

# Lidong Zhang

## List of Publications by Year in descending order

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130  
docs citations

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times ranked

7823  
citing authors

#	ARTICLE	IF	CITATIONS
1	Mesoporous Co-Mn Spinel Oxides as Efficient Catalysts for Low Temperature Propane Oxidation. Catalysis Letters, 2022, 152, 2695-2704.	2.6	3
2	Experimental and kinetic modeling studies of 2-acetylfuran pyrolysis at atmospheric pressure. Combustion and Flame, 2022, 236, 111824.	5.2	6
3	Converting CO <sub>2</sub> Hydrogenation Products from Paraffins to Olefins: Modification of Zeolite Surface Properties by a UiO-66 Membrane. ACS Catalysis, 2022, 12, 5894-5902.	11.2	10
4	A theoretical kinetics study on low-temperature oxidation of n-C <sub>4</sub> H <sub>9</sub> radicals. Proceedings of the Combustion Institute, 2021, 38, 681-689.	3.9	12
5	Experimental and kinetic modeling study of methyl heptanoate low-temperature oxidation in a jet-stirred reactor. Fuel, 2021, 283, 118885.	6.4	10
6	Catalytic combustion of methyl butanoate over HZSM-5 zeolites. Chemical Communications, 2021, 57, 2233-2244.	4.1	11
7	Unique Coordination Structure of Cobalt Single-Atom Catalyst Supported on Dopant-Free Carbon. Journal of Physical Chemistry C, 2021, 125, 6735-6742.	3.1	1
8	Optimized rapid flame synthesis of morphology-controlled $\gamma$ -MoO <sub>3</sub> layered nanoflakes. Journal of Nanoparticle Research, 2021, 23, 1.	1.9	5
9	Toward the Mechanism Study of Pd/ $\gamma$ -Al <sub>2</sub> O <sub>3</sub> -Assisted Bioalcohol Combustion in a Flow Reactor. Energy & Fuels, 2021, 35, 14954-14962.	5.1	6
10	Unraveling the low-temperature oxidation mechanism between methyl crotonate radicals and O <sub>2</sub> . Combustion and Flame, 2021, 231, 111473.	5.2	9
11	Toward high-level theoretical studies on the reaction kinetics of PAHs growth based on HACA pathway: An ONIOM[G3(MP2,CC)//B3LYP:DFT] method developed. Fuel, 2021, 301, 121052.	6.4	15
12	Theoretical investigation of chemical reaction kinetics of CO <sub>2</sub> and vinyl radical under catalytic combustion. Fuel, 2021, 305, 121566.	6.4	3
13	Flame In Situ Synthesis of Metal-Anchored CuO Nanowires for CO Catalytic Oxidation and Kinetic Analysis. ACS Applied Energy Materials, 2021, 4, 13226-13238.	5.1	9
14	Highly active and stable Co <sub>3</sub> O <sub>4</sub> catalyst for the Low-temperature oxidative dehydrogenation of propane. Inorganic Chemistry Communication, 2020, 112, 107725.	3.9	9
15	Theoretical study of transition metals supported on g-C <sub>3</sub> N <sub>4</sub> as electrochemical catalysts for CO <sub>2</sub> reduction to CH <sub>3</sub> OH and CH <sub>4</sub> . Journal of CO <sub>2</sub> Utilization, 2020, 36, 116-123.	6.8	59
16	Influence of Torsional Anharmonicity on the Reactions of Methyl Butanoate with Hydroperoxyl Radical. Journal of Physical Chemistry A, 2020, 124, 8643-8652.	2.5	8
17	Dynamic Surface Reconstruction of Single-Atom Bimetallic Alloy under <i>Operando</i> Electrochemical Conditions. Nano Letters, 2020, 20, 8319-8325.	9.1	28
18	Theoretical investigations of electrochemical CO <sub>2</sub> reduction by transition metals anchored on CNTs. Sustainable Energy and Fuels, 2020, 4, 6156-6164.	4.9	13

