Xiang-Yuan Li

List of Publications by Citations

160	2,164	25	38
papers	citations	h-index	g-index
166	2,502	3.5	5.11
ext. papers	ext. citations	avg, IF	L-index

#	Paper	IF	Citations
160	H S-Activable MOF Nanoparticle Photosensitizer for Effective Photodynamic Therapy against Cancer with Controllable Singlet-Oxygen Release. *Angewandte Chemie - International Edition*, **2017**, 56, 13752-13756	16.4	210
159	Reactive molecular dynamics simulation and chemical kinetic modeling of pyrolysis and combustion of n-dodecane. *Combustion and Flame*, **2011**, 158, 217-226	5.3	138
158	ReaxFF molecular dynamics simulations of oxidation of toluene at high temperatures. *Journal of Physical Chemistry A*, **2012**, 116, 9811-8	2.8	87
157	A shock tube study of the autoignition characteristics of RP-3 jet fuel. *Proceedings of the Combustion Institute*, **2015**, 35, 3151-3158	5.9	63
156	A new type of surface-enhanced Raman scattering sensor for the enantioselective recognition of d/l-cysteine and d/l-asparagine based on a helically arranged Ag NPs@homochiral MOF. *Chemical Communications*, **2016**, 52, 5432-5	5.8	52
155	H2S-Activable MOF Nanoparticle Photosensitizer for Effective Photodynamic Therapy against Cancer with Controllable Singlet-Oxygen Release. *Angewandte Chemie*, **2017**, 129, 13940-13944	3.6	49
154	Electron transfer in poly(p-phenylene) oligomers: effect of external electric field and application of Koopmans theorem. *Chemical Physics*, **1999**, 248, 137-146	2.3	45
153	Ab initio calculation for inner reorganization energy of gas-phase electron transfer in organic molecule□n systems. *Chemical Physics*, **2000**, 260, 283-294	2.3	37
152	Catalytic cracking of RP-3 jet fuel over wall-coated Pt/ZrO2□TiO2□Al2O3 catalysts with different Al2O3 ratios. *Journal of Analytical and Applied Pyrolysis*, **2015**, 111, 100-107	6	36
151	Theoretical Kinetic Study of Thermal Decomposition of Cyclohexane. *Energy & Fuels*, **2012**, 26, 2811-2820	4.2	35
150	Linker-Eliminated Nano Metal-Organic Framework Fluorescent Probe for Highly Selective and Sensitive Phosphate Ratiometric Detection in Water and Body Fluids. *Analytical Chemistry*, **2020**, 92, 3722-3727	7.8	33
149	Continuous medium theory for nonequilibrium solvation: I. How to correctly evaluate solvation free energy of nonequilibrium. *Journal of Computational Chemistry*, **2004**, 25, 500-9	3.5	33
148	Time-dependent density functional theory study on intramolecular charge transfer and solvent effect of dimethylaminobenzophenone. *Journal of Chemical Physics*, **2005**, 122, 84314	3.9	33
147	Recyclable Diels□Alder Furan/Maleimide Polymer Networks with Shape Memory Effect. *Industrial & Engineering Chemistry Research*, **2014**, 53, 16156-16163	3.9	32
146	Theoretical calculation of reorganization energy for electron self-exchange reaction by constrained density functional theory and constrained equilibrium thermodynamics. *Journal of Physical Chemistry A*, **2013**, 117, 8017-25	2.8	32
145	Low- and intermediate-temperature oxidation of ethylcyclohexane: A theoretical study. *Combustion and Flame*, **2015**, 162, 4167-4182	5.3	31
144	Characterization of CVD TiN coating at different deposition temperatures and its application in hydrocarbon pyrolysis. *Surface and Coatings Technology*, **2014**, 258, 1060-1067	4.4	30

143	Correlation between structure, acidity and activity of Mo-promoted Pt/ZrO2-TiO2-Al2O3 catalysts for n-decane catalytic cracking. *Applied Thermal Engineering*, **2017**, 111, 811-818	5.8	30
