

Xiang-Yuan Li

List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

160
papers

2,164
citations

25
h-index

38
g-index

166
ext. papers

2,502
ext. citations

3.5
avg, IF

5.11
L-index

#	Paper	IF	Citations
160	Two new cycloartane triterpenoid glycosides from the rhizomes of .. <i>Natural Product Research</i> , 2022 , 1-8	2.3	0
159	A comparative study on the autoignition characteristics of cyclopropane and propane at high temperatures. <i>Combustion and Flame</i> , 2022 , 237, 111881	5.3	0
158	The kinetic model of cyclohexene-air combustion over a wide temperature range.. <i>RSC Advances</i> , 2021 , 11, 39907-39916	3.7	1
157	High-pressure limit rate rules for intramolecular H-migration reactions of β -hydroxyalkylperoxy radicals. <i>Theoretical Chemistry Accounts</i> , 2021 , 140, 1	1.9	
156	Combined strategy and Ni NPs/SiO ₂ aerogel catalyst for cracking hydrocarbon fuels. <i>Journal of Power Sources</i> , 2021 , 506, 230172	8.9	2
155	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. <i>Journal of Physical Chemistry A</i> , 2021 , 125, 8942-8958	2.8	2
154	A theoretical study of β -hydroxybutenyl with O ₂ on the HO-C ₄ H ₆ O ₂ -potential energy surface. <i>Theoretical Chemistry Accounts</i> , 2021 , 140, 1	1.9	
153	Enhanced cracking conversion of supercritical fuel over stabilized Pt nanoparticles supported SiO ₂ -Al ₂ O ₃ catalyst coating. <i>Applied Surface Science</i> , 2021 , 559, 149950	6.7	4
152	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. <i>Journal of Physical Chemistry A</i> , 2021 , 125, 8959-8977	2.8	3
151	Theoretical Study of Radical-Molecule Reactions with Negative Activation Energies in Combustion: Hydroxyl Radical Addition to Alkenes. <i>ACS Omega</i> , 2020 , 5, 12777-12788	3.9	2
150	Rate rules for hydrogen abstraction reaction kinetics of polycyclic aromatic hydrocarbons and vinyl radical. <i>Theoretical Chemistry Accounts</i> , 2020 , 139, 1	1.9	4
149	Soulioside U, a new cycloartane triterpene glycoside from. <i>Natural Product Research</i> , 2020 , 1-6	2.3	1
148	Linker-Eliminated Nano Metal-Organic Framework Fluorescent Probe for Highly Selective and Sensitive Phosphate Ratiometric Detection in Water and Body Fluids. <i>Analytical Chemistry</i> , 2020 , 92, 3722-3727	7.8	33
147	High catalytic activity and stability quasi homogeneous alkali metal promoted Ni/SiO ₂ aerogel catalysts for catalytic cracking of n-decane. <i>Fuel</i> , 2020 , 268, 117384	7.1	10
146	Investigation on the Thermal Cracking of n -Decane under Supercritical Pressure by a Developed Online-Sampling Experimental Method. <i>Petroleum Chemistry</i> , 2020 , 60, 39-44	1.1	0
145	Rate rules for hydrogen abstraction reaction kinetics of alkenes from allylic sites by HO ₂ radical. <i>Computational and Theoretical Chemistry</i> , 2020 , 1179, 112795	2	2
144	A Comprehensive Investigation of the Pyrolysis Effect on Heat Transfer Characteristics for n-Decane in the Horizon Mini-Channel. <i>Energy & Fuels</i> , 2020 , 34, 199-210	4.1	6