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19	Abatement of <i>n</i> -Butane by Catalytic Combustion over Co-ZSM-5 Catalysts. <i>Energy &amp; Fuels</i> , 2020, 34, 12880-12890.	5.1	20
20	Theoretical calculation of low-temperature oxidation of heptyl radicals and O <sub>2</sub> . <i>Combustion and Flame</i> , 2020, 217, 274-284.	5.2	14
21	Au@Pt Nanotubes within CoZn-Based Metal-Organic Framework for Highly Efficient Semi-hydrogenation of Acetylene. <i>IScience</i> , 2020, 23, 101233.	4.1	12
22	Theoretical chemical kinetics for catalytic pyrolysis of methyl acetate over H-ZSM-5 zeolites. <i>Fuel</i> , 2020, 277, 118101.	6.4	7
23	A thorough theoretical mechanistic study of OH-initiated oxidative degradation mechanism for large polycyclic aromatic hydrocarbons. <i>Computational and Theoretical Chemistry</i> , 2020, 1175, 112730.	2.5	5
24	A theoretical investigation on Bell-Evans-Polanyi correlations for hydrogen abstraction reactions of large biodiesel molecules by H and OH radicals. <i>Combustion and Flame</i> , 2020, 214, 394-406.	5.2	18
25	Coordination-Engineered Cu <sup>II</sup> Single-Site Catalyst for Enhancing Oxygen Reduction Reaction. <i>ACS Applied Energy Materials</i> , 2019, 2, 6497-6504.	5.1	58
26	Interfacial engineering of cobalt sulfide/graphene hybrids for highly efficient ammonia electrosynthesis. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2019, 116, 6635-6640.	7.1	242
27	Towards high-level theoretical studies of large biodiesel molecules: an ONIOM/RRKM/Master-equation approach to the isomerization and dissociation kinetics of methyl decanoate radicals. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 5232-5242.	2.8	13
28	Theoretical Study on Criegee Intermediate's Role in Ozonolysis of Acrylic Acid. <i>Journal of Physical Chemistry A</i> , 2019, 123, 1929-1936.	2.5	7
29	Experimental and Theoretical Investigation of the Pyrolysis of Furfural. <i>Journal of Physical Chemistry A</i> , 2019, 123, 103-110.	2.5	21
30	Utilization of generalized energy-based fragmentation method on the study of hydrogen abstraction reactions of large methyl esters. <i>Combustion and Flame</i> , 2018, 190, 467-476.	5.2	17
31	Experimental and modeling studies of small typical methyl esters pyrolysis: Methyl butanoate and methyl crotonate. <i>Combustion and Flame</i> , 2018, 191, 160-174.	5.2	48
32	Ab initio kinetics on low temperature oxidation of iso-pentane: The first oxygen addition. <i>Combustion and Flame</i> , 2018, 190, 119-132.	5.2	25
33	Theoretical studies on the reaction kinetics of methyl crotonate with hydroxyl radical. <i>Sustainable Energy and Fuels</i> , 2018, 2, 392-402.	4.9	24
34	Oxygen Vacancies Confined in Nickel Molybdenum Oxide Porous Nanosheets for Promoted Electrocatalytic Urea Oxidation. <i>ACS Catalysis</i> , 2018, 8, 1-7.	11.2	372
35	Toward High-Level Theoretical Studies of Large Biodiesel Molecules: An ONIOM [QCISD(T)/CBS:DFT] Study of the Reactions between Unsaturated Methyl Esters (C <sub>n</sub> H <sub>2n-1</sub> COOCH <sub>3</sub> ) and Hydrogen Radical. <i>Journal of Physical Chemistry A</i> , 2018, 122, 4882-4893.	2.5	18
36	A theoretical kinetics study on low-temperature reactions of methyl acetate radicals with molecular oxygen. <i>Combustion and Flame</i> , 2018, 196, 45-53.	5.2	20

