Xiang-Yuan Li

List of Publications by Year
in descending order

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166	2,875	218592	233338
papers	citations	26 h-index	45 g-index

166	166	166	2797
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	H₂Sâ€Activable MOF Nanoparticle Photosensitizer for Effective Photodynamic Therapy against Cancer with Controllable Singletâ€Oxygen Release. Angewandte Chemie - International Edition, 2017, 56, 13752-13756.	7.2	283
2	Reactive molecular dynamics simulation and chemical kinetic modeling of pyrolysis and combustion of n-dodecane. Combustion and Flame, 2011, 158, 217-226.	2.8	196
3	ReaxFF Molecular Dynamics Simulations of Oxidation of Toluene at High Temperatures. Journal of Physical Chemistry A, 2012, 116, 9811-9818.	1.1	117
4	A shock tube study of the autoignition characteristics of RP-3 jet fuel. Proceedings of the Combustion Institute, 2015, 35, 3151-3158.	2.4	90
5	Linker-Eliminated Nano Metalâ€“Organic Framework Fluorescent Probe for Highly Selective and Sensitive Phosphate Ratiometric Detection in Water and Body Fluids. Analytical Chemistry, 2020, 92, 3722-3727.	3.2	84
6	A new type of surface-enhanced Raman scattering sensor for the enantioselective recognition of <scp>d</scp>/<scp>l</scp>-cysteine and <scp>d</scp>/<scp>l</scp>-asparagine based on a helically arranged Ag NPs@homochiral MOF. Chemical Communications, 2016, 52, 5432-5435.	2.2	61
7	H₂Sâ€Activable MOF Nanoparticle Photosensitizer for Effective Photodynamic Therapy against Cancer with Controllable Singletâ€Oxygen Release. Angewandte Chemie, 2017, 129, 13940-13944.	1.6	59
8	Molecular-level modeling investigation of n-decane pyrolysis at high temperature. Journal of Analytical and Applied Pyrolysis, 2017, 128, 412-422.	2.6	59
9	Electron transfer in poly(p-phenylene) oligomers: effect of external electric field and application of Koopmans theorem. Chemical Physics, 1999, 248, 137-146.	0.9	48
10	Theoretical Kinetic Study of Thermal Decomposition of Cyclohexane. Energy & Fuels, 2012, 26, 2811-2820.	2.5	44
11	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, 8017-8025.	1.1	40
12	Characterization of CVD TiN coating at different deposition temperatures and its application in hydrocarbon pyrolysis. Surface and Coatings Technology, 2014, 258, 1060-1067.	2.2	40
13	Ab initio calculation for inner reorganization energy of gas-phase electron transfer in organic moleculeâ€“ion systems. Chemical Physics, 2000, 260, 283-294.	0.9	39
14	Recyclable Dielsâ€“Alder Furan/Maleimide Polymer Networks with Shape Memory Effect. Industrial & Engineering Chemistry Research, 2014, 53, 16156-16163.	1.8	39
15	Low- and intermediate-temperature oxidation of ethylcyclohexane: A theoretical study. Combustion and Flame, 2015, 162, 4167-4182.	2.8	39
16	Effects of Fuel Additives on the Thermal Cracking of n-Decane from Reactive Molecular Dynamics. Journal of Physical Chemistry A, 2012, 116, 3794-3801.	1.1	37
17	Catalytic cracking of RP-3 jet fuel over wall-coated Pt/ZrO2â€“TiO2â€“Al2O3 catalysts with different Al2O3 ratios. Journal of Analytical and Applied Pyrolysis, 2015, 111, 100-107.	2.6	37
18	Time-dependent density functional theory study on intramolecular charge transfer and solvent effect of dimethylaminobenzophenone. Journal of Chemical Physics, 2005, 122, 084314.	1.2	36