142	Inhibition Effect of APCVD Titanium Nitride Coating on Coke Growth during n-Hexane Thermal Cracking under Supercritical Conditions. *Industrial & Engineering Chemistry Research*, **2014**, 53, 5432-5442	3.9	29
141	Molecular Orbital Analysis in Evaluation of Electron-Transfer Matrix Element by Koopmans' Theory. *Journal of Physical Chemistry A*, **2004**, 108, 4125-4131	2.8	29
140	Curing kinetics and shape-memory behavior of an intrinsically toughened epoxy resin system. *Journal of Thermal Analysis and Calorimetry*, **2015**, 119, 537-546	4.1	27
139	Molecular-level modeling investigation of n-decane pyrolysis at high temperature. *Journal of Analytical and Applied Pyrolysis*, **2017**, 128, 412-422	6	26
138	Effects of fuel additives on the thermal cracking of n-decane from reactive molecular dynamics. *Journal of Physical Chemistry A*, **2012**, 116, 3794-801	2.8	26
137	Theoretical Prediction of Rate Constants for Hydrogen Abstraction by OH, H, O, CH3, and HO2 Radicals from Toluene. *Journal of Physical Chemistry A*, **2016**, 120, 3424-32	2.8	26
136	Kerosene cracking over supported monolithic Pt catalysts: Effects of SrO and BaO promoters. *Chinese Journal of Catalysis*, **2013**, 34, 1139-1147	11.3	25
135	Electron transfer between biphenyl and biphenyl anion radicals: Reorganization energies and electron transfer matrix elements. *Journal of Computational Chemistry*, **1999**, 20, 597-603	3.5	24
134	Spectral shifts of the n -j□ and □j□ transitions of uracil based on a modified form of solvent reorganization energy. *Physical Chemistry Chemical Physics*, **2012**, 14, 13284-91	3.6	23
133	Thermal, mechanical and shape memory properties of an intrinsically toughened epoxy/anhydride system. *Journal of Polymer Research*, **2014**, 21, 1	2.7	22
132	Catalytic Cracking of RP-3 Jet Fuel over Pt/CeO2□Al2O3by Adding Cu/ZSM-5. *Energy & Fuels*, **2014**, 28, 5382-5388	4.1	22
131	Electric field dependence of the diabatic potential energy surface for gas-phase electron transfer O2O2□jO2□2. *Chemical Physics Letters*, **1995**, 233, 227-230	2.5	22
130	An overview of continuum models for nonequilibrium solvation: Popular theories and new challenge. *International Journal of Quantum Chemistry*, **2015**, 115, 700-721	2.1	21
129	Experimental and modeling study of thermal and catalytic cracking of n-decane. *Journal of Analytical and Applied Pyrolysis*, **2014**, 110, 463-469	6	21
128	Continuous medium theory for nonequilibrium solvation: II. Interaction energy between solute charge and reaction field and single-sphere model for spectral shift. *Journal of Computational Chemistry*, **2004**, 25, 835-42	3.5	21
127	Electron transfer between tryptophan and tyrosine: Theoretical calculation of electron transfer matrix element for intramolecular hole transfer. *Journal of Computational Chemistry*, **2001**, 22, 565-579	3.5	21
126	Shock-Tube Study of Dimethoxymethane Ignition at High Temperatures. *Energy & Fuels*, **2014**, 28, 4603-4610	4.1	20

125	Spectral shift of the n -j* transition for acetone and formic acid with an explicit solvent model. *Journal of Physical Chemistry A*, **2011**, 115, 232-43	2.8	19
124	Solvent effect on the UV/Vis absorption spectra in aqueous solution: The nonequilibrium polarization with an explicit representation of the solvent environment. *Computational and Theoretical Chemistry*, **2011**, 971, 65-72	2	18
123	CONTINUOUS MEDIUM THEORY FOR NONEQUILIBRIUM SOLVATION: NEW FORMULATIONS AND AN OVERVIEW OF THEORIES AND APPLICATIONS. *Journal of Theoretical and Computational Chemistry*, **2005**, 04, 907-983	1.8	18
122	SOLVATION ENERGY OF NONEQUILIBRIUM POLARIZATION: OLD QUESTION, NEW ANSWER. *Journal of Theoretical and Computational Chemistry*, **2010**, 09, 23-37	1.8	17