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37	Experimental and kinetic modeling investigation on methyl decanoate pyrolysis at low and atmospheric pressures. <i>Fuel</i> , 2018, 232, 333-340.	6.4	27
38	Theoretical Studies on Isomerization and Decomposition Reactions of 2-Methyl-1-butanol Radicals. <i>Energy &amp; Fuels</i> , 2018, 32, 7652-7659.	5.1	3
39	Predictive kinetics on the formation and decomposition of ethylbenzene. <i>Proceedings of the Combustion Institute</i> , 2017, 36, 533-542.	3.9	15
40	Hydroperoxide Measurements During Low-Temperature Gas-Phase Oxidation of <i>n</i> -Heptane and <i>n</i> -Decane. <i>Journal of Physical Chemistry A</i> , 2017, 121, 1861-1876.	2.5	31
41	Theoretical kinetic studies for low temperature oxidation of two typical methylcyclohexyl radicals. <i>Combustion and Flame</i> , 2017, 182, 216-224.	5.2	32
42	Atomically Dispersed Iron–Nitrogen Species as Electrocatalysts for Bifunctional Oxygen Evolution and Reduction Reactions. <i>Angewandte Chemie - International Edition</i> , 2017, 56, 610-614.	13.8	950
43	Experimental and kinetic modeling studies of furan pyrolysis: Fuel decomposition and aromatic ring formation. <i>Fuel</i> , 2017, 206, 239-247.	6.4	38
44	Regulating Water–Reduction Kinetics in Cobalt Phosphide for Enhancing HER Catalytic Activity in Alkaline Solution. <i>Advanced Materials</i> , 2017, 29, 1606980.	21.0	220
45	3D Nitrogen–Anion–Decorated Nickel Sulfides for Highly Efficient Overall Water Splitting. <i>Advanced Materials</i> , 2017, 29, 1701584.	21.0	478
46	Pyrolysis of <i>n</i> -butane investigated using synchrotron threshold photoelectron photoion coincidence spectroscopy. <i>RSC Advances</i> , 2017, 7, 28746-28753.	3.6	7
47	Spin-State Regulation of Perovskite Cobaltite to Realize Enhanced Oxygen Evolution Activity. <i>Chem</i> , 2017, 3, 812-821.	11.7	225
48	Roaming-Mediated CH <sub>2</sub> NH Elimination from the Ionization of Aromatic Ethylamines. <i>ChemistryOpen</i> , 2017, 6, 40-45.	1.9	2
49	Theoretical studies for reaction kinetics of cy-C <sub>6</sub> H <sub>11</sub> CH <sub>2</sub> radical with O <sub>2</sub> . <i>Proceedings of the Combustion Institute</i> , 2017, 36, 179-186.	3.9	25
50	New insights into the low-temperature oxidation of 2-methylhexane. <i>Proceedings of the Combustion Institute</i> , 2017, 36, 373-382.	3.9	36
51	Experimental and kinetic modeling study of laminar premixed decalin flames. <i>Proceedings of the Combustion Institute</i> , 2017, 36, 1193-1202.	3.9	14
52	Phase–Transformation Engineering in Cobalt Diselenide Realizing Enhanced Catalytic Activity for Hydrogen Evolution in an Alkaline Medium. <i>Advanced Materials</i> , 2016, 28, 7527-7532.	21.0	307
53	Experimental and Kinetic Modeling Study of Nitroethane Pyrolysis at a Low Pressure: Competition Reactions in the Primary Decomposition. <i>Energy &amp; Fuels</i> , 2016, 30, 7738-7745.	5.1	12
54	Metallic Nickel Hydroxide Nanosheets Give Superior Electrocatalytic Oxidation of Urea for Fuel Cells. <i>Angewandte Chemie - International Edition</i> , 2016, 55, 12465-12469.	13.8	356

