Andrzej L Sobolewski

List of Publications by Year
in descending order

190 papers	10,866 citations	30070 54 h-index	33894 99 g-index
195 all docs	195 docs citations	195 times ranked	5141 citing authors

#	Article	IF	Citations
1	Excited-state hydrogen detachment and hydrogen transfer driven by repulsive 1Ï€Ïƒ* states: A new paradigm for nonradiative decay in aromatic biomolecules. Physical Chemistry Chemical Physics, 2002, 4, 1093-1100.	2.8	881
2	Efficient Deactivation of a Model Base Pair via Excited-State Hydrogen Transfer. Science, 2004, 306, 1765-1768.	12.6	330
3	Ab Initio Studies on the Radiationless Decay Mechanisms of the Lowest Excited Singlet States of 9H-Adenine. Journal of the American Chemical Society, 2005, 127, 6257-6265.	13.7	306
4	Tautomeric selectivity of the excited-state lifetime of guanine/cytosine base pairs: The role of electron-driven proton-transfer processes. Proceedings of the National Academy of Sciences of the United States of America, 2005, 102, 17903-17906.	7.1	290
5	Photoinduced Electron and Proton Transfer in Phenol and Its Clusters with Water and Ammonia. Journal of Physical Chemistry A, 2001, 105, 9275-9283.	2.5	273
6	Ab initio studies on the photophysics of the guanineâ€“cytosine base pair. Physical Chemistry Chemical Physics, 2004, 6, 2763-2771.	2.8	273
7	Ab initio potential-energy functions for excited state intramolecular proton transfer: a comparative study of o-hydroxybenzaldehyde, salicylic acid and 7-hydroxy-1-indanone. Physical Chemistry Chemical Physics, 1999, 1, 3065-3072.	2.8	246
8	Computational Studies of the Photophysics of Hydrogen-Bonded Molecular Systems. Journal of Physical Chemistry A, 2007, 111, 11725-11735.	2.5	227
9	Conical intersections induced by repulsive 1Ï€Ïƒ* states in planar organic molecules: malonaldehyde, pyrrole and chlorobenzene as photochemical model systems. Chemical Physics, 2000, 259, 181-191.	1.9	221
10	Ab initio investigations on the photophysics of indole. Chemical Physics Letters, 1999, 315, 293-298.	2.6	213
11	Conical Intersections in Thymine. Journal of Physical Chemistry A, 2006, 110, 13238-13244.	2.5	200
12	Characterization of theS1â€“S2conical intersection in pyrazine usingabinitiomulticonfiguration selfâ€consistentâ€field and multireference configurationâ€interaction methods. Journal of Chemical Physics, 1994, 100, 1400-1413.	3.0	193
13	Role of Electron-Driven Proton-Transfer Processes in the Excited-State Deactivation of the Adenineâ‹¯Thymine Base Pair. Journal of Physical Chemistry A, 2006, 110, 9031-9038.	2.5	180
14	Charge transfer in aminobenzonitriles: do they twist?. Chemical Physics Letters, 1996, 250, 428-436.	2.6	179
15	Time-dependent quantum wave-packet description of the Ï€1Ïƒ* photochemistry of phenol. Journal of Chemical Physics, 2005, 122, 224315.	3.0	177
16	Photostability of 9H-adenine: mechanisms of the radiationless deactivation of the lowest excited singlet states. Chemical Physics, 2005, 313, 107-112.	1.9	170
17	Ab initio study of the excited-state coupled electronâ€“proton-transfer process in the 2-aminopyridine dimer. Chemical Physics, 2003, 294, 73-83.	1.9	166
18	CHEMISTRY: Unraveling the Molecular Mechanisms of Photoacidity. Science, 2003, 302, 1693-1694.	12.6	158

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19	Ab Initio Investigation of the Structure and Spectroscopy of Hydroniumâˆ'Water Clusters. Journal of Physical Chemistry A, 2002, 106, 4158-4167.	2.5	154