143	Preparation of Al ₂ O ₃ coating on TiN coating by polymer-assisted deposition to improve oxidation resistance in coking inhibition applications. <i>Ceramics International</i> , 2020 , 46, 7774-7782	5.1	5
142	An experimental and modeling study of ethylene-air combustion over a wide temperature range. <i>Combustion and Flame</i> , 2020 , 221, 20-40	5.3	8
141	Development of a detailed pyrolysis mechanism for C ₁₀ -C ₁₄ hydrocarbons under a wide range of temperature and pressure. <i>International Journal of Chemical Kinetics</i> , 2020 , 52, 796-821	1.4	0
140	Investigation on Carburization during the Repeated Coking and Decoking Process. <i>Industrial & Engineering Chemistry Research</i> , 2020 , 59, 13051-13059	3.9	3
139	Kinetic Analysis for Reaction of Cyclopentadiene with Hydroperoxyl Radical under Low- and Medium-Temperature Combustion. <i>Journal of Physical Chemistry A</i> , 2020 , 124, 8280-8291	2.8	2
138	Reactions of Hydroxypropyl radicals with O ₂ on the HO(CH ₂) ₃ OO potential energy surfaces: A theoretical study. <i>Combustion and Flame</i> , 2020 , 211, 202-217	5.3	5
137	Pressure-Dependent Rate Rules for the Intramolecular H-Shift Reactions of Hydroperoxy-Alkenyl-Peroxy Radicals in Low Temperature. <i>Energy & Fuels</i> , 2019 , 33, 5597-5609	4.1	3
136	Theoretical Study on Reactions of Alkylperoxy Radicals. <i>Journal of Physical Chemistry A</i> , 2019 , 123, 3949-3958	3.5	5
135	Pressure-dependent rate rules for cycloaddition, intramolecular H-shift, and concerted elimination reactions of alkenyl peroxy radicals at low temperature. <i>Physical Chemistry Chemical Physics</i> , 2019 , 21, 10693-10705	3.6	10
134	Theoretical study of hydrogen abstraction by small radicals from cyclohexane-carbonyl-hydroperoxide. <i>Theoretical Chemistry Accounts</i> , 2019 , 138, 1	1.9	1
133	Pressure-dependent rate rules for intramolecular H-migration reactions of normal-alkyl cyclohexylperoxy radicals. <i>Combustion and Flame</i> , 2019 , 204, 176-188	5.3	13
132	The performance comparison in predicting n-decane pyrolysis process between three ANNs methods: MLP, RBFN and GRNN. <i>Petroleum Science and Technology</i> , 2019 , 37, 1053-1058	1.4	
131	Novel nonequilibrium solvation theory for calculating the solvatochromic Stokes shift by State-specific TD-DFT. <i>Chemical Physics Letters</i> , 2019 , 732, 136640	2.5	2
130	Experimental and numerical analysis on flow characteristics and pyrolysis mechanism of hydrocarbon fuel with a novel online hybrid method. <i>Energy Conversion and Management</i> , 2019 , 198, 111817	10.6	11
129	Catalytic Cracking of n-Decane over Monometallic and Bimetallic Pt ₂ Ni/MoO ₃ /LaAl ₂ O ₃ Catalysts: Correlations of Surface Properties and Catalytic Behaviors. <i>Industrial & Engineering Chemistry Research</i> , 2019 , 58, 1823-1833	3.9	15
128	Relationship between Energetic Performance and Clustering Effects on Incremental Nitramine Groups: A Theoretical Perspective. <i>Journal of Physical Chemistry A</i> , 2019 , 123, 742-749	2.8	4
127	Experimental and numerical investigation on the isobaric heat capacity for methylcyclohexane at high temperature and high pressure. <i>Applied Thermal Engineering</i> , 2019 , 146, 613-621	5.8	1
126	Solvent effects for vertical absorption and emission processes in solution using a self-consistent state specific method based on constrained equilibrium thermodynamics. <i>Physical Chemistry Chemical Physics</i> , 2018 , 20, 13178-13190	3.6	7