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19	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.	1.8	36
20	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, 3424-3432.	1.1	36
21	Continuous medium theory for nonequilibrium solvation: I. How to correctly evaluate solvation free energy of nonequilibrium. Journal of Computational Chemistry, 2004, 25, 500-509.	1.5	33
22	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.	3.0	32
23	Molecular Orbital Analysis in Evaluation of Electron-Transfer Matrix Element by Koopmans' Theory. Journal of Physical Chemistry A, 2004, 108, 4125-4131.	1.1	31
24	Curing kinetics and shape-memory behavior of an intrinsically toughened epoxy resin system. Journal of Thermal Analysis and Calorimetry, 2015, 119, 537-546.	2.0	30
25	Kerosene cracking over supported monolithic Pt catalysts: Effects of SrO and BaO promoters. Chinese Journal of Catalysis, 2013, 34, 1139-1147.	6.9	27
26	Thermal, mechanical and shape memory properties of an intrinsically toughened epoxy/anhydride system. Journal of Polymer Research, 2014, 21, 1.	1.2	27
27	Experimental and modeling study of thermal and catalytic cracking of n-decane. Journal of Analytical and Applied Pyrolysis, 2014, 110, 463-469.	2.6	27
28	Shock-Tube Study of Dimethoxymethane Ignition at High Temperatures. Energy & Fuels, 2014, 28, 4603-4610.	2.5	26
29	An overview of continuum models for nonequilibrium solvation: Popular theories and new challenge. International Journal of Quantum Chemistry, 2015, 115, 700-721.	1.0	26
30	Electron transfer between biphenyl and biphenyl anion radicals: Reorganization energies and electron transfer matrix elements. Journal of Computational Chemistry, 1999, 20, 597-603.	1.5	25
31	Pressure-Dependent Kinetics of Initial Reactions in Iso-octane Pyrolysis. Journal of Physical Chemistry A, 2015, 119, 4093-4107.	1.1	25
32	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.	1.1	24
33	Spectral shifts of the n â†' Ï€* and Ï€ â†' Ï€* transitions of uracil based on a modified form of solvent reorganization energy. Physical Chemistry Chemical Physics, 2012, 14, 13284.	1.3	24
34	Pressure-dependent rate rules for intramolecular H-migration reactions of normal-alkyl cyclohexylperoxy radicals. Combustion and Flame, 2019, 204, 176-188.	2.8	24
35	Catalytic Cracking of RP-3 Jet Fuel over Pt/CeO₂â€“Al₂O₃ by Adding Cu/ZSM-5. Energy & Fuels, 2014, 28, 5382-5388.	2.5	23
36	Electric field dependence of the diabatic potential energy surface for gas-phase electron transfer O2O2â^' â†' O2â^'O2. Chemical Physics Letters, 1995, 233, 227-230.	1.2	22

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37	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.	1.5	22
38	Flow distribution of hydrocarbon fuel in parallel minichannels heat exchanger. AICHE Journal, 2018, 64, 2781-2791.	1.8	22
39	An experimental and modeling study of ethyleneâ€“air combustion over a wide temperature range. Combustion and Flame, 2020, 221, 20-40.	2.8	22
40	High catalytic activity and stability quasi homogeneous alkali metal promoted Ni/SiO2 aerogel catalysts for catalytic cracking of n-decane. Fuel, 2020, 268, 117384.	3.4	22
41	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, 835-842.	1.5	21
42	Spectral Shift of the n â†' Ï€* Transition for Acetone and Formic Acid with an Explicit Solvent Model. Journal of Physical Chemistry A, 2011, 115, 232-243.	1.1	21
43	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	20
44	A modified two-sphere model for solvent reorganization energy in electron transfer. Physical Chemistry Chemical Physics, 2012, 14, 5538.	1.3	20
45	Pressure-Dependent Rate Rules for Intramolecular H-Migration Reactions of Hydroperoxyalkylperoxy Radicals in Low Temperature. Journal of Physical Chemistry A, 2017, 121, 3001-3018.	1.1	20
46	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.	4.4	20
47	Mechanism construction and simulation for high-temperature combustion of n-propylcyclohexane. Chemical Research in Chinese Universities, 2014, 30, 480-488.	1.3	19
48	Catalytic Cracking of n-Decane over Monometallic and Bimetallic Ptâ€“Ni/MoO₃/Laâ€“Al₂O₃ Catalysts: Correlations of Surface Properties and Catalytic Behaviors. Industrial & Engineering Chemistry Research, 2019, 58, 1823-1833.	1.8	18
49	SOLVATION ENERGY OF NONEQUILIBRIUM POLARIZATION: OLD QUESTION, NEW ANSWER. Journal of Theoretical and Computational Chemistry, 2010, 09, 23-37.	1.8	17
50	Nonequilibrium solvation energy by means of constrained equilibrium thermodynamics and its application to self-exchange electron transfer reactions. Physical Chemistry Chemical Physics, 2010, 12, 1341-1350.	1.3	17
51	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.	2.6	17
52	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.	2.3	17
53	Quantum Chemical Study on Excited States and Electronic Coupling Matrix Element in a Catecholâ^'Bridgeâ^'Dicyanoethylene System. Journal of Physical Chemistry A, 2005, 109, 4154-4161.	1.1	16
54	Shock tube study of n-nonane/air ignition over a wide range of temperatures. Fuel, 2017, 188, 567-574.	3.4	16