20	Promotion of intramolecular charge transfer in dimethylamino derivatives: twisting versus acceptor-group rehybridization. Chemical Physics Letters, 1996, 259, 119-127.	2.6	143
21	On the nature and signatures of the solvated electron in water. Physical Chemistry Chemical Physics, 2012, 14, 22-34.	2.8	141
22	Ab initioinvestigation of potentialâ€energy surfaces involved in the photophysics of benzene and pyrazine. Journal of Chemical Physics, 1993, 98, 5627-5641.	3.0	140
23	Hydrated hydronium: a cluster model of the solvated electron?. Physical Chemistry Chemical Physics, 2002, 4, 4-10.	2.8	133
24	Photophysics of intramolecularly hydrogen-bonded aromatic systems: ab initio exploration of the excited-state deactivation mechanisms of salicylic acid. Physical Chemistry Chemical Physics, 2006, 8, 3410.	2.8	131
25	Ab Initio Investigation of Reaction Pathways for Intramolecular Charge Transfer in Dimethylanilino Derivatives. Journal of Physical Chemistry A, 1998, 102, 2716-2722.	2.5	129
26	Photochemistry of pyrrole: Time-dependent quantum wave-packet description of the dynamics at the Ï€1Ïƒ*-S0 conical intersections. Journal of Chemical Physics, 2005, 123, 144307.	3.0	120
27	Ab initio study of excited-state intramolecular proton dislocation in salicylic acid. Chemical Physics, 1998, 232, 257-265.	1.9	115
28	Abinitiocharacterization of theS1â€“S2conical intersection in pyrazine and calculation of spectra. Journal of Chemical Physics, 1992, 96, 5298-5309.	3.0	110
29	Nonradiative Decay Mechanisms of the Biologically Relevant Tautomer of Guanine. Journal of Physical Chemistry A, 2008, 112, 11965-11968.	2.5	109
30	Photophysics of Organic Photostabilizers. Ab Initio Study of the Excited-State Deactivation Mechanisms of 2-(2â€˜-Hydroxyphenyl)benzotriazole. Journal of Physical Chemistry A, 2006, 110, 6301-6306.	2.5	107
31	Ab initio characterization of the conical intersections involved in the photochemistry of phenol. Journal of Chemical Physics, 2008, 129, 224307.	3.0	105
32	Photophysics of Malonaldehyde:Â An ab Initio Study. Journal of Physical Chemistry A, 1999, 103, 4494-4504.	2.5	104
33	Theoretical investigation of potential energy surfaces relevant for excited-state hydrogen transfer in o-hydroxybenzaldehyde. Chemical Physics, 1994, 184, 115-124.	1.9	100
34	Intramolecular Hydrogen Bonding in the S1(Ï€Ï€*) Excited State of Anthranilic Acid and Salicylic Acid:â€‰TDDFT Calculation of Excited-State Geometries and Infrared Spectra. Journal of Physical Chemistry A, 2004, 108, 10917-10922.	2.5	100
35	AbinitioStudy of the Excited-State Deactivation Pathways of Protonated Tryptophan and Tyrosine. Journal of the American Chemical Society, 2007, 129, 6223-6231.	13.7	99
36	The chemical physics of the photostability of life. Europhysics News, 2006, 37, 20-23.	0.3	93

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37	Singletâ€“Triplet Inversion in Heptazine and in Polymeric Carbon Nitrides. Journal of Physical Chemistry A, 2019, 123, 8099-8108.	2.5	87
38	Effect of Chemical Substituents on the Energetical Landscape of a Molecular Photoswitch: An Ab Initio Study. Journal of Physical Chemistry A, 2010, 114, 11879-11889.	2.5	86
39	Molecular mechanisms of the photostability of indigo. Physical Chemistry Chemical Physics, 2011, 13, 1618-1628.	2.8	86
40	Mechanism of Photocatalytic Water Splitting with Graphitic Carbon Nitride: Photochemistry of the Heptazineâ€“Water Complex. Journal of Physical Chemistry A, 2017, 121, 4754-4764.	2.5	85