125	Flow distribution of hydrocarbon fuel in parallel minichannels heat exchanger. <i>AIChE Journal</i> , 2018 , 64, 2781-2791	3.6	13
124	Investigations on the thermal cracking and pyrolysis mechanism of China No.3 aviation kerosene under supercritical conditions. <i>Petroleum Science and Technology</i> , 2018 , 36, 1396-1404	1.4	1
123	Shock tube measurements and kinetic modeling study on autoignition characteristics of cyclohexanone. <i>Combustion and Flame</i> , 2018 , 192, 358-368	5.3	11
122	Novel nonequilibrium solvation theory for calculating the vertical ionization energies of alkali metal cations and DNA bases in aqueous. <i>Theoretical Chemistry Accounts</i> , 2018 , 137, 1	1.9	2
121	Shock tube study of n-nonane/air ignition over a wide range of temperatures. <i>Fuel</i> , 2017 , 188, 567-574	7.1	12
120	Pressure-Dependent Rate Rules for Intramolecular H-Migration Reactions of Hydroperoxyalkylperoxy Radicals in Low Temperature. <i>Journal of Physical Chemistry A</i> , 2017 , 121, 3001-3018	3.8	16
119	An experimental and simulated investigation on pyrolysis of blended cyclohexane and benzene under supercritical pressure. <i>Petroleum Chemistry</i> , 2017 , 57, 71-78	1.1	4
118	Calculation of the rate constants for concerted elimination reaction class of hydroperoxyl-alkyl-peroxyl radicals. <i>Theoretical Chemistry Accounts</i> , 2017 , 136, 1	1.9	3
117	Photoinduced charge-transfer electronic excitation of tetracyanoethylene/tetramethylethylene complex in dichloromethane. <i>Chemical Physics Letters</i> , 2017 , 679, 158-163	2.5	7
116	Theoretical study on electronic excitation spectra: A matrix form of numerical algorithm for spectral shift. <i>Chemical Physics</i> , 2017 , 492, 27-34	2.3	3
115	H ₂ S-Activable MOF Nanoparticle Photosensitizer for Effective Photodynamic Therapy against Cancer with Controllable Singlet-Oxygen Release. <i>Angewandte Chemie - International Edition</i> , 2017 , 56, 13752-13756	16.4	210
114	H ₂ S-Activable MOF Nanoparticle Photosensitizer for Effective Photodynamic Therapy against Cancer with Controllable Singlet-Oxygen Release. <i>Angewandte Chemie</i> , 2017 , 129, 13940-13944	3.6	49
113	Catalytic cracking of n-decane over NiO/MoO ₃ modified Pt/ZrO ₂ -TiO ₂ -Al ₂ O ₃ catalyst with different Al ₂ O ₃ ratios. <i>Petroleum Chemistry</i> , 2017 , 57, 666-672	1.1	1
112	Molecular-level modeling investigation of n-decane pyrolysis at high temperature. <i>Journal of Analytical and Applied Pyrolysis</i> , 2017 , 128, 412-422	6	26
111	Solvent effects on excitation energies obtained using the state-specific TD-DFT method with a polarizable continuum model based on constrained equilibrium thermodynamics. <i>Physical Chemistry Chemical Physics</i> , 2017 , 19, 32242-32252	3.6	5
110	Correlation between structure, acidity and activity of Mo-promoted Pt/ZrO ₂ -TiO ₂ -Al ₂ O ₃ catalysts for n-decane catalytic cracking. <i>Applied Thermal Engineering</i> , 2017 , 111, 811-818	5.8	30
109	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. <i>Chemical Communications</i> , 2016 , 52, 5432-5	5.8	52
108	Theoretical Prediction of Rate Constants for Hydrogen Abstraction by OH, H, O, CH ₃ , and HO ₂ Radicals from Toluene. <i>Journal of Physical Chemistry A</i> , 2016 , 120, 3424-32	2.8	26