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55	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.	1.3	16
56	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, 368-374.	1.5	15
57	Vertical Detachment Energy of Hydrated Electron Based on a Modified Form of Solvent Reorganization Energy. Journal of Physical Chemistry B, 2010, 114, 2189-2197.	1.2	15
58	Ab initio study on electron excitation and electron transfer in tryptophanâ€“tyrosine system. Chemical Physics, 2002, 284, 543-554.	0.9	14
59	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, 13061-13068.	1.1	14
60	Reaction of ketenyl radical with hydroxyl radical over C2H2O2 potential energy surface: A theoretical study. Combustion and Flame, 2014, 161, 885-897.	2.8	14
61	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, 3161-3170.	1.1	14
62	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.	1.3	14
63	Investigation on Carburization during the Repeated Coking and Decoking Process. Industrial & Engineering Chemistry Research, 2020, 59, 13051-13059.	1.8	14
64	Theoretical Study of Radicalâ€“Molecule Reactions with Negative Activation Energies in Combustion: Hydroxyl Radical Addition to Alkenes. ACS Omega, 2020, 5, 12777-12788.	1.6	14
65	An anti-quinoid structure in dual fluorescence of fluozazene molecule and solvent effect of intramolecular charge transfer. Chemical Physics, 2007, 332, 325-335.	0.9	13
66	An ab initio/Riceâ€“Ramspergerâ€“Kasselâ€“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.	1.2	13
67	Kinetic study of the formation of triphenylene from the condensation of C12H10+C6H5. Computational and Theoretical Chemistry, 2012, 985, 1-7.	1.1	13
68	Theoretical and kinetic study of reaction C2HÂ+ÂC3H6 on the C5H7 potential energy surface. Theoretical Chemistry Accounts, 2015, 134, 1.	0.5	12
69	Photoinduced charge-transfer electronic excitation of tetracyanoethylene/tetramethylethylene complex in dichloromethane. Chemical Physics Letters, 2017, 679, 158-163.	1.2	12
70	Shock tube measurements and kinetic modeling study on autoignition characteristics of cyclohexanone. Combustion and Flame, 2018, 192, 358-368.	2.8	12
71	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.	1.5	11
72	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.	1.5	11