41	Time-dependent quantum wave-packet description of the1Ï€Ïƒ* photochemistry of pyrrole. Faraday Discussions, 2004, 127, 283-293.	3.2	78
42	Mechanisms of Ultrafast Excited-State Deactivation in Adenosine. Journal of Physical Chemistry A, 2014, 118, 122-127.	2.5	76
43	Photochemistry of hydrogen-bonded aromatic pairs: Quantum dynamical calculations for the pyrroleâ€“pyridine complex. Proceedings of the National Academy of Sciences of the United States of America, 2008, 105, 12707-12712.	7.1	74
44	A Computational Study on the Mechanism of Intramolecular Oxoâˆ’Hydroxy Phototautomerism Driven by Repulsive Ï€Ïƒ* State. Journal of Physical Chemistry A, 2008, 112, 13655-13661.	2.5	70
45	Photoinduced charge separation in indoleâ€“water clusters. Chemical Physics Letters, 2000, 329, 130-137.	2.6	68
46	Reversible molecular switch driven by excited-state hydrogen transfer. Physical Chemistry Chemical Physics, 2008, 10, 1243.	2.8	68
47	The mechanism of excited-state hydrogen transfer in 2-hydroxypyridine. Chemical Physics Letters, 1993, 211, 293-299.	2.6	66
48	Photophysics of Eumelanin: Ab Initio Studies on the Electronic Spectroscopy and Photochemistry of 5,6-Dihydroxyindole. ChemPhysChem, 2007, 8, 756-762.	2.1	65
49	Efficient Excited-State Deactivation of the Gly-Phe-Ala Tripeptide via an Electron-Driven Proton-Transfer Process. Journal of the American Chemical Society, 2009, 131, 1374-1375.	13.7	65
50	Relevance of Electron-Driven Proton-Transfer Processes for the Photostability of Proteins. ChemPhysChem, 2006, 7, 561-564.	2.1	64
51	Comparison of the non-radiative decay mechanisms of 4-pyrimidinone and uracil: an ab initio study. Physical Chemistry Chemical Physics, 2010, 12, 5007.	2.8	61
52	Photophysics of 2-Hydroxypyridine:Â Anab InitioStudy. The Journal of Physical Chemistry, 1996, 100, 3933-3941.	2.9	60
53	Computational Studies of the Photophysics of Neutral and Zwitterionic Amino Acids in an Aqueous Environment: Tyrosineâˆ’(H2O)2 and Tryptophanâˆ’(H2O)2 Clusters. Journal of Physical Chemistry A, 2009, 113, 542-550.	2.5	57
54	Photoejection of electrons from pyrrole into an aqueous environment: ab initio results on pyrrole-water clusters. Chemical Physics Letters, 2000, 321, 479-484.	2.6	56

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55	Ab initio study of the amino group twisting and wagging reaction paths in the intramolecular charge transfer of 4-(N,N-dimethylamino)benzonitrile. Chemical Physics, 1999, 240, 9-18.	1.9	54
56	On the mechanism of rapid non-radiative decay in intramolecularly hydrogen-bonded Ї€ systems. Chemical Physics Letters, 1999, 300, 533-539.	2.6	53
57	A Bistable Molecular Switch Driven by Photoinduced Hydrogenâ€Atom Transfer. ChemPhysChem, 2009, 10, 2290-2295.	2.1	53
58	Bowlâ€Shaped Pentagonâ€and Heptagonâ€Embedded Nanographene Containing a Central Pyrrolo[3,2â€b]pyrrole Core. Angewandte Chemie - International Edition, 2021, 60, 14998-15005.	13.8	53
59	Double-proton-transfer in [2,2â€²-bipyridine]-3,3â€²-diol: an ab initio study. Chemical Physics Letters, 1996, 252, 33-41.	2.6	51
60	Computational investigation of the photoinduced homolytic dissociation of water in the pyridineâ€“water complex. Physical Chemistry Chemical Physics, 2013, 15, 5957.	2.8	51
61	Proton-Coupled Electron Transfer from Water to a Model Heptazine-Based Molecular Photocatalyst. Journal of Physical Chemistry Letters, 2018, 9, 6257-6261.	4.6	51
62	Photophysically relevant potential energy functions of low-lying singlet states of benzene, pyridine and pyrazine: an ab initio study. Chemical Physics Letters, 1991, 180, 381-386.	2.6	50