121	Nonequilibrium solvation energy by means of constrained equilibrium thermodynamics and its application to self-exchange electron transfer reactions. *Physical Chemistry Chemical Physics*, **2010**, 12, 1341-50	3.6	17
120	Pressure-Dependent Rate Rules for Intramolecular H-Migration Reactions of Hydroperoxyalkylperoxy Radicals in Low Temperature. *Journal of Physical Chemistry A*, **2017**, 121, 3001-3018	2.8	16
119	A modified two-sphere model for solvent reorganization energy in electron transfer. *Physical Chemistry Chemical Physics*, **2012**, 14, 5538-44	3.6	15
118	Vertical detachment energy of hydrated electron based on a modified form of solvent reorganization energy. *Journal of Physical Chemistry B*, **2010**, 114, 2189-97	3.4	15
117	Continuous medium theory for nonequilibrium solvation: IV. Solvent reorganization energy of electron transfer based on conductor-like screening model. *Journal of Computational Chemistry*, **2006**, 27, 368-74	3.5	15
116	Quantum chemical study on excited states and electronic coupling matrix element in a catechol-bridge-dicyanoethylene system. *Journal of Physical Chemistry A*, **2005**, 109, 4154-61	2.8	15
115	Catalytic Cracking of n-Decane over Monometallic and Bimetallic Pt□Ni/MoO3/La□Al2O3 Catalysts: Correlations of Surface Properties and Catalytic Behaviors. *Industrial & Engineering Chemistry Research*, **2019**, 58, 1823-1833	3.9	15
114	Pressure-dependent kinetics of initial reactions in iso-octane pyrolysis. *Journal of Physical Chemistry A*, **2015**, 119, 4093-107	2.8	14
113	Mechanism construction and simulation for high-temperature combustion of n-propylcyclohexane. *Chemical Research in Chinese Universities*, **2014**, 30, 480-488	2.2	14
112	Ab initio study on electron excitation and electron transfer in tryptophan□yrosine system. *Chemical Physics*, **2002**, 284, 543-554	2.3	14
111	Pressure-dependent rate rules for intramolecular H-migration reactions of normal-alkyl cyclohexylperoxy radicals. *Combustion and Flame*, **2019**, 204, 176-188	5.3	13
110	Flow distribution of hydrocarbon fuel in parallel minichannels heat exchanger. *AICHE Journal*, **2018**, 64, 2781-2791	3.6	13
109	Influence of TiN coating on products distribution for hydrocarbon fuel cracking under high temperature and pressure. *Journal of Analytical and Applied Pyrolysis*, **2014**, 107, 197-203	6	13
108	Multichannel photoinduced intramolecular electron-transfer excitations in a bis-naphthalimide spermine conjugate by time-dependent density functional theory. *Journal of Physical Chemistry A*, **2007**, 111, 13061-8	2.8	13

107	Shock tube study of n-nonane/air ignition over a wide range of temperatures. *Fuel*, **2017**, 188, 567-574	7.1	12
106	An ab initio/Rice-Ramsperger-Kassel-Marcus prediction of rate constant and product branching ratios for unimolecular decomposition of propen-2-ol and related H + CH2COHCH2 reaction. *Journal of Chemical Physics*, **2008**, 129, 234301	3.9	12
105	An anti-quinoid structure in dual fluorescence of fluozazene molecule and solvent effect of intramolecular charge transfer. *Chemical Physics*, **2007**, 332, 325-335	2.3	12
104	Temperature and pressure dependent rate coefficients for the reaction of C2H4 + HO2 on the C2H4O2H potential energy surface. *Journal of Physical Chemistry A*, **2015**, 119, 3161-70	2.8	11
103	Shock tube measurements and kinetic modeling study on autoignition characteristics of cyclohexanone. *Combustion and Flame*, **2018**, 192, 358-368	5.3	11