107	An experimental and numerical investigation on thermal cracking of n-decane in the microchannel. <i>Petroleum Science and Technology</i> , 2016 , 34, 555-561	1.4	7
106	Curing kinetics and shape-memory behavior of an intrinsically toughened epoxy resin system. <i>Journal of Thermal Analysis and Calorimetry</i> , 2015 , 119, 537-546	4.1	27
105	Theoretical and kinetic study of reaction C ₂ H + C ₃ H ₆ on the C ₅ H ₇ potential energy surface. <i>Theoretical Chemistry Accounts</i> , 2015 , 134, 1	1.9	10
104	An overview of continuum models for nonequilibrium solvation: Popular theories and new challenge. <i>International Journal of Quantum Chemistry</i> , 2015 , 115, 700-721	2.1	21
103	Pressure-dependent kinetics of initial reactions in iso-octane pyrolysis. <i>Journal of Physical Chemistry A</i> , 2015 , 119, 4093-107	2.8	14
102	Temperature and pressure dependent rate coefficients for the reaction of C ₂ H ₄ + HO ₂ on the C ₂ H ₄ O ₂ H potential energy surface. <i>Journal of Physical Chemistry A</i> , 2015 , 119, 3161-70	2.8	11
101	Low- and intermediate-temperature oxidation of ethylcyclohexane: A theoretical study. <i>Combustion and Flame</i> , 2015 , 162, 4167-4182	5.3	31
100	Catalytic cracking of RP-3 jet fuel over wall-coated Pt/ZrO ₂ /TiO ₂ /Al ₂ O ₃ catalysts with different Al ₂ O ₃ ratios. <i>Journal of Analytical and Applied Pyrolysis</i> , 2015 , 111, 100-107	6	36
99	A shock tube study of the autoignition characteristics of RP-3 jet fuel. <i>Proceedings of the Combustion Institute</i> , 2015 , 35, 3151-3158	5.9	63
98	Thermal, mechanical and shape memory properties of an intrinsically toughened epoxy/anhydride system. <i>Journal of Polymer Research</i> , 2014 , 21, 1	2.7	22
97	Influence of TiN coating on products distribution for hydrocarbon fuel cracking under high temperature and pressure. <i>Journal of Analytical and Applied Pyrolysis</i> , 2014 , 107, 197-203	6	13
96	Reaction of ketyenyl radical with hydroxyl radical over C ₂ H ₂ O ₂ potential energy surface: A theoretical study. <i>Combustion and Flame</i> , 2014 , 161, 885-897	5.3	10
95	Characterization of CVD TiN coating at different deposition temperatures and its application in hydrocarbon pyrolysis. <i>Surface and Coatings Technology</i> , 2014 , 258, 1060-1067	4.4	30
94	Inhibition Effect of APCVD Titanium Nitride Coating on Coke Growth during n-Hexane Thermal Cracking under Supercritical Conditions. <i>Industrial & Engineering Chemistry Research</i> , 2014 , 53, 5432-5442	3.9	29
93	Experimental and modeling study of thermal and catalytic cracking of n-decane. <i>Journal of Analytical and Applied Pyrolysis</i> , 2014 , 110, 463-469	6	21
92	Recyclable Diels-Alder Furan/Maleimide Polymer Networks with Shape Memory Effect. <i>Industrial & Engineering Chemistry Research</i> , 2014 , 53, 16156-16163	3.9	32
91	Numerical solution of solvent reorganization energy and its application in electron transfer reaction. <i>Theoretical Chemistry Accounts</i> , 2014 , 133, 1	1.9	5
90	Catalytic Cracking of RP-3 Jet Fuel over Pt/CeO ₂ /Al ₂ O ₃ by Adding Cu/ZSM-5. <i>Energy & Fuels</i> , 2014 , 28, 5382-5388	4.1	22