63	Excitedâ€State Intramolecular Proton Transfer: Photoswitching in Salicylidene Methylamine Derivatives. ChemPhysChem, 2014, 15, 1643-1652.	2.1	49
64	Theoretical investigations of proton transfer reactions in a hydrogen bonded complex of cytosine with water. Journal of Chemical Physics, 1995, 102, 5708-5718.	3.0	48
65	Computational studies of aqueous-phase photochemistry and the hydrated electron in finite-size clusters. Physical Chemistry Chemical Physics, 2007, 9, 3818.	2.8	48
66	Evidence for the need of a non-Bornâ€”Oppenheimer description of excited-state hydrogen transfer. Chemical Physics Letters, 1993, 211, 82-87.	2.6	46
67	Ab initio studies of the photophysics of 2-aminopurine. Molecular Physics, 2006, 104, 1113-1121.	1.7	46
68	Photophysics of Schiff Bases: Theoretical Study of Salicylidene Methylamine. ChemPhysChem, 2012, 13, 4287-4294.	2.1	45
69	Are Heptazine-Based Organic Light-Emitting Diode Chromophores Thermally Activated Delayed Fluorescence or Inverted Singletâ€“Triplet Systems?. Journal of Physical Chemistry Letters, 2021, 12, 6852-6860.	4.6	45
70	Molecular mechanisms of the photostability of life. Physical Chemistry Chemical Physics, 2010, 12, 4897.	2.8	44
71	Ab initio characterization of electronically excited states in highly unsaturated hydrocarbons. Journal of Chemical Physics, 1995, 102, 394-399.	3.0	43
72	Photocatalytic Water Splitting with the Acridine Chromophore: A Computational Study. Journal of Physical Chemistry B, 2015, 119, 10664-10672.	2.6	41

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73	Photochemistry of HCl(H2O)4:Â Cluster Model of the Photodetachment of the Chloride Anion in Water. Journal of Physical Chemistry A, 2003, 107, 1557-1562.	2.5	40
74	Photophysics of inter- and intra-molecularly hydrogen-bonded systems: Computational studies on the pyrroleâ€“pyridine complex and 2(2â€²-pyridyl)pyrrole. Chemical Physics, 2008, 347, 413-421.	1.9	40
75	On the Origin of Radiationless Transitions in Porphycenes. Journal of Physical Chemistry A, 2009, 113, 7714-7716.	2.5	40
76	Molecular-dynamics simulations of solvent effects in the intramolecular charge transfer of 4-(N,N-dimethylamino)benzonitrile. Physical Chemistry Chemical Physics, 2000, 2, 4341-4353.	2.8	39
77	Internal conversion funnel in benzene and pyrazine: adiabatic and diabatic representation. Chemical Physics Letters, 1993, 203, 220-226.	2.6	38
78	Computational Study on the Photophysics of Protonated Benzene. Journal of Physical Chemistry A, 2009, 113, 5865-5873.	2.5	38
79	Onset of the Electronic Absorption Spectra of Isolated and Ï€-Stacked Oligomers of 5,6-Dihydroxyindole: An Ab Initio Study of the Building Blocks of Eumelanin. Journal of Physical Chemistry B, 2016, 120, 3493-3502.	2.6	37
80	The infrared spectroscopy of HNCCC: matrix isolation and density functional theory study. Chemical Physics Letters, 2001, 344, 625-630.	2.6	36
81	Photochemical Mechanisms of Radiationless Deactivation Processes in Urocanic Acid. Journal of Physical Chemistry B, 2014, 118, 976-985.	2.6	35
82	Mechanism of photocatalytic water splitting with triazine-based carbon nitrides: insights from ab initio calculations for the triazineâ€“water complex. Physical Chemistry Chemical Physics, 2018, 20, 14420-14430.	2.8	35
83	Photophysics of xanthine: computational study of the radiationless decay mechanisms. Physical Chemistry Chemical Physics, 2009, 11, 10165.	2.8	34