102	Experimental and numerical analysis on flow characteristics and pyrolysis mechanism of hydrocarbon fuel with a novel online hybrid method. *Energy Conversion and Management*, **2019**, 198, 111817	10.6	11
101	New formulation for nonequilibrium solvation: a consistent expression of electrostatic free energy by different methods and its application to solvent reorganization energy and spectral shifts in solution. *Computational and Theoretical Chemistry*, **2005**, 715, 157-175		11
100	Continuous medium theory for nonequilibrium solvation: III. Solvation shift by monopole approximation and multipole expansion in spherical cavity. *Journal of Computational Chemistry*, **2005**, 26, 399-409	3.5	11
99	Pressure-dependent rate rules for cycloaddition, intramolecular H-shift, and concerted elimination reactions of alkenyl peroxy radicals at low temperature. *Physical Chemistry Chemical Physics*, **2019**, 21, 10693-10705	3.6	10
98	Theoretical and kinetic study of reaction C2H + C3H6 on the C5H7 potential energy surface. *Theoretical Chemistry Accounts*, **2015**, 134, 1	1.9	10
97	High catalytic activity and stability quasi homogeneous alkali metal promoted Ni/SiO2 aerogel catalysts for catalytic cracking of n-decane. *Fuel*, **2020**, 268, 117384	7.1	10
96	Reaction of ketenyl radical with hydroxyl radical over C2H2O2 potential energy surface: A theoretical study. *Combustion and Flame*, **2014**, 161, 885-897	5.3	10
95	The performance of Pt/ZrxTixAl1−xO2 as Kerosene cracking catalysts. *Chinese Journal of Catalysis*, **2014**, 35, 175-184	11.3	10
94	Reaction mechanism on the activation of ethane C–H and C–C bonds by a diplatinum cluster. *Theoretical Chemistry Accounts*, **2013**, 132, 1	1.9	9
93	Solvent effect on UV/Vis absorption and emission spectra in aqueous solution based on a modified form of solvent reorganization energy. *Chemical Physics Letters*, **2013**, 583, 213-217	2.5	9
92	Unimolecular decomposition mechanism of vinyl alcohol by computational study. *Theoretical Chemistry Accounts*, **2011**, 128, 341-348	1.9	9
91	A theoretical search for stable bent and linear structures of low-lying electronic states of the titanium dioxide (TiO2) molecule. *RSC Advances*, **2011**, 1, 1228	3.7	9
90	Single-sphere model for absorption spectrum of interfacial molecules with application to predictions of orientational angles. *Journal of Physical Chemistry B*, **2006**, 110, 10088-94	3.4	9

89	Theoretical study of photoinduced electron transfer from tetramethylethylene to tetracyanoethylene. *Journal of Chemical Physics*, **2003**, 119, 8854-8863	3.9	9
88	Activation of propane C□H and C□C bonds by a diplatinum cluster: potential energy surfaces and reaction mechanisms. *Structural Chemistry*, **2014**, 25, 471-481	1.8	8
87	Kinetic study of the formation of triphenylene from the condensation of C12H10 + C6H5. *Computational and Theoretical Chemistry*, **2012**, 985, 1-7	2	8
86	Thermodynamics for nonequilibrium solvation and numerical evaluation of solvent reorganization energy. *Science in China Series B: Chemistry*, **2008**, 51, 1246-1256		8
85	NEW FORMULATION FOR NON-EQUILIBRIUM SOLVATION: SPECTRAL SHIFTS AND CAVITY RADII OF 6-PROPANOYL-2-(N,N-DIMETHYLAMINO) NAPHTHALENE AND 4-(N,N-DIMETHYLAMINO) BENZONITRILE. *Journal of Theoretical and Computational Chemistry*, **2006**, 05, 355-374	1.8	8
84	Investigation of photoinduced electron transfer in model system of vitamin E-duroquinone by time-dependent density functional theory. *Journal of Chemical Physics*, **2004**, 120, 10025-32	3.9	8
83	Theoretical investigation of electron transfer transition in tetracyanoethylene-contained organic complexes. *Journal of Computational Chemistry*, **2002**, 23, 874-86	3.5	8