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73	Unimolecular decomposition mechanism of vinyl alcohol by computational study. Theoretical Chemistry Accounts, 2011, 128, 341-348.	0.5	11
74	Theoretical Study on Reactions of Alkylperoxy Radicals. Journal of Physical Chemistry A, 2019, 123, 3949-3958.	1.1	11
75	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.	2.5	11
76	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.	1.7	10
77	Reaction mechanism on the activation of ethane Câ€“H and Câ€“C bonds by a diplatinum cluster. Theoretical Chemistry Accounts, 2013, 132, 1.	0.5	10
78	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.	1.2	10
79	The performance of Pt/ZrxTixAl1â€“2xO2 as Kerosene cracking catalysts. Chinese Journal of Catalysis, 2014, 35, 175-184.	6.9	10
80	An experimental and numerical investigation on thermal cracking of n-decane in the microchannel. Petroleum Science and Technology, 2016, 34, 555-561.	0.7	10
81	Reactions of Î²-hydroxypropyl radicals with O2 on the HOC3H6OOâ€¢ potential energy surfaces: A theoretical study. Combustion and Flame, 2020, 211, 202-217.	2.8	10
82	Combined strategy and Ni NPs/SiO2 aerogel catalyst for cracking hydrocarbon fuels. Journal of Power Sources, 2021, 506, 230172.	4.0	10
83	Enhanced cracking conversion of supercritical fuel over stabilized Pt nanoparticles supported SiO2-Al2O3 catalyst coating. Applied Surface Science, 2021, 559, 149950.	3.1	10
84	Theoretical investigation of electron transfer transition in tetracyanoethylene-contained organic complexes. Journal of Computational Chemistry, 2002, 23, 874-886.	1.5	9
85	Theoretical study of photoinduced electron transfer from tetramethylethylene to tetracyanoethylene. Journal of Chemical Physics, 2003, 119, 8854-8863.	1.2	9
86	Investigation of photoinduced electron transfer in model system of vitamin E-duroquinone by time-dependent density functional theory. Journal of Chemical Physics, 2004, 120, 10025-10032.	1.2	9
87	Single-Sphere Model for Absorption Spectrum of Interfacial Molecules with Application to Predictions of Orientational Angles. Journal of Physical Chemistry B, 2006, 110, 10088-10094.	1.2	9
88	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	9
89	Activation of propane Câ€“H and Câ€“C bonds by a diplatinum cluster: potential energy surfaces and reaction mechanisms. Structural Chemistry, 2014, 25, 471-481.	1.0	9
90	High-Pressure-Limit and Pressure-Dependent Rate Rules for Unimolecular Reactions Related to Hydroperoxy Alkyl Radicals in Normal Alkyl Cyclohexane Combustion. 1. Concerted HO2 Elimination Reaction Class and Î²-Scission Reaction Class. Journal of Physical Chemistry A, 2021, 125, 8942-8958.	1.1	9

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91	A comparative study on the autoignition characteristics of cyclopropane and propane at high temperatures. Combustion and Flame, 2022, 237, 111881.	2.8	9
92	Electron transfer integral between two zero-overlap states. Journal of Computational Chemistry, 1996, 17, 1108-1111.	1.5	8
93	Thermodynamics for nonequilibrium solvation and numerical evaluation of solvent reorganization energy. Science in China Series B: Chemistry, 2008, 51, 1246-1256.	0.8	8
94	Shock-Tube Study of the Ignition of Gas-Phase 1,3,5-Trimethylbenzene in Air. Energy & Fuels, 2014, 28, 6707-6713.	2.5	8
95	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.	1.1	8
96	Electron transfer NO 2 + +NOâ†'N02+NO+ in aromatic nitration. Science in China Series B: Chemistry, 1997, 40, 523-528.	0.8	7
97	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.	1.5	7
98	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.	1.0	7
99	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.	1.5	7
100	A study on orientation and absorption spectrum of interfacial molecules by using continuum model. Journal of Computational Chemistry, 2008, 29, 198-210.	1.5	7
101	An experimental and simulated investigation on pyrolysis of blended cyclohexane and benzene under supercritical pressure. Petroleum Chemistry, 2017, 57, 71-78.	0.4	7
102	Structure and Formation Mechanism of Antimicrobial Peptides Temporin B- and L-Induced Tubular Membrane Protrusion. International Journal of Molecular Sciences, 2021, 22, 11015.	1.8	7
103	Ab initio study of long-range electron transfer between biphenyl anion radical and naphthalene. Science in China Series B: Chemistry, 1999, 42, 441-448.	0.8	6
104	Application of Koopmansâ€™ theorem in evaluating electron transfer matrix element of long-range electron transfer. Computational and Theoretical Chemistry, 2000, 530, 49-58.	1.5	6
105	Accurate prediction of thermodynamic properties of alkyl peroxides by combining density functional theory calculation with leastâ€square calibration. Journal of Computational Chemistry, 2009, 30, 1007-1015.	1.5	6
106	Shock tube study of n-decane ignition at low pressures. Acta Mechanica Sinica/Lixue Xuebao, 2012, 28, 79-82.	1.5	6
107	Numerical solution of solvent reorganization energy and its application in electron transfer reaction. Theoretical Chemistry Accounts, 2014, 133, 1.	0.5	6
108	Calculation of the rate constants for concerted elimination reaction class of hydroperoxyl-alkyl-peroxyl radicals. Theoretical Chemistry Accounts, 2017, 136, 1.	0.5	6