89	Mechanism construction and simulation for high-temperature combustion of n-propylcyclohexane. <i>Chemical Research in Chinese Universities</i> , 2014 , 30, 480-488	2.2	14
88	Shock-Tube Study of Dimethoxymethane Ignition at High Temperatures. <i>Energy & Fuels</i> , 2014 , 28, 4603-4610	4.1	20
87	Spectral Shift of π Transition for p-Nitroaniline Based on a New Expression of Nonequilibrium Solvation Energy. <i>Chinese Journal of Chemical Physics</i> , 2014 , 27, 181-188	0.9	3
86	Shock-Tube Study of the Ignition of Gas-Phase 1,3,5-Trimethylbenzene in Air. <i>Energy & Fuels</i> , 2014 , 28, 6707-6713	4.1	5
85	The performance of Pt/Zr _x Ti _x Al _{1-x} O ₂ as Kerosene cracking catalysts. <i>Chinese Journal of Catalysis</i> , 2014 , 35, 175-184	11.3	10
84	Activation of propane C-H and C-C bonds by a diplatinum cluster: potential energy surfaces and reaction mechanisms. <i>Structural Chemistry</i> , 2014 , 25, 471-481	1.8	8
83	Reaction mechanism on the activation of ethane C-H and C-C bonds by a diplatinum cluster. <i>Theoretical Chemistry Accounts</i> , 2013 , 132, 1	1.9	9
82	Kerosene cracking over supported monolithic Pt catalysts: Effects of SrO and BaO promoters. <i>Chinese Journal of Catalysis</i> , 2013 , 34, 1139-1147	11.3	25
81	Theoretical calculation of reorganization energy for electron self-exchange reaction by constrained density functional theory and constrained equilibrium thermodynamics. <i>Journal of Physical Chemistry A</i> , 2013 , 117, 8017-25	2.8	32
80	Quasi-classical trajectory calculation of the chemical reaction Ba + m-C ₆ H ₄ ClCH ₃ . <i>Canadian Journal of Chemistry</i> , 2013 , 91, 206-210	0.9	
79	Solvent effect on UV/Vis absorption and emission spectra in aqueous solution based on a modified form of solvent reorganization energy. <i>Chemical Physics Letters</i> , 2013 , 583, 213-217	2.5	9
78	Theoretical Kinetic Study of Thermal Decomposition of Cyclohexane. <i>Energy & Fuels</i> , 2012 , 26, 2811-2820	3.5	35
77	Spectral shifts of the n- π^* and π - π^* transitions of uracil based on a modified form of solvent reorganization energy. <i>Physical Chemistry Chemical Physics</i> , 2012 , 14, 13284-91	3.6	23
76	A modified two-sphere model for solvent reorganization energy in electron transfer. <i>Physical Chemistry Chemical Physics</i> , 2012 , 14, 5538-44	3.6	15
75	Kinetic study of the formation of triphenylene from the condensation of C ₁₂ H ₁₀ + C ₆ H ₅ . <i>Computational and Theoretical Chemistry</i> , 2012 , 985, 1-7	2	8
74	ReaxFF molecular dynamics simulations of oxidation of toluene at high temperatures. <i>Journal of Physical Chemistry A</i> , 2012 , 116, 9811-8	2.8	87
73	Effects of fuel additives on the thermal cracking of n-decane from reactive molecular dynamics. <i>Journal of Physical Chemistry A</i> , 2012 , 116, 3794-801	2.8	26
72	Shock tube study of n-decane ignition at low pressures. <i>Acta Mechanica Sinica/Lixue Xuebao</i> , 2012 , 28, 79-82	2	5

71	Spectral shift of the n- π^* transition for acetone and formic acid with an explicit solvent model. <i>Journal of Physical Chemistry A</i> , 2011 , 115, 232-43	2.8	19
70	Solvent effect on the UV/Vis absorption spectra in aqueous solution: The nonequilibrium polarization with an explicit representation of the solvent environment. <i>Computational and Theoretical Chemistry</i> , 2011 , 971, 65-72	2	18
69	Unimolecular decomposition mechanism of vinyl alcohol by computational study. <i>Theoretical Chemistry Accounts</i> , 2011 , 128, 341-348	1.9	9
68	Molecular orientations at interfaces by extended polarizable continuum model. <i>International Journal of Quantum Chemistry</i> , 2011 , 111, 2187-2195	2.1	
67	A theoretical search for stable bent and linear structures of low-lying electronic states of the titanium dioxide (TiO ₂) molecule. <i>RSC Advances</i> , 2011 , 1, 1228	3.7	9
66	Reactive molecular dynamics simulation and chemical kinetic modeling of pyrolysis and combustion of n-dodecane. <i>Combustion and Flame</i> , 2011 , 158, 217-226	5.3	138
65	Time-Dependent Stokes Shift from Solvent Dielectric Relaxation. <i>Chinese Journal of Chemical Physics</i> , 2010 , 23, 297-302	0.9	1
64	SOLVATION ENERGY OF NONEQUILIBRIUM POLARIZATION: OLD QUESTION, NEW ANSWER. <i>Journal of Theoretical and Computational Chemistry</i> , 2010 , 09, 23-37	1.8	17
63	Vertical detachment energy of hydrated electron based on a modified form of solvent reorganization energy. <i>Journal of Physical Chemistry B</i> , 2010 , 114, 2189-97	3.4	15
62	Nonequilibrium solvation energy by means of constrained equilibrium thermodynamics and its application to self-exchange electron transfer reactions. <i>Physical Chemistry Chemical Physics</i> , 2010 , 12, 1341-50	3.6	17
61	Polarizable continuum model associated with the self-consistent-reaction field for molecular adsorbates at the interface. <i>Physical Chemistry Chemical Physics</i> , 2010 , 12, 207-14	3.6	2
60	Vertical ionization energies of halogen anions in solution. <i>Science China Chemistry</i> , 2010 , 53, 1316-1321	7.9	5
59	Theoretical Study on Reactivity of Electron Transfer in Model-System of Oxidation of β -Amino Carbon-centered Radical by O ₂ . <i>Chinese Journal of Chemistry</i> , 2010 , 20, 834-840	4.9	1
58	Theoretical Study on Electron Transfer Matrix Element in Oxidation of β -Amino Carbon-Centered Radical by O ₂ . <i>Chinese Journal of Chemistry</i> , 2010 , 20, 972-977	4.9	
57	Accurate prediction of enthalpies of formation for a large set of organic compounds. <i>Journal of Computational Chemistry</i> , 2010 , 31, 2585-92	3.5	2
56	Continuum Model for Electronic Polarization Based on a Novel Dielectric Response Function. <i>Chinese Journal of Chemical Physics</i> , 2009 , 22, 481-488	0.9	1
55	Analytical Dielectric Spectrum Formula Based on Representative Frequencies. <i>Chinese Journal of Chemical Physics</i> , 2009 , 22, 262-268	0.9	1
54	Accurate prediction of thermodynamic properties of alkyl peroxides by combining density functional theory calculation with least-square calibration. <i>Journal of Computational Chemistry</i> , 2009 , 30, 1007-15	3.5	3