82	Electron transfer integral between two zero-overlap states. *Journal of Computational Chemistry*, **1996**, 17, 1108-1111	3.5	8
81	An experimental and modeling study of ethylene□ir combustion over a wide temperature range. *Combustion and Flame*, **2020**, 221, 20-40	5.3	8
80	Photoinduced charge-transfer electronic excitation of tetracyanoethylene/tetramethylethylene complex in dichloromethane. *Chemical Physics Letters*, **2017**, 679, 158-163	2.5	7
79	Solvent effects for vertical absorption and emission processes in solution using a self-consistent state specific method based on constrained equilibrium thermodynamics. *Physical Chemistry Chemical Physics*, **2018**, 20, 13178-13190	3.6	7
78	New formulation for non-equilibrium solvation: dielectric constant change during charging process and influence of slow response of polarization upon solvent reorganization energy of electron transfer. *Computational and Theoretical Chemistry*, **2004**, 671, 239-248		7
77	An experimental and numerical investigation on thermal cracking of n-decane in the microchannel. *Petroleum Science and Technology*, **2016**, 34, 555-561	1.4	7
76	Electron transfer NO +2 +NO-N02+NO+ in aromatic nitration. *Science in China Series B: Chemistry*, **1997**, 40, 523-528		6
75	A study on orientation and absorption spectrum of interfacial molecules by using continuum model. *Journal of Computational Chemistry*, **2008**, 29, 198-210	3.5	6
74	Ab initio study of hydrogen bonding interaction and photoinduced electron transfer between 4-nitroquinoline-1-oxide and tryptophan. *International Journal of Quantum Chemistry*, **2004**, 98, 33-43	2.1	6
73	A theoretical study of solvent effect and reaction mechanism of electron transfer reaction between indole side chain and phenol side chain of peptide involving tryptophan and tyrosine. *Journal of Computational Chemistry*, **2001**, 22, 1067-1081	3.5	6
72	Application of Koopmans□theorem in evaluating electron transfer matrix element of long-range electron transfer. *Computational and Theoretical Chemistry*, **2000**, 530, 49-58		6

71	Ab initio study of long-range electron transfer between biphenyl anion radical and naphthalene. *Science in China Series B: Chemistry*, **1999**, 42, 441-448		6
70	A Comprehensive Investigation of the Pyrolysis Effect on Heat Transfer Characteristics for n-Decane in the Horizon Mini-Channel. *Energy & Fuels*, **2020**, 34, 199-210	4.1	6
69	Theoretical Study on Reactions of Alkylperoxy Radicals. *Journal of Physical Chemistry A*, **2019**, 123, 3949-3958	2.8	5
68	Numerical solution of solvent reorganization energy and its application in electron transfer reaction. *Theoretical Chemistry Accounts*, **2014**, 133, 1	1.9	5
67	Solvent effects on excitation energies obtained using the state-specific TD-DFT method with a polarizable continuum model based on constrained equilibrium thermodynamics. *Physical Chemistry Chemical Physics*, **2017**, 19, 32242-32252	3.6	5
66	Shock-Tube Study of the Ignition of Gas-Phase 1,3,5-Trimethylbenzene in Air. *Energy & Fuels*, **2014**, 28, 6707-6713	4.1	5
65	Shock tube study of n-decane ignition at low pressures. *Acta Mechanica Sinica/Lixue Xuebao*, **2012**, 28, 79-82	2	5
64	Vertical ionization energies of halogen anions in solution. *Science China Chemistry*, **2010**, 53, 1316-1321	7.9	5
63	Intramolecular electron transfer in cyclopeptide involving tryptophan and tyrosine and corrected two-sphere model for solvent reorganization energy. *Chemical Physics*, **2005**, 312, 21-29	2.3	5