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109	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.	1.3	6
110	Novel nonequilibrium solvation theory for calculating the solvatochromic Stokes shift by State-specific TD-DFT. Chemical Physics Letters, 2019, 732, 136640.	1.2	6
111	Pressure-Dependent Rate Rules for the Intramolecular H-Shift Reactions of Hydroperoxy-Alkenyl-Peroxy Radicals in Low Temperature. Energy & Fuels, 2019, 33, 5597-5609.	2.5	6
112	Relationship between Energetic Performance and Clustering Effects on Incremental Nitramine Groups: A Theoretical Perspective. Journal of Physical Chemistry A, 2019, 123, 742-749.	1.1	6
113	Rate rules for hydrogen abstraction reaction kinetics of polycyclic aromatic hydrocarbons and vinyl radical. Theoretical Chemistry Accounts, 2020, 139, 1.	0.5	6
114	Catalyzed Michael addition, polycondensation, and the related performance of Dielsâ€“Alder selfâ€healing crosslinked polyamides. Polymer Engineering and Science, 2022, 62, 1269-1280.	1.5	6
115	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.	1.5	5
116	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.	0.5	5
117	Intramolecular electron transfer in cyclopeptide involving tryptophan and tyrosine and corrected two-sphere model for solvent reorganization energy. Chemical Physics, 2005, 312, 21-29.	0.9	5
118	Prediction of HIVâ€1 Protease Inhibitors Using Machine Learning Approaches. QSAR and Combinatorial Science, 2009, 28, 1346-1357.	1.5	5
119	Vertical ionization energies of halogen anions in solution. Science China Chemistry, 2010, 53, 1316-1321.	4.2	5
120	Investigation on the Thermal Cracking of n -Decane under Supercritical Pressure by a Developed Online-Sampling Experimental Method. Petroleum Chemistry, 2020, 60, 39-44.	0.4	5
121	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.	1.5	4
122	Nonequilibrium solvation theory: Comparison, modification and application. Science Bulletin, 2003, 48, 965-970.	1.7	4
123	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
124	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.	0.7	4
125	Rate rules for hydrogen abstraction reaction kinetics of alkenes from allylic sites by HO2 radical. Computational and Theoretical Chemistry, 2020, 1179, 112795.	1.1	4
126	Electronic coupling matrix elements of U-shaped donor-bridge-acceptor molecules and influence of mediated benzene solvent. Chemical Physics Letters, 2005, 414, 71-75.	1.2	3