53	Influence of contaminations on combustion kinetics in hydrogen-fueled engine. <i>Science Bulletin</i> , 2009 , 54, 1317-1321	10.6	
52	Prediction of HIV-1 Protease Inhibitors Using Machine Learning Approaches. <i>QSAR and Combinatorial Science</i> , 2009 , 28, 1346-1357		4
51	COMMENT ON "VARIATIONAL ELECTROSTATICS FOR CHARGE SOLVATION". <i>Journal of Theoretical and Computational Chemistry</i> , 2009 , 08, 1099-1101	1.8	
50	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 + CH ₂ COHCH ₂ reaction. <i>Journal of Chemical Physics</i> , 2008 , 129, 234301	3.9	12
49	A THEORETICAL STUDY ON DUAL FLUORESCENCE OF 4-DIMETHYLAMINOPYRIDINE BY POLARIZABLE CONTINUUM MODEL. <i>Journal of Theoretical and Computational Chemistry</i> , 2008 , 07, 821-832	1.8	4
48	Solvent Reorganization Energy and Electronic Coupling for Intramolecular Electron Transfer in Biphenyl-Acceptor Anion Radicals. <i>Chinese Journal of Chemical Physics</i> , 2008 , 21, 45-54	0.9	1
47	Thermodynamics for nonequilibrium solvation and numerical evaluation of solvent reorganization energy. <i>Science in China Series B: Chemistry</i> , 2008 , 51, 1246-1256		8
46	Solvent Reorganization Energy of Intramolecular Electron Transfer in Peptides Involving Tryptophan and Tyrosine. <i>Chinese Journal of Chemistry</i> , 2008 , 26, 2003-2008	4.9	1
45	A study on orientation and absorption spectrum of interfacial molecules by using continuum model. <i>Journal of Computational Chemistry</i> , 2008 , 29, 198-210	3.5	6
44	Multichannel photoinduced intramolecular electron-transfer excitations in a bis-naphthalimide spermine conjugate by time-dependent density functional theory. <i>Journal of Physical Chemistry A</i> , 2007 , 111, 13061-8	2.8	13
43	Solvent reorganization energy of electron transfer by a modified ellipsoidal cavity model. <i>Computational and Theoretical Chemistry</i> , 2007 , 819, 32-40		
42	An anti-quinoid structure in dual fluorescence of fluozazene molecule and solvent effect of intramolecular charge transfer. <i>Chemical Physics</i> , 2007 , 332, 325-335	2.3	12
41	Absorption Spectra and Photoreactivity of p-Aminobenzophenone by Time-dependent Density Functional Theory. <i>Chinese Journal of Chemical Physics</i> , 2007 , 20, 273-278	0.9	2
40	Single-sphere model for solvent reorganization energy and its application to electron transfer. <i>Science Bulletin</i> , 2006 , 51, 902-905		
39	Explicit solvent model for spectral shift of acrolein and simulation with molecular dynamics. <i>Science Bulletin</i> , 2006 , 51, 2951-2958		2
38	Continuous medium theory for nonequilibrium solvation: IV. Solvent reorganization energy of electron transfer based on conductor-like screening model. <i>Journal of Computational Chemistry</i> , 2006 , 27, 368-74	3.5	15
37	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. <i>Journal of Theoretical and Computational Chemistry</i> , 2006 , 05, 355-374	1.8	8
36	Single-sphere model for absorption spectrum of interfacial molecules with application to predictions of orientational angles. <i>Journal of Physical Chemistry B</i> , 2006 , 110, 10088-94	3.4	9