62	Self-consistent reaction field calculation of solvent reorganization energy in electron transfer: a dipole-reaction field interaction model. *Theoretical Chemistry Accounts*, **2000**, 105, 77-85	1.9	5
61	A preliminary study of electron transfer reactions between indole and phenol and their consequences for tryptophan and tyrosine. *Computational and Theoretical Chemistry*, **1999**, 459, 123-129		5
60	Preparation of Al2O3 coating on TiN coating by polymer-assisted deposition to improve oxidation resistance in coking inhibition applications. *Ceramics International*, **2020**, 46, 7774-7782	5.1	5
59	Reactions of □hydroxypropyl radicals with O2 on the HOC3H6OO□potential energy surfaces: A theoretical study. *Combustion and Flame*, **2020**, 211, 202-217	5.3	5
58	An experimental and simulated investigation on pyrolysis of blended cyclohexane and benzene under supercritical pressure. *Petroleum Chemistry*, **2017**, 57, 71-78	1.1	4
57	Rate rules for hydrogen abstraction reaction kinetics of polycyclic aromatic hydrocarbons and vinyl radical. *Theoretical Chemistry Accounts*, **2020**, 139, 1	1.9	4
56	Prediction of HIV-1 Protease Inhibitors Using Machine Learning Approaches. *QSAR and Combinatorial Science*, **2009**, 28, 1346-1357		4
55	A THEORETICAL STUDY ON DUAL FLUORESCENCE OF 4-DIMETHYLAMINOPYRIDINE BY POLARIZABLE CONTINUUM MODEL. *Journal of Theoretical and Computational Chemistry*, **2008**, 07, 821-832	1.8	4
54	Nonequilibrium solvation theory: Comparison, modification and application. *Science Bulletin*, **2003**, 48, 965-970		4

53	Study on photochemistry of concerted [1,j] and [i,j] sigmatropic rearrangements by the classical path method. *Computational and Theoretical Chemistry*, **1995**, 342, 181-186		4
52	Relationship between Energetic Performance and Clustering Effects on Incremental Nitramine Groups: A Theoretical Perspective. *Journal of Physical Chemistry A*, **2019**, 123, 742-749	2.8	4
51	Enhanced cracking conversion of supercritical fuel over stabilized Pt nanoparticles supported SiO2-Al2O3 catalyst coating. *Applied Surface Science*, **2021**, 559, 149950	6.7	4
50	Calculation of the rate constants for concerted elimination reaction class of hydroperoxyl-alkyl-peroxyl radicals. *Theoretical Chemistry Accounts*, **2017**, 136, 1	1.9	3
49	Theoretical study on electronic excitation spectra: A matrix form of numerical algorithm for spectral shift. *Chemical Physics*, **2017**, 492, 27-34	2.3	3
48	Pressure-Dependent Rate Rules for the Intramolecular H-Shift Reactions of Hydroperoxy-Alkenyl-Peroxy Radicals in Low Temperature. *Energy & Fuels*, **2019**, 33, 5597-5609	4.1	3
47	Spectral Shift of □ Transition for p-Nitroaniline Based on a New Expression of Nonequilibrium Solvation Energy. *Chinese Journal of Chemical Physics*, **2014**, 27, 181-188	0.9	3
46	Accurate prediction of thermodynamic properties of alkyl peroxides by combining density functional theory calculation with least-square calibration. *Journal of Computational Chemistry*, **2009**, 30, 1007-15	3.5	3
45	Electronic coupling matrix elements of U-shaped donor-bridge-acceptor molecules and influence of mediated benzene solvent. *Chemical Physics Letters*, **2005**, 414, 71-75	2.5	3
44	Investigation on Carburization during the Repeated Coking and Decoking Process. *Industrial & Engineering Chemistry Research*, **2020**, 59, 13051-13059	3.9	3
43	High-Pressure-Limit and Pressure-Dependent Rate Rules for Unimolecular Reactions Related to Hydroperoxy Alkyl Radicals in Normal-Alkyl Cyclohexane Combustion. 2. Cyclization Reaction Class. *Journal of Physical Chemistry A*, **2021**, 125, 8959-8977	2.8	3