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55	Manganous oxide nanoparticles encapsulated in few-layer carbon as an efficient electrocatalyst for oxygen reduction in alkaline media. Journal of Materials Chemistry A, 2016, 4, 11775-11781.	10.3	27
56	Experimental and kinetic modeling investigation on decalin pyrolysis at low to atmospheric pressures. Combustion and Flame, 2016, 167, 228-237.	5.2	18
57	Additional chain-branching pathways in the low-temperature oxidation of branched alkanes. Combustion and Flame, 2016, 164, 386-396.	5.2	94
58	Online Study on the Catalytic Pyrolysis of Bituminous Coal over HUSY and HZSM-5 with Photoionization Time-of-Flight Mass Spectrometry. Energy & Fuels, 2016, 30, 1598-1604.	5.1	45
59	Pyrolysis of 2-methyl-1-butanol at low and atmospheric pressures: Mass spectrometry and modeling studies. Proceedings of the Combustion Institute, 2015, 35, 409-417.	3.9	14
60	Experimental and kinetic modeling study of premixed o-xylene flames. Proceedings of the Combustion Institute, 2015, 35, 1745-1752.	3.9	45
61	Investigation on primary decomposition of ethylcyclohexane at atmospheric pressure. Proceedings of the Combustion Institute, 2015, 35, 367-375.	3.9	47
62	Experimental and kinetic modeling study of the low- and intermediate-temperature oxidation of dimethyl ether. Combustion and Flame, 2015, 162, 1113-1125.	5.2	120
63	Kinetics of ethylcyclohexane pyrolysis and oxidation: An experimental and detailed kinetic modeling study. Combustion and Flame, 2015, 162, 2873-2892.	5.2	70
64	Molecular co-catalyst accelerating hole transfer for enhanced photocatalytic H <sub>2</sub> evolution. Nature Communications, 2015, 6, 8647.	12.8	172
65	Towards high-level theoretical studies of large biodiesel molecules: an ONIOM [QCISD(T)/CBS:DFT] study of hydrogen abstraction reactions of C <sub>n</sub> H <sub>2n+1</sub> COOC <sub>m</sub> H <sub>2m+1</sub> + H. Physical Chemistry Chemical Physics, 2015, 17, 200-208.	2.8	26
66	Hydrogen dangling bonds induce ferromagnetism in two-dimensional metal-free graphitic-C <sub>3</sub> N <sub>4</sub> nanosheets. Chemical Science, 2015, 6, 283-287.	7.4	62
67	Density functional theory study of the reactions of 2-azido- N , N -dimethylethanamine with nitric acid and nitrogen dioxide. Combustion and Flame, 2015, 162, 237-248.	5.2	8
68	A theoretical kinetics study of the reactions of methylbutanoate with hydrogen and hydroxyl radicals. Proceedings of the Combustion Institute, 2015, 35, 481-489.	3.9	40
69	Experimental and kinetic modeling study of i-butanol pyrolysis and combustion. Combustion and Flame, 2014, 161, 1955-1971.	5.2	28
70	Experimental and kinetic modeling study on methylcyclohexane pyrolysis and combustion. Combustion and Flame, 2014, 161, 84-100.	5.2	126
71	Large Negative Magnetoresistance Induced by Anionic Solid Solutions in Two-Dimensional Spin-Frustrated Transition Metal Chalcogenides. Physical Review Letters, 2014, 113, 157202.	7.8	39
72	Kinetics of Homoallylic/Homobenzylic Rearrangement Reactions under Combustion Conditions. Journal of Physical Chemistry A, 2014, 118, 6741-6748.	2.5	16

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73	Experimental and kinetic modeling study of pyrolysis and oxidation of n-decane. Combustion and Flame, 2014, 161, 1701-1715.	5.2	87
74	Interactions of disulfide-constrained cyclic tetrapeptides with Cu <sup>2+</sup> . Journal of Biological Inorganic Chemistry, 2013, 18, 277-286.	2.6	4
75	Experimental and kinetic modeling study of tetralin pyrolysis at low pressure. Proceedings of the Combustion Institute, 2013, 34, 1739-1748.	3.9	53
76	An experimental and modeling study of methyl propanoate pyrolysis at low pressure. Combustion and Flame, 2013, 160, 1958-1966.	5.2	50
77	Experimental and kinetic modeling study of 2-butanol pyrolysis and combustion. Combustion and Flame, 2013, 160, 1939-1957.	5.2	58
78	An experimental and theoretical study of pyrrolidine pyrolysis at low pressure. Proceedings of the Combustion Institute, 2013, 34, 641-648.	3.9	9
79	An experimental and kinetic modeling study of premixed nitroethane flames at low pressure. Proceedings of the Combustion Institute, 2013, 34, 617-624.	3.9	29
80	An experimental and kinetic modeling investigation on a rich premixed n-propylbenzene flame at low pressure. Proceedings of the Combustion Institute, 2013, 34, 1785-1793.	3.9	41
81	Experimental and theoretical studies of pyrolysis of chrysophanol and its derivatives. Journal of Analytical and Applied Pyrolysis, 2013, 100, 237-244.	5.5	2
82	Kinetics of Decomposition and Isomerization of Methylcyclohexane: Starting Point for Studying Monoalkylated Cyclohexanes Combustion. Energy & Fuels, 2013, 27, 1679-1687.	5.1	44
83	Product Identification and Mass Spectrometric Analysis of <i>n</i> -Butane and <i>i</i> -Butane Pyrolysis at Low Pressure. Chinese Journal of Chemical Physics, 2013, 26, 151-156.	1.3	9
84	Experimental and Theoretical Study on Pyrolysis of Isopsoralen. Chinese Journal of Chemical Physics, 2012, 25, 249-253.	1.3	1
85	VUV Photoionization and Dissociation of Tyramine and Dopamine: the Joint Experimental and Theoretical Studies. Chinese Journal of Chemical Physics, 2012, 25, 11-18.	1.3	5
86	Thermal Decomposition of 1-Pentanol and Its Isomers: A Theoretical Study. Journal of Physical Chemistry A, 2012, 116, 9238-9244.	2.5	44
87	Experimental and Kinetic Modeling Study of <i>n</i> -Butanol Pyrolysis and Combustion. Energy & Fuels, 2012, 26, 5550-5568.	5.1	123
88	Experimental and kinetic modeling study of tert-butanol combustion at low pressure. Energy, 2012, 43, 94-102.	8.8	29
89	Theoretical Studies on the Unimolecular Decomposition of Propanediols and Glycerol. Journal of Physical Chemistry A, 2012, 116, 4457-4465.	2.5	13
90	Theoretical Studies on the Unimolecular Decomposition of Ethylene Glycol. Journal of Physical Chemistry A, 2012, 116, 55-63.	2.5	30

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91	Synchrotron vacuum ultraviolet (VUV) photo-induced fragmentation of cyclic dipeptides radical cations. <i>Amino Acids</i> , 2012, 43, 279-287.	2.7	2
92	An experimental and kinetic modeling study of three butene isomers pyrolysis at low pressure. <i>Combustion and Flame</i> , 2012, 159, 905-917.	5.2	141
93	An experimental and kinetic modeling study of cyclohexane pyrolysis at low pressure. <i>Combustion and Flame</i> , 2012, 159, 2243-2253.	5.2	110
94	Pyrolysis of <i>n</i> -Heptane: Experimental and Theoretical Study. <i>Journal of Physical Chemistry A</i> , 2011, 115, 1593-1601.	2.5	50
95	Unimolecular Decomposition of Ethyl Hydroperoxide: Ab Initio/Rice-Kramers/Marcus Theoretical Prediction of Rate Constants. <i>Journal of Physical Chemistry A</i> , 2011, 115, 602-611.	2.5	19
96	Experimental and theoretical studies on decomposition of pyrrolidine. <i>Proceedings of the Combustion Institute</i> , 2011, 33, 415-423.	3.9	16
97	Experimental and modeling investigation on premixed ethylbenzene flames at low pressure. <i>Proceedings of the Combustion Institute</i> , 2011, 33, 617-624.	3.9	56
98	Investigation on chemical structures of premixed toluene flames at low pressure. <i>Proceedings of the Combustion Institute</i> , 2011, 33, 593-600.	3.9	113
99	VUV photon-induced ionization/dissociation of antipyrine and propyphenazone: mass spectrometric and theoretical insights. <i>Journal of Mass Spectrometry</i> , 2010, 45, 734-739.	1.6	9
100	Investigation on fuel-rich premixed flames of monocyclic aromatic hydrocarbons: Part I. Intermediate identification and mass spectrometric analysis. <i>Combustion and Flame</i> , 2010, 157, 143-154.	5.2	83
101	Kinetic modeling study of toluene pyrolysis at low pressure. <i>Combustion and Flame</i> , 2010, 157, 1686-1697.	5.2	111
102	Determination of absolute photoionization cross-sections of alkanes and cycloalkanes. <i>Rapid Communications in Mass Spectrometry</i> , 2010, 24, 1335-1342.	1.5	53
103	Photoionisation and photodissociation studies of nonvolatile organic molecules by synchrotron VUV photoionisation mass spectrometry and theoretical calculations. <i>International Reviews in Physical Chemistry</i> , 2010, 29, 369-401.	2.3	20
104	Vacuum Ultraviolet Photofragmentation of Sarcosine: Photoionization Mass Spectrometric and Theoretical Insights. <i>Journal of Physical Chemistry A</i> , 2010, 114, 3411-3417.	2.5	14
105	THEORETICAL STUDIES ON PHOTOIONIZATION OF GUANINE TAUTOMERS AND INTERCONVERSION OF CATION RADICALS. <i>Journal of Theoretical and Computational Chemistry</i> , 2009, 08, 1103-1115.	1.8	6
106	Photoionization and Dissociative Photoionization Study of Cholesterol by IR Laser Desorption/Tunable Synchrotron VUV Photoionization Mass Spectrometry. <i>Chinese Journal of Chemical Physics</i> , 2009, 22, 129-133.	1.3	3
107	Identification of Intermediates in Pyridine Pyrolysis with Molecular-beam Mass Spectrometry and Tunable Synchrotron VUV Photoionization. <i>Chinese Journal of Chemical Physics</i> , 2009, 22, 204-209.	1.3	12
108	An experimental study of the rich premixed ethylbenzene flame at low pressure. <i>Proceedings of the Combustion Institute</i> , 2009, 32, 647-655.	3.9	51



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109	An experimental and kinetic modeling study of a premixed nitromethane flame at low pressure. Proceedings of the Combustion Institute, 2009, 32, 311-318.	3.9	70
110	Investigation of the rich premixed laminar acetylene/oxygen/argon flame: Comprehensive flame structure and special concerns of polyynes. Proceedings of the Combustion Institute, 2009, 32, 1293-1300.	3.9	66
111	An experimental and kinetic modeling study of premixed NH <sub>3</sub> /CH <sub>4</sub> /O <sub>2</sub> /Ar flames at low pressure. Combustion and Flame, 2009, 156, 1413-1426.	5.2	359
112	An experimental and theoretical study of toluene pyrolysis with tunable synchrotron VUV photoionization and molecular-beam mass spectrometry. Combustion and Flame, 2009, 156, 2071-2083.	5.2	111
113	Conformation-Specific Pathways of Î <sup>2</sup> -Alanine: A Vacuum Ultraviolet Photoionization and Theoretical Study. Journal of Physical Chemistry A, 2009, 113, 5838-5845.	2.5	22
114	An Experimental and Theoretical Study of Pyrrole Pyrolysis with Tunable Synchrotron VUV Photoionization and Molecular-Beam Mass Spectrometry. Journal of Physical Chemistry A, 2009, 113, 5397-5405.	2.5	35
115	Experimental Study of a Fuel-Rich Premixed Toluene Flame at Low Pressure. Energy & Fuels, 2009, 23, 1473-1485.	5.1	184
116	Intramolecular hydrogen transfer in the ionization process of Î±-alanine. Physical Chemistry Chemical Physics, 2009, 11, 1189.	2.8	22
117	Photoionization studies on various quinones by an infrared laser desorption/tunable VUV photoionization TOF mass spectrometry. Journal of Mass Spectrometry, 2008, 43, 1701-1710.	1.6	25
118	Dissociative Photoionization Mechanism of 1,8-Dihydroxyanthraquinone: An Experimental and Theoretical Study. Journal of Physical Chemistry A, 2008, 112, 10977-10984.	2.5	7
119	Pyrolysis of Methyl tert-Butyl Ether (MTBE). 2. Theoretical Study of Decomposition Pathways. Journal of Physical Chemistry A, 2008, 112, 10495-10501.	2.5	19
120	Pyrolysis of Methyl tert-Butyl Ether (MTBE). 1. Experimental Study with Molecular-Beam Mass Spectrometry and Tunable Synchrotron VUV Photoionization. Journal of Physical Chemistry A, 2008, 112, 10487-10494.	2.5	74
121	Theoretical Study of the AlEt <sub>3</sub> -Promoted Tandem Reductive Rearrangement of Epoxides. Chinese Journal of Chemical Physics, 2008, 21, 547-554.	1.3	3
122	Molecular Dynamics and Density Functional Studies of Substrate Binding and Catalysis of Arginine Deiminase. Journal of Physical Chemistry B, 2007, 111, 3267-3273.	2.6	10
123	Supermolecule density functional calculations suggest a key role for solvent in alkaline hydrolysis of p-nitrophenyl phosphate. Chemical Communications, 2007, , 1638.	4.1	42
124	Electronic Excitations of Green Fluorescent Proteins: Modeling Solvatochromatic Shifts of Red Fluorescent Protein Chromophore Model Compound in Aqueous Solutions. Journal of Physical Chemistry B, 2007, 111, 14055-14063.	2.6	21
125	A computational investigation on the sequential rearrangement mechanism of 2-allyl-2,4,5-hexatrienaldehyde involving [1,5]-hydrogen migration and 8Î€-electrocyclization. Journal of Computational Chemistry, 2007, 28, 2164-2169.	3.3	5
126	ELECTRONIC EXCITATIONS OF GREEN FLUORESCENT PROTEINS: MODELING SOLVATOCHROMATIC SHIFTS OF CHROMOPHORE MODEL COMPOUNDS IN SOLUTIONS. Journal of Theoretical and Computational Chemistry, 2006, 05, 375-390.	1.8	7



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127	Density functional theory study of proton transfer in carbonic anhydrase. Science Bulletin, 2005, 50, 2557.	1.7	0
128	Theoretical Study of General Base-Catalyzed Hydrolysis of Aryl Esters and Implications for Enzymatic Reactions. Journal of Physical Chemistry B, 2005, 109, 5259-5266.	2.6	11
129	Reactivity of Metaphosphate and Thiometaphosphate in Water: A DFT Study. Journal of Physical Chemistry A, 2005, 109, 11295-11303.	2.5	14