84	Ab initio study of the potential energy functions relevant for hydrogen transfer in formamide, its dimer and its complex with water. Journal of Photochemistry and Photobiology A: Chemistry, 1995, 89, 89-97.	3.9	33
85	Photoinduced Oxidation of Water in the Pyridineâ€“Water Complex: Comparison of the Singlet and Triplet Photochemistries. Journal of Physical Chemistry A, 2014, 118, 7788-7795.	2.5	33
86	Mechanisms of Photostability in Kynurenines: A Joint Electronic-Structure and Dynamics Study. Journal of Physical Chemistry B, 2015, 119, 2112-2124.	2.6	33
87	A theoretical study on the structure of acetonitrile (CH3CN) and its anion CH3CNâ¯. Chemical Physics, 1995, 196, 1-11.	1.9	31
88	Photoinduced Electron and Proton Transfer in the Hydrogen-Bonded Pyridineâ¯Pyrrole System. Journal of Physical Chemistry B, 2007, 111, 6110-6112.	2.6	31
89	7-Hydroxyquinoline-8-carbaldehydes. 1. Ground- and Excited-State Long-Range Prototropic Tautomerization. Journal of Physical Chemistry A, 2013, 117, 9127-9146.	2.5	31
90	Solar Energy Harvesting with Carbon Nitrides and Nâ€Heterocyclic Frameworks: Do We Understand the Mechanism?. ChemPhotoChem, 2019, 3, 10-23.	3.0	31

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91	Anionic water clusters with large vertical electron binding energies and their electronic spectra: (H2O)11â€“ and (H2O)14â€–. Physical Chemistry Chemical Physics, 2003, 5, 1130-1136.	2.8	30
92	Tailoring the Schiff base photoswitching â€“ a non-adiabatic molecular dynamics study of substituent effect on excited state proton transfer. Physical Chemistry Chemical Physics, 2017, 19, 5318-5325.	2.8	30
93	Role of excited-state hydrogen detachment and hydrogen-transfer processes for the excited-state deactivation of an aromatic dipeptide: N-acetyl tryptophan methyl amide. Physical Chemistry Chemical Physics, 2010, 12, 4899.	2.8	29
94	Photochemistry of 2-Aminooxazole, a Hypothetical Prebiotic Precursor of RNA Nucleotides. Journal of Physical Chemistry Letters, 2013, 4, 2785-2788.	4.6	29
95	Ultrafast dynamics of the ESIPT photoswitch N-(3-pyridinyl)-2-pyridinecarboxamide. Physical Chemistry Chemical Physics, 2018, 20, 2646-2655.	2.8	29
96	Spectroscopy meets theory. Nature Chemistry, 2013, 5, 257-258.	13.6	28
97	Nonadiabatic dynamics simulation of keto isocytosine: a comparison of dynamical performance of different electronic-structure methods. Physical Chemistry Chemical Physics, 2017, 19, 19168-19177.	2.8	28
98	Triangular boron carbon nitrides: an unexplored family of chromophores with unique properties for photocatalysis and optoelectronics. Physical Chemistry Chemical Physics, 2021, 23, 12968-12975.	2.8	28
99	Modern Theoretical Approaches to Modeling the Excited-State Intramolecular Proton Transfer: An Overview. Molecules, 2021, 26, 5140.	3.8	28
100	Sequential electron transfer governs the UV-induced self-repair of DNA photolesions. Chemical Science, 2018, 9, 3131-3140.	7.4	27
101	Photochemistry of water: The (H2O)5 cluster. Journal of Chemical Physics, 2005, 122, 184320.	3.0	25
102	Photochemistry of MCl(H2O)4, M = H, Li, Na clusters: finite-size models of the photodetachment of the chloride anion in salt solutions. Physical Chemistry Chemical Physics, 2005, 7, 970.	2.8	25
103	Photoinduced water splitting with oxotitanium porphyrin: a computational study. Physical Chemistry Chemical Physics, 2012, 14, 12807.	2.8	25
104	An ab initio study of the potential energy surface in the S1 state of 2-hydroxypyridine. Chemical Physics, 1996, 213, 193-201.	1.9	24