35	Quantum chemical study on excited states and electronic coupling matrix element in a catechol-bridge-dicyanoethylene system. <i>Journal of Physical Chemistry A</i> , 2005 , 109, 4154-61	2.8	15
34	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. <i>Computational and Theoretical Chemistry</i> , 2005 , 715, 157-175		11
33	Theoretical investigation of excitation states of tetracyanoethylenenBiphenylene (n=0,1,2) system. <i>Computational and Theoretical Chemistry</i> , 2005 , 715, 219-226		
32	Intramolecular electron transfer in cyclopeptide involving tryptophan and tyrosine and corrected two-sphere model for solvent reorganization energy. <i>Chemical Physics</i> , 2005 , 312, 21-29	2.3	5
31	Electronic coupling matrix elements of U-shaped donor-bridge-acceptor molecules and influence of mediated benzene solvent. <i>Chemical Physics Letters</i> , 2005 , 414, 71-75	2.5	3
30	Continuous medium theory for nonequilibrium solvation: III. Solvation shift by monopole approximation and multipole expansion in spherical cavity. <i>Journal of Computational Chemistry</i> , 2005 , 26, 399-409	3.5	11
29	Time-dependent density functional theory study on intramolecular charge transfer and solvent effect of dimethylaminobenzophenone. <i>Journal of Chemical Physics</i> , 2005 , 122, 84314	3.9	33
28	CONTINUOUS MEDIUM THEORY FOR NONEQUILIBRIUM SOLVATION: NEW FORMULATIONS AND AN OVERVIEW OF THEORIES AND APPLICATIONS. <i>Journal of Theoretical and Computational Chemistry</i> , 2005 , 04, 907-983	1.8	18
27	Investigation of photoinduced electron transfer in model system of vitamin E-duroquinone by time-dependent density functional theory. <i>Journal of Chemical Physics</i> , 2004 , 120, 10025-32	3.9	8
26	SOLVENT REORGANIZATION ENERGY WITH DIELECTRIC GREEN FUNCTIONAL AND ITS APPLICATION TO RETURN ELECTRON TRANSFER IN TETRACYANOETHYLENE-HEXAMETHYLBENZENE SYSTEM. <i>Journal of Theoretical and Computational Chemistry</i> , 2004 , 03, 609-627	1.8	1
25	Ab initio study of hydrogen bonding interaction and photoinduced electron transfer between 4-nitroquinoline-1-oxide and tryptophan. <i>International Journal of Quantum Chemistry</i> , 2004 , 98, 33-43	2.1	6
24	Continuous medium theory for nonequilibrium solvation: I. How to correctly evaluate solvation free energy of nonequilibrium. <i>Journal of Computational Chemistry</i> , 2004 , 25, 500-9	3.5	33
23	Continuous medium theory for nonequilibrium solvation: II. Interaction energy between solute charge and reaction field and single-sphere model for spectral shift. <i>Journal of Computational Chemistry</i> , 2004 , 25, 835-42	3.5	21
22	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. <i>Computational and Theoretical Chemistry</i> , 2004 , 671, 239-248		7
21	Molecular Orbital Analysis in Evaluation of Electron-Transfer Matrix Element by Koopmans' Theory. <i>Journal of Physical Chemistry A</i> , 2004 , 108, 4125-4131	2.8	29
20	One approach to calculating the solvent reorganization energy of intramolecular electron transfer. <i>Science Bulletin</i> , 2003 , 48, 35-38		1
19	Nonequilibrium solvation theory: Comparison, modification and application. <i>Science Bulletin</i> , 2003 , 48, 965-970		4
18	Theoretical investigation of charge transfer excitation and charge recombination in acenaphthyleneBetracyanoethylene complex. <i>International Journal of Quantum Chemistry</i> , 2003 , 94, 23-35	2.1	1