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127	Spectral Shift of Ï€â†'Ï€* Transition forp-Nitroaniline Based on a New Expression of Nonequilibrium Solvation Energy. Chinese Journal of Chemical Physics, 2014, 27, 181-188.	0.6	3
128	Theoretical study on electronic excitation spectra: A matrix form of numerical algorithm for spectral shift. Chemical Physics, 2017, 492, 27-34.	0.9	3
129	Kinetic Analysis for Reaction of Cyclopentadiene with Hydroperoxyl Radical under Low- and Medium-Temperature Combustion. Journal of Physical Chemistry A, 2020, 124, 8280-8291.	1.1	3
130	Soulieoside U, a new cycloartane triterpene glycoside from Actaea vaginata. Natural Product Research, 2020, , 1-6.	1.0	3
131	The kinetic model of cyclohexeneâ€“air combustion over a wide temperature range. RSC Advances, 2021, 11, 39907-39916.	1.7	3
132	Numerical Investigations on the Molecular Reaction Model for Thermal Cracking of n-Decane at Supercritical Pressures. ACS Omega, 2022, 7, 22351-22362.	1.6	3
133	Theoretical investigation of charge transfer excitation and charge recombination in acenaphthylene-tetracyanoethylene complex. International Journal of Quantum Chemistry, 2003, 94, 23-35.	1.0	2
134	Prediction of Antitumor Activity for Epothilone Analogues Based on 3D Molecular Descriptors. Acta Physico-chimica Sinica, 2006, 22, 397-402.	0.6	2
135	Explicit solvent model for spectral shift of acrolein and simulation with molecular dynamics. Science Bulletin, 2006, 51, 2951-2958.	1.7	2
136	Absorption Spectra and Photoreactivity ofp-Aminobenzophenone by Time-dependent Density Functional Theory. Chinese Journal of Chemical Physics, 2007, 20, 273-278.	0.6	2
137	Accurate prediction of enthalpies of formation for a large set of organic compounds. Journal of Computational Chemistry, 2010, 31, 2585-2592.	1.5	2
138	Polarizable continuum model associated with the self-consistent-reaction field for molecular adsorbates at the interface. Physical Chemistry Chemical Physics, 2010, 12, 207-214.	1.3	2
139	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.	0.5	2
140	Development of a detailed pyrolysis mechanism for C 1 â€“C 4 hydrocarbons under a wide range of temperature and pressure. International Journal of Chemical Kinetics, 2020, 52, 796-821.	1.0	2
141	Two new cycloartane triterpenoid glycosides from the rhizomes of Actaea vaginata. Natural Product Research, 2022, , 1-8.	1.0	2
142	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.	0.5	1
143	One approach to calculating the solvent reorganization energy of intramolecular electron transfer. Science Bulletin, 2003, 48, 35-38.	1.7	1
144	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

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145	Theoretical investigation of excitation states of tetracyanoethylenenâ^'â€“biphenylene (n=0,1,2) system. Computational and Theoretical Chemistry, 2005, 715, 219-226.	1.5	1
146	Solvent Reorganization Energy of Intramolecular Electron Transfer in Peptides Involving Tryptophan and Tyrosine. Chinese Journal of Chemistry, 2008, 26, 2003-2008.	2.6	1
147	Solvent Reorganization Energy and Electronic Coupling for Intramolecular Electron Transfer in Biphenyl-Acceptor Anion Radicals. Chinese Journal of Chemical Physics, 2008, 21, 45-54.	0.6	1
148	Continuum Model for Electronic Polarization Based on a Novel Dielectric Response Function. Chinese Journal of Chemical Physics, 2009, 22, 481-488.	0.6	1
149	Analytical Dielectric Spectrum Formula Based on Representative Frequencies. Chinese Journal of Chemical Physics, 2009, 22, 262-268.	0.6	1
150	Theoretical Study on Reactivity of Electron Transfer in Modelâ€System of Oxidation of Î± â€Amino Carbonâ€centered Radical by O₂. Chinese Journal of Chemistry, 2002, 20, 834-840.	2.6	1
151	Time-Dependent Stokes Shift from Solvent Dielectric Relaxation. Chinese Journal of Chemical Physics, 2010, 23, 297-302.	0.6	1
152	Catalytic cracking of n-decane over NiOâ€“MoO3 modified Pt/ZrO2â€“TiO2â€“Al2O3 catalyst with different Al2O3 ratios. Petroleum Chemistry, 2017, 57, 666-672.	0.4	1
153	Theoretical study of hydrogen abstraction by small radicals from cyclohexane-carbonyl-hydroperoxide. Theoretical Chemistry Accounts, 2019, 138, 1.	0.5	1
154	Experimental and numerical investigation on the isobaric heat capacity for methylcyclohexane at high temperature and high pressure. Applied Thermal Engineering, 2019, 146, 613-621.	3.0	1
155	Theoretical Study on Reactions of Î±-Site Hydroxyethyl and Hydroxypropyl Radicals with O2. Journal of Physical Chemistry A, 2021, 125, 5423-5437.	1.1	1
156	Single-sphere model for solvent reorganization energy and its application to electron transfer. Science Bulletin, 2006, 51, 902-905.	1.7	0
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