105	Dual Fluorescence in Aromatic Nitriles:Â The Role of the Charge-Transfer State. Journal of Physical Chemistry A, 1997, 101, 8221-8226.	2.5	24
106	An Ab initio study on the photophysics of tris(salicylideneaniline). Physical Chemistry Chemical Physics, 2018, 20, 25164-25168.	2.8	24
107	Photophysical transformations induced by chemical substitution to salicylaldimines. Physical Chemistry Chemical Physics, 2020, 22, 6698-6705.	2.8	23
108	Barrierless Heptazine-Driven Excited State Proton-Coupled Electron Transfer: Implications for Controlling Photochemistry of Carbon Nitrides and Aza-Arenes. Journal of Physical Chemistry C, 2019, 123, 29580-29588.	3.1	21

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109	Theoretical investigations of the proton transfer reaction in the hydrogen-bonded complex of 2-pyrimidinone with water. The Journal of Physical Chemistry, 1995, 99, 14277-14284.	2.9	20
110	Simulation of the resonance Raman spectrum of the hydrated electron in the hydrated-hydronium cluster model. Physical Chemistry Chemical Physics, 2004, 6, 5297.	2.8	20
111	Electronically excited states and photochemical reaction mechanisms of Î²-glucose. Physical Chemistry Chemical Physics, 2014, 16, 38-47.	2.8	20
112	Molecular Design of Heptazine-Based Photocatalysts: Effect of Substituents on Photocatalytic Efficiency and Photostability. Journal of Physical Chemistry A, 2020, 124, 3698-3710.	2.5	20
113	Effect of chemical substitutions on photo-switching properties of 3-hydroxy-picolinic acid studied by ab initio methods. Journal of Chemical Physics, 2014, 140, 084301.	3.0	19
114	Unravelling the ambiguity of the emission pattern of donorâ€“acceptor salicylaldimines. Journal of Molecular Liquids, 2021, 343, 117532.	4.9	19
115	Potent strategy towards strongly emissive nitroaromatics through a weakly electron-deficient core. Chemical Science, 2021, 12, 14039-14049.	7.4	19
116	Resonances in molecular photoionization. I. Model calculations and analysis of general phenomena. Journal of Chemical Physics, 1987, 86, 176-187.	3.0	18
117	Resonances in molecular photoionization. III. Multichannel extension and application to polyatomic molecules. Journal of Chemical Physics, 1988, 88, 5571-5579.	3.0	18
118	Photodynamics of alternative DNA base isoguanine. Physical Chemistry Chemical Physics, 2019, 21, 13474-13485.	2.8	18
119	Control of Excited-State Proton-Coupled Electron Transfer by Ultrafast Pump-Push-Probe Spectroscopy in Heptazine-Phenol Complexes: Implications for Photochemical Water Oxidation. Journal of Physical Chemistry C, 2020, 124, 9151-9160.	3.1	18
120	Glycine in an Electronically Excited State:â€‰Ab Initio Electronic Structure and Dynamical Calculations. Journal of Physical Chemistry A, 2007, 111, 5259-5269.	2.5	17
121	Computational Model of Photocatalytic Water Splitting. Journal of Physical Chemistry A, 2008, 112, 7311-7313.	2.5	17
122	Photooxidation of water with heptazine-based molecular photocatalysts: Insights from spectroscopy and computational chemistry. Journal of Chemical Physics, 2020, 153, 100902.	3.0	17
123	Photoinduced water oxidation in pyrimidineâ€“water clusters: a combined experimental and theoretical study. Physical Chemistry Chemical Physics, 2020, 22, 12502-12514.	2.8	16
124	Role of the Intermolecular Vibrations in the Hydrogen Transfer Rate:Â The 3-Methylindoleâ‹¯NH3Complex. Journal of Physical Chemistry A, 2006, 110, 9383-9387.	2.5	15