17	Theoretical study of photoinduced electron transfer from tetramethylethylene to tetracyanoethylene. <i>Journal of Chemical Physics</i> , 2003 , 119, 8854-8863	3.9	9
16	Theoretical investigation of electron transfer transition in tetracyanoethylene-contained organic complexes. <i>Journal of Computational Chemistry</i> , 2002 , 23, 874-86	3.5	8
15	Dipole-reaction field interaction model for the solvent reorganization energy and its application to the benzoquinone-benzoquinone anion radical system. <i>Theoretical Chemistry Accounts</i> , 2002 , 107, 282-290	1.9	1
14	Ab initio study on electron excitation and electron transfer in tryptophan-tyrosine system. <i>Chemical Physics</i> , 2002 , 284, 543-554	2.3	14
13	Electron transfer between tryptophan and tyrosine: Theoretical calculation of electron transfer matrix element for intramolecular hole transfer. <i>Journal of Computational Chemistry</i> , 2001 , 22, 565-579	3.5	21
12	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. <i>Journal of Computational Chemistry</i> , 2001 , 22, 1067-1081	3.5	6
11	Ab initio calculation for inner reorganization energy of gas-phase electron transfer in organic molecule- π systems. <i>Chemical Physics</i> , 2000 , 260, 283-294	2.3	37
10	Application of Koopmans's theorem in evaluating electron transfer matrix element of long-range electron transfer. <i>Computational and Theoretical Chemistry</i> , 2000 , 530, 49-58		6
9	Self-consistent reaction field calculation of solvent reorganization energy in electron transfer: a dipole-reaction field interaction model. <i>Theoretical Chemistry Accounts</i> , 2000 , 105, 77-85	1.9	5
8	Electron transfer in poly(p-phenylene) oligomers: effect of external electric field and application of Koopmans theorem. <i>Chemical Physics</i> , 1999 , 248, 137-146	2.3	45
7	Ab initio study of long-range electron transfer between biphenyl anion radical and naphthalene. <i>Science in China Series B: Chemistry</i> , 1999 , 42, 441-448		6
6	A preliminary study of electron transfer reactions between indole and phenol and their consequences for tryptophan and tyrosine. <i>Computational and Theoretical Chemistry</i> , 1999 , 459, 123-129		5
5	Electron transfer between biphenyl and biphenyl anion radicals: Reorganization energies and electron transfer matrix elements. <i>Journal of Computational Chemistry</i> , 1999 , 20, 597-603	3.5	24
4	Electron transfer $\text{NO} + 2 + \text{NO} \rightarrow \text{NO}_2 + \text{NO} +$ in aromatic nitration. <i>Science in China Series B: Chemistry</i> , 1997 , 40, 523-528		6
3	Electron transfer integral between two zero-overlap states. <i>Journal of Computational Chemistry</i> , 1996 , 17, 1108-1111	3.5	8
2	Study on photochemistry of concerted $[1, j]$ and $[i, j]$ sigmatropic rearrangements by the classical path method. <i>Computational and Theoretical Chemistry</i> , 1995 , 342, 181-186		4
1	Electric field dependence of the diabatic potential energy surface for gas-phase electron transfer $\text{O}_2 + \text{O} \rightarrow \text{O}_2^- + \text{O}^+$. <i>Chemical Physics Letters</i> , 1995 , 233, 227-230	2.5	22