Yong-Qing Li

List of Publications by Year
in descending order

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78	1,854	270111	325983
papers	citations	25 h-index	40 g-index

79	79	79	1317
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	An accurate many-body expansion potential energy surface for SiH₂ (1¹ Aâ€²) using a switching function formalism. Physical Chemistry Chemical Physics, 2022, 24, 7759-7767.	1.3	1
2	Solvent dependence of ESIPT process in 2-(2-carbonmethoxy-3,4-dichloro-6-hydroxyphenyl) compounds. Journal of Molecular Liquids, 2022, 354, 118807.	2.3	31
3	Globally Accurate Potential Energy Surface for BH₂⁺2(1³Aâ€²) Using the Switching Function Formalism. Journal of Physical Chemistry A, 2022, 126, 53-60.	1.1	1
4	The theoretical study of excited-state intramolecular proton transfer of N, N,-bis (salicylidene)-(2-(3â€³4â€²-diaminophenyl) benzothiazole). Journal of Luminescence, 2021, 230, 117741.	1.5	62
5	The direct evidence for ESPT route and ICT emission of N6-Methyladenine in aqueous solution. Journal of Luminescence, 2021, 229, 117698.	1.5	26
6	Fluorescence probes detecting O2â€¢_ based on intramolecular charge transfer and excited-state intramolecular proton transfer mechanisms. Journal of Molecular Liquids, 2021, 322, 114886.	2.3	19
7	Substituent Effects on Excited-State Intramolecular Proton Transfer Reaction of 2-Aryloxazoline Derivatives. Journal of Physical Chemistry A, 2021, 125, 2743-2750.	1.1	30
8	The global potential energy surface of PH2+(21Aâ€²) extrapolated to the complete basis set limit. Journal of Physics B: Atomic, Molecular and Optical Physics, 2021, 54, 075101.	0.6	1
9	Substituent effect on ESIPT mechanisms and photophysical properties of HBT derivatives. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2021, 250, 119375.	2.0	45
10	Accurate High-Level Ab Initio-Based Global Potential Energy Surface and Quantum Dynamics Calculation for the First Excited State of CH2+. Journal of Physical Chemistry A, 2021, 125, 5490-5498.	1.1	3
11	Systematic theoretical investigation of two novel molecules BtyC-1 and BtyC-2 based on ESIPT mechanism. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2021, 258, 119810.	2.0	16
12	Accurate global adiabatic potential energy surface for the ground state of AlH2+ by extrapolation to the complete basis set limit. Molecular Physics, 2020, 118, e1655599.	0.8	1
13	The effects of amino group meta- and para-substitution on ESIPT mechanisms of amino 2-(2â€™-hydroxyphenyl) benzazole derivatives. Journal of Luminescence, 2020, 218, 116836.	1.5	59
14	Globally accurate potential energy surface for PH₂⁺ (1¹ Aâ€²) by using the switching function formalism. Molecular Physics, 2020, 118, e1688875.	0.8	3
15	Accurate global adiabatic potential energy surfaces for three low-lying electronic states of AlH₂ free radicals. Physical Chemistry Chemical Physics, 2020, 22, 26544-26551.	1.3	6
16	Theoretical insights into ESIPT mechanism of the two protons system BH-BA in dichloromethane solution. Journal of Molecular Liquids, 2020, 319, 114145.	2.3	20
17	Effect of solvent environment on excited state intramolecular proton transfer in 2-(4-(dimethylamino)phenyl)-3-hydroxy-6,7-dimethoxy-4h-chromen-4-one. Physical Chemistry Chemical Physics, 2019, 21, 17711-17719.	1.3	23
18	The effect of different environments on excited-state intramolecular proton transfer in 4â€²-methoxy-3-hydroxyflavone. Organic Chemistry Frontiers, 2019, 6, 218-225.	2.3	28

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19	Colorimetric fluorescence probe detecting Hg2+ and OClâ€“ based on intramolecular charge transfer and excited-state intramolecular proton transfer mechanisms. Journal of Luminescence, 2019, 209, 102-108.	1.5	37
20	Fluorescence deactivation mechanism for a new probe detecting phosgene based on ESIPT and TICT. Organic Chemistry Frontiers, 2019, 6, 597-602.	2.3	50
21	Revelation solvent effects: excited state hydrogen bond and proton transfer of 2-(benzo[d]thiazol-2-yl)-3-methoxynaphthalen-1-ol. Organic Chemistry Frontiers, 2019, 6, 2780-2787.	2.3	19
22	The novel excited state intramolecular proton transfer broken by intermolecular hydrogen bonds in HOF system. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2019, 219, 164-172.	2.0	36
23	Accurate global potential energy surface by extrapolation to the complete basis set limit and dynamics studies for ground state of H2Sâ‹†. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2019, 219, 267-273.	2.0	8
24	The solvent effect on the excited-state intramolecular proton transfer of cyanine derivative molecules. Organic Chemistry Frontiers, 2019, 6, 1674-1680.	2.3	27
25	A detecting Al3+ ion luminophor 2-(Anthracen-1-yliminomethyl)-phenol: Theoretical investigation on the fluorescence properties and ESIPT mechanism. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2019, 208, 309-314.	2.0	22
26	Under different solvents excited-state intramolecular proton transfer mechanism and solvatochromic effect of 2-(2-hydroxyphenyl) benzothiazole molecule. Journal of Luminescence, 2019, 206, 326-334.	1.5	48
27	Accurate global potential energy surface for the ground state of CH₂⁺ by extrapolation to the complete basis set limit. RSC Advances, 2018, 8, 13635-13642.	1.7	16
28	Theoretical Investigation of the Reaction Mechanism of Photodeamination Induced by Excited-State Intramolecular Proton Transfer of Cresol Derivatives. Journal of Physical Chemistry A, 2018, 122, 1011-1018.	1.1	49
29	Effects of different substituents of methyl 5-R-salicylates on the excited state intramolecular proton transfer process. Physical Chemistry Chemical Physics, 2018, 20, 4208-4215.	1.3	82
30	Stimuli-responsive luminescent coumarin thiazole hybrid dye: Mechanism of excited-state intramolecular double proton transfer. Journal of Luminescence, 2018, 201, 189-195.	1.5	35
31	Theoretical investigation on excited state intramolecular proton transfer of 1-aryl-2-(furan-2-yl) butane-1, 3-diones substitutions. Journal of Molecular Structure, 2018, 1173, 341-344.	1.8	20
32	Allâ€Solidâ€State Synaptic Transistor with Ultralow Conductance for Neuromorphic Computing. Advanced Functional Materials, 2018, 28, 1804170.	7.8	335
33	Excited state intramolecular proton transfer mechanism of o-hydroxynaphthyl phenanthroimidazole. Chinese Physics B, 2018, 27, 023103.	0.7	19
34	The order of multiple excited state proton transfer in ternary complex of norharmane and acetic acids. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2018, 202, 30-35.	2.0	20
35	Reaction Mechanism of Photodeamination Induced by Excited-State Intramolecular Proton Transfer of the Anthrol Molecule. Journal of Physical Chemistry A, 2018, 122, 5409-5417.	1.1	18
36	The theoretical study of excited-state intramolecular proton transfer of 2,5-bis(benzoxazol-2-yl)thiophene-3,4-diol. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2017, 183, 37-44.	2.0	29

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37	The new competitive mechanism of hydrogen bonding interactions and transition process for the hydroxyphenyl imidazo [1, 2-a] pyridine in mixed liquid solution. Scientific Reports, 2017, 7, 1574.	1.6	31
38	Isotopic Effects on Stereodynamics of the C + + H 2 â†' CH + + H Reaction. Communications in Theoretical Physics, 2017, 67, 549.	1.1	3
39	Effect of Different Substituted Groups on Excited-State Intramolecular Proton Transfer of 1-(Acylamino)-anthraquinons. Journal of Physical Chemistry C, 2017, 121, 14779-14786.	1.5	72
40	Proton-Transfer and Photo-deamination Reactive Mechanisms Studies of Amines Compounds. Communications in Computational Chemistry, 2017, 5, 37-45.	1.0	7
41	Accurate ab initio-based potential energy curve and spectroscopic properties of NO(X²Î) via extrapolation to the complete basis set limit. The Journal of Atomic and Molecular Sciences, 2017, 8, 75-83.	0.1	0
42	Accurate potential energy function and spectroscopic properties of NS (X²Î) via extrapolation to the complete basis set limit. The Journal of Atomic and Molecular Sciences, 2017, 8, 88-96.	0.1	0
43	Energy and rotation-dependent stereodynamics of reaction. Chinese Physics B, 2016, 25, 023401.	0.7	1
44	How was the proton transfer process in bis-3, 6-(2- benzoxazolyl)-pyrocatechol, single or double proton transfer?. Scientific Reports, 2016, 6, 25568.	1.6	29
45	Theoretical Study of the ESIPT Process for a New Natural Product Quercetin. Scientific Reports, 2016, 6, 32152.	1.6	84
46	The investigation of excited state proton transfer mechanism in water-bridged 7-azaindole. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2016, 153, 147-151.	2.0	26
47	Photoinduced Charge Transport in a BHJ Solar Cell Controlled by an External Electric Field. Scientific Reports, 2015, 5, 13970.	1.6	33
48	Vector correlations study of the reaction N(² D)+H ₂ (X ¹ Î£) Tj ETQq0 0 0 rgBT /Overlock 10 Tf and reagent vibration excitations. Chinese Physics B, 2015, 24, 113402.	0.7	0
49	Accurate high level ab initio-based global potential energy surface and dynamics calculations for ground state of CH2+. Journal of Chemical Physics, 2015, 142, 124302.	1.2	38
50	Time-Resolved Photoluminescence Spectroscopy of Excitonâ€“Plasmon Coupling Dynamics. Plasmonics, 2015, 10, 271-280.	1.8	5
51	Stereodynamics of the reactions: F + H ₂ /HD/HTâ†'FH + H/D/T. Chinese Physics B, 2015, 24, 053401.	0.7	1
52	Accurate adiabatic potential energy surface for 12Aâ€² state of FH2 based on ab initio data extrapolated to the complete basis set limit. European Physical Journal D, 2015, 69, 1.	0.6	8
53	Theoretical study of stereodynamics for the N + H 2 /D 2 /T 2 reactions. Chinese Physics B, 2014, 23, 123401.	0.7	0
54	Accurate equilibrium inversion barrier of ammonia by extrapolation to the one-electron basis set limit. Chinese Physics B, 2014, 23, 023301.	0.7	3

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55	Accurate ab initio-based DMBE potential energy surface for HLi2(X â€‰2Aâ€²) via scaling of the external correlation. European Physical Journal D, 2014, 68, 1.	0.6	13
56	Unusual Raman spectra of para-nitroaniline by sequential Fermi resonances. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 120, 616-620.	2.0	2
57	Insight into vibration mode-resolved plasmon enhanced Raman optical activity. Journal of Colloid and Interface Science, 2014, 415, 165-168.	5.0	2
58	Bioorganic dye-sensitized solar cell of carotenoidâ€“pheophytin aâ€“TiO₂. RSC Advances, 2014, 4, 63016-63024.	1.7	15
59	Accurate double manyâ€body expansion potential energy surface by extrapolation to the complete basis set limit and dynamics calculations for ground state of NH₂. Journal of Computational Chemistry, 2013, 34, 1686-1696.	1.5	32
60	Remote-Excitation Time-Dependent Surface Catalysis Reaction Using Plasmonic Waveguide on Sites of Single-Crystalline Crossed Nanowires. Plasmonics, 2013, 8, 249-254.	1.8	17
61	Accurate ab initio-based adiabatic global potential energy surface for the 22Aâ€³ state of NH2 by extrapolation to the complete basis set limit. Journal of Chemical Physics, 2013, 139, 154305.	1.2	29
62	Simple formula for the ionization rate of diatomic molecules in an intense laser field using the velocity gauge. Chinese Physics B, 2013, 22, 084203.	0.7	0
63	INTERMOLECULAR CHARGE TRANSFER ENHANCED RESONANCE RAMAN SCATTERING OF CHARGE TRANSFER COMPLEX. Journal of Theoretical and Computational Chemistry, 2012, 11, 273-282.	1.8	4
64	Molecular modeling of two-photon absorption and third-order nonlinearities of polymethine dyes for all-optical switching. Journal of Molecular Modeling, 2012, 18, 4141-4149.	0.8	6
65	Nonlinear resonances in electrochemical SERS of SCNâ¯, rotation-resolved Raman and anti-Stokes Raman of SCNâ¯ in HV-TERS. RSC Advances, 2012, 2, 12160.	1.7	2
66	Visualizations of charge transfer for the model of poly(3,4-alkylenedioxythiophene)s in neutral and various oxidation states. RSC Advances, 2012, 2, 12983.	1.7	8
67	Accurate ab initioâ€based double manyâ€body expansion adiabatic potential energy surface for the 2² A^{â€²} state of NH₂ by extrapolation to the complete basis set limit. International Journal of Quantum Chemistry, 2012, 112, 2932-2939.	1.0	13
68	Ab initio-based double many-body expansion potential energy surface for the first excited triplet state of the ammonia molecule. Journal of Chemical Physics, 2012, 136, 194705.	1.2	25
69	Timeâ€dependent Density Functional Theory Study on the Hydrogenâ€bonded Dimers Formed by Gaucheâ€1PA and Transâ€1PA. Journal of the Chinese Chemical Society, 2012, 59, 494-499.	0.8	1
70	Electron transport properties of three-dimensional topological insulators. Frontiers of Physics, 2012, 7, 165-174.	2.4	26
71	Refining to near spectroscopic accuracy the double many-body expansion potential energy surface for ground-state NH2. Chemical Physics Letters, 2011, 516, 17-22.	1.2	14
72	Ab-Initio-Based Global Double Many-Body Expansion Potential Energy Surface for the Electronic Ground State of the Ammonia Molecule. Journal of Physical Chemistry A, 2010, 114, 6669-6680.	1.1	22

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73	Accurate Potential Energy Surface for the 1²Aâ€² State of NH₂: Scaling of External Correlation Versus Extrapolation to the Complete Basis Set Limit. Journal of Physical Chemistry A, 2010, 114, 9644-9654.	1.1	29
74	-related Quantum Interference of 2 [Case(a)] Diatom on Rotational Energy Transfer. Chinese Journal of Chemical Physics, 2009, 22, 13-18.	0.6	0
75	Intramolecular Charge Transfer of Caroteneâ€porphyrinâ€fullerene Triad: Sequential or Superexchange Cechanism. Chinese Journal of Chemistry, 2008, 26, 1011-1018.	2.6	2
76	Electronic Structure and Photophysical Properties of 2-(N,N-diethylanilin-4-yl)-4,6-bis(3,5-dimethylpyrazol-1-yl)-1,3,5-triazine. Chinese Journal of Chemical Physics, 2007, 20, 59-64.	0.6	3
77	Differential Interference Angle of Collision-induced Rotational Energy Transfer in Na2(A1u+,v=8 b3Ou,v=14)-Na System. Chinese Journal of Chemical Physics, 2006, 19, 469-472.	0.6	1
78	Time-dependent wave packet investigation for N(2D)â€‰+â€‰H2(X1Î£+ g) reaction on the NH2(12Aâ€²) surface. Molecular Physics, 0, , e1928313.	0.8	2