125	Ab initio study on the excited state proton transfer mediated photophysics of 3-hydroxy-picolinic acid. Chemical Physics, 2012, 409, 41-48.	1.9	15
126	Electronic Spectra and Reversible Photoisomerization of Protonated Naphthalenes in Solid Neon. Journal of Physical Chemistry A, 2013, 117, 351-360.	2.5	15

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127	Photoinduced water splitting with oxotitanium tetraphenylporphyrin. Physical Chemistry Chemical Physics, 2014, 16, 15256-15262.	2.8	15
128	Electric field control of proton-transfer molecular switching: molecular dynamics study on salicylidene aniline. Physical Chemistry Chemical Physics, 2015, 17, 14484-14488.	2.8	15
129	Substituent effects on the photophysical properties of tris(salicylideneanilines). Physical Chemistry Chemical Physics, 2021, 23, 1156-1164.	2.8	15
130	Ab initio Studies of Reaction Paths in Excited-State Hydrogen-Transfer Processes. , 1995, , 257-282.		15
131	Resonances in molecular photoionization. IV. Theory of oneâ€color and twoâ€color nearâ€threshold photoionization of molecules. Journal of Chemical Physics, 1988, 89, 6209-6219.	3.0	14
132	Franckâ€“Condon analysis of laser-induced fluorescence excitation spectrum of anthranilic acid: Evaluation of geometry change upon S0â†'S1 excitation. Journal of Chemical Physics, 2009, 130, 054307.	3.0	14
133	Bowlâ€Shaped Pentagonâ€and Heptagonâ€Embedded Nanographene Containing a Central Pyrrolo[3,2â€b]pyrrole Core. Angewandte Chemie, 2021, 133, 15125-15132.	2.0	14
134	Development of an effective single-electron model of the electronic structure of hydronium and hydroniumâ€“water clusters. Chemical Physics Letters, 2002, 356, 556-562.	2.6	13
135	Solvent effects on the photochemistry of 4-aminoimidazole-5-carbonitrile, a prebiotically plausible precursor of purines. Physical Chemistry Chemical Physics, 2014, 16, 17617-17626.	2.8	13
136	Switching the conductance of a molecular junction using a proton transfer reaction. Journal of Molecular Modeling, 2014, 20, 2163.	1.8	13
137	Effect of conformational flexibility on photophysics of bis-coumarins. Physical Chemistry Chemical Physics, 2018, 20, 14491-14503.	2.8	13
138	MQDT analysis of radiationless decay rates of autoionizing rydberg states of polyatomic molecules. Chemical Physics Letters, 1989, 162, 336-341.	2.6	12
139	Photochemical Synâ^'Anti Isomerization Reaction in 1-Methyl-N4-hydroxycytosine. An Experimental Matrix Isolation and Theoretical Density Functional Theory Study. Journal of Physical Chemistry A, 2000, 104, 9459-9466.	2.5	12
140	Ab initio study of the energetics of photoinduced electron and proton transfer processes in a bio-inspired model of photochemical water splitting. Chemical Physics Letters, 2009, 479, 144-148.	2.6	12
141	Photophysics of indole-2-carboxylic acid in an aqueous environment studied by fluorescence spectroscopy in combination with ab initio calculations. Physical Chemistry Chemical Physics, 2012, 14, 2078.	2.8	12
142	Conical-Intersection Topographies Suggest That Ribose Exhibits Enhanced UV Photostability. Journal of Physical Chemistry B, 2016, 120, 10729-10735.	2.6	12
143	The Coumarinâ€Dimer Springâ€”The Struggle between Charge Transfer and Steric Interactions. Chemistry - A European Journal, 2017, 23, 9174-9184.	3.3	12
144	7-Hydroxyquinoline-8-carbaldehydes. 2. Prototropic Equilibria. Journal of Physical Chemistry A, 2013, 117, 9147-9155.	2.5	11

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145	Environmentâ€Sensitive Behavior of DCNP in Solvