzene. *Journal of Physical Organic Chemistry*, **1996**, 9, 801-810 | 2.1 | 47 |
| 32 | 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 |
| 31 | Theoretical study of reactions of N2O with NO and OH radicals. *International Journal of Chemical Kinetics*, **1996**, 28, 693-703 | 1.4 | 17 |
| 30 | 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 |
| 29 | 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 |
| 28 | THE REACTIONS OF THE CN RADICAL WITH MOLECULES RELEVANT TO COMBUSTION AND ATMOSPHERIC CHEMISTRY. *Advanced Series in Physical Chemistry*, **1996**, 164-213 | | 3 |
| 27 | Theoretical study of the thermal isomerization of fulvene to benzene **1996**, 9, 801 | | 1 |
| 26 | Ab initio molecular orbital study of the O + C6H5O reaction. *Journal of Physical Organic Chemistry*, **1995**, 8, 407-420 | 2.1 | 26 |
| 25 | 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 |
| 24 | 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 |
| 23 | Modification of the gaussian□ theoretical model: The use of coupled-cluster energies, density-functional geometries, and frequencies. *Journal of Chemical Physics*, **1995**, 103, 7414-7421 | 3.9 | 437 |
| 22 | 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 |
| 21 | The Adsorption and Thermal Decomposition of CH2CO (CD2CO) on Si(111)-7 □. *Journal of the Chinese Chemical Society*, **1995**, 42, 309-316 | 1.5 | 4 |

| | | | |
|---|---|---|---|
| 20 | Kinetic modeling of the CH3 + C2H2 reaction data with sensitivity analyses. *International Journal of Chemical Kinetics*, **1995**, 27, 855-866 | 1.4 | 8 |
| 19 | 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 |
| 18 | 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 |
| 17 | Kinetics of the reaction of C6H5 with HBr and DBr. *International Journal of Chemical Kinetics*, **1994**, 26, 771-778 | 1.4 | 20 |
| 16 | Absolute rate constant for the reaction of Phenyl radical with Acetylene. *International Journal of Chemical Kinetics*, **1994**, 26, 1095-1104 | 1.4 | 47 |
| 15 | 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 |
| 14 | LPCVD of InN on GaAs(110) Using HN3 and TMIn: Comparison with Si(100) Results. *Materials Research Society Symposia Proceedings*, **1993**, 335, 21 | | 3 |
| 13 | Thermal reaction of HNCO with NO2 at moderate temperatures. *International Journal of Chemical Kinetics*, **1993**, 25, 845-863 | 1.4 | 27 |
| 12 | Kinetics of the reaction of C6H5 with HBr. *International Journal of Chemical Kinetics*, **1993**, 25, 875-880 | 1.4 | 32 |
| 11 | Kinetics of CN radical reactions with formaldehyde and 1,3,5-trioxane. *International Journal of Chemical Kinetics*, **1993**, 25, 1053-1064 | 1.4 | 9 |
| 10 | 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 |
| 9 | 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 |
| 8 | 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 |
| 7 | Kinetics of CN reactions with N2O and CO2. *International Journal of Chemical Kinetics*, **1991**, 23, 151-160 | 1.4 | 30 |
| 6 | 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 |
| 5 | The thermal reaction of HNCO at moderate temperatures. *International Journal of Chemical Kinetics* , **1991**, 23, 1129-1149 | 1.4 | 21 |
| 4 | A shock tube study of the CH2O + NO2 reaction at high temperatures. *International Journal of Chemical Kinetics*, **1990**, 22, 455-482 | 1.4 | 49 |
| 3 | Homogeneous pyrolysis of acetylacetone at high temperatures in shock waves. *International Journal of Chemical Kinetics*, **1990**, 22, 491-504 | 1.4 | 10 |

| | | | |
|---|---|---|---|
| 2 | 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 |
| 1 | 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 |