42	Theoretical Study of Radical-Molecule Reactions with Negative Activation Energies in Combustion: Hydroxyl Radical Addition to Alkenes. *ACS Omega*, **2020**, 5, 12777-12788	3.9	2
41	Rate rules for hydrogen abstraction reaction kinetics of alkenes from allylic sites by HO2 radical. *Computational and Theoretical Chemistry*, **2020**, 1179, 112795	2	2
40	Novel nonequilibrium solvation theory for calculating the solvatochromic Stokes shift by State-specific TD-DFT. *Chemical Physics Letters*, **2019**, 732, 136640	2.5	2
39	Polarizable continuum model associated with the self-consistent-reaction field for molecular adsorbates at the interface. *Physical Chemistry Chemical Physics*, **2010**, 12, 207-14	3.6	2
38	Accurate prediction of enthalpies of formation for a large set of organic compounds. *Journal of Computational Chemistry*, **2010**, 31, 2585-92	3.5	2
37	Explicit solvent model for spectral shift of acrolein and simulation with molecular dynamics. *Science Bulletin*, **2006**, 51, 2951-2958		2
36	Absorption Spectra and Photoreactivity of p-Aminobenzophenone by Time-dependent Density Functional Theory. *Chinese Journal of Chemical Physics*, **2007**, 20, 273-278	0.9	2

35	Kinetic Analysis for Reaction of Cyclopentadiene with Hydroperoxyl Radical under Low- and Medium-Temperature Combustion. *Journal of Physical Chemistry A*, **2020**, 124, 8280-8291	2.8	2
34	Novel nonequilibrium solvation theory for calculating the vertical ionization energies of alkali metal cations and DNA bases in aqueous. *Theoretical Chemistry Accounts*, **2018**, 137, 1	1.9	2
33	Combined strategy and Ni NPs/SiO2 aerogel catalyst for cracking hydrocarbon fuels. *Journal of Power Sources*, **2021**, 506, 230172	8.9	2
32	High-Pressure-Limit and Pressure-Dependent Rate Rules for Unimolecular Reactions Related to Hydroperoxy Alkyl Radicals in Normal Alkyl Cyclohexane Combustion. 1. Concerted HO Elimination Reaction Class and Scission Reaction Class. *Journal of Physical Chemistry A*, **2021**, 125, 8942-8958	2.8	2
31	Theoretical study of hydrogen abstraction by small radicals from cyclohexane-carbonyl-hydroperoxide. *Theoretical Chemistry Accounts*, **2019**, 138, 1	1.9	1
30	Soulieoside U, a new cycloartane triterpene glycoside from. *Natural Product Research*, **2020**, 1-6	2.3	1
29	Investigations on the thermal cracking and pyrolysis mechanism of China No.3 aviation kerosene under supercritical conditions. *Petroleum Science and Technology*, **2018**, 36, 1396-1404	1.4	1
28	Catalytic cracking of n-decane over NiOMoO3 modified Pt/ZrO2TiO2Al2O3 catalyst with different Al2O3 ratios. *Petroleum Chemistry*, **2017**, 57, 666-672	1.1	1
27	Time-Dependent Stokes Shift from Solvent Dielectric Relaxation. *Chinese Journal of Chemical Physics*, **2010**, 23, 297-302	0.9	1
26	Continuum Model for Electronic Polarization Based on a Novel Dielectric Response Function. *Chinese Journal of Chemical Physics*, **2009**, 22, 481-488	0.9	1
25	Analytical Dielectric Spectrum Formula Based on Representative Frequencies. *Chinese Journal of Chemical Physics*, **2009**, 22, 262-268	0.9	1
24	Theoretical Study on Reactivity of Electron Transfer in Model-System of Oxidation of Amino Carbon-centered Radical by O2. *Chinese Journal of Chemistry*, **2010**, 20, 834-840	4.9	1
23	Solvent Reorganization Energy and Electronic Coupling for Intramolecular Electron Transfer in Biphenyl-Acceptor Anion Radicals. *Chinese Journal of Chemical Physics*, **2008**, 21, 45-54	0.9	1
22	Solvent Reorganization Energy of Intramolecular Electron Transfer in Peptides Involving Tryptophan and Tyrosine. *Chinese Journal of Chemistry*, **2008**, 26, 2003-2008	4.9	1
21	SOLVENT REORGANIZATION ENERGY WITH DIELECTRIC GREEN FUNCTIONAL AND ITS APPLICATION TO RETURN ELECTRON TRANSFER IN TETRACYANOETHYLENE-HEXAMETHYLBENZENE SYSTEM. *Journal of Theoretical and Computational Chemistry*, **2004**, 03, 609-627	1.8	1
20	Dipole reaction field interaction model for the solvent reorganization energy and its application to the benzoquinone benzoquinone anion radical system. *Theoretical Chemistry Accounts*, **2002**, 107, 282-290	1.9	1
19	One approach to calculating the solvent reorganization energy of intramolecular electron transfer. *Science Bulletin*, **2003**, 48, 35-38		1
18	Theoretical investigation of charge transfer excitation and charge recombination in acenaphthylene tetracyanoethylene complex. *International Journal of Quantum Chemistry*, **2003**, 94, 23-35	2.1	1

17	The kinetic model of cyclohexene-air combustion over a wide temperature range.. *RSC Advances*, **2021**, 11, 39907-39916	3.7	1
16	Experimental and numerical investigation on the isobaric heat capacity for methylcyclohexane at high temperature and high pressure. *Applied Thermal Engineering*, **2019**, 146, 613-621	5.8	1
15	Investigation on the Thermal Cracking of n -Decane under Supercritical Pressure by a Developed Online-Sampling Experimental Method. *Petroleum Chemistry*, **2020**, 60, 39-44	1.1	0
14	Two new cycloartane triterpenoid glycosides from the rhizomes of .. *Natural Product Research*, **2022**, 1-8	2.3	0
13	A comparative study on the autoignition characteristics of cyclopropane and propane at high temperatures. *Combustion and Flame*, **2022**, 237, 111881	5.3	0
12	Development of a detailed pyrolysis mechanism for C1–4 hydrocarbons under a wide range of temperature and pressure. *International Journal of Chemical Kinetics*, **2020**, 52, 796-821	1.4	0
11	The performance comparison in predicting n-decane pyrolysis process between three ANNs methods: MLP, RBFN and GRNN. *Petroleum Science and Technology*, **2019**, 37, 1053-1058	1.4	
10	Quasi-classical trajectory calculation of the chemical reaction Ba + m-C6H4ClCH3. *Canadian Journal of Chemistry*, **2013**, 91, 206-210	0.9	
9	Molecular orientations at interfaces by extended polarizable continuum model. *International Journal of Quantum Chemistry*, **2011**, 111, 2187-2195	2.1	
8	Influence of contaminations on combustion kinetics in hydrogen-fueled engine. *Science Bulletin*, **2009**, 54, 1317-1321	10.6	
7	COMMENT ON "VARIATIONAL ELECTROSTATICS FOR CHARGE SOLVATION". *Journal of Theoretical and Computational Chemistry*, **2009**, 08, 1099-1101	1.8	
6	Theoretical Study on Electron Transfer Matrix Element in Oxidation of α-Amino Carbon-Centered Radical by O2. *Chinese Journal of Chemistry*, **2010**, 20, 972-977	4.9	
5	Solvent reorganization energy of electron transfer by a modified ellipsoidal cavity model. *Computational and Theoretical Chemistry*, **2007**, 819, 32-40		
4	Single-sphere model for solvent reorganization energy and its application to electron transfer. *Science Bulletin*, **2006**, 51, 902-905		
3	Theoretical investigation of excitation states of tetracyanoethylene–biphenylene (n=0,1,2) system. *Computational and Theoretical Chemistry*, **2005**, 715, 219-226		
2	High-pressure limit rate rules for intramolecular H-migration reactions of ȤȤhydroxyalkylperoxy radicals. *Theoretical Chemistry Accounts*, **2021**, 140, 1	1.9	
1	A theoretical study of ȤȤhydroxybutenyl with O2 on the HOC4H6OO·potential energy surface. *Theoretical Chemistry Accounts*, **2021**, 140, 1	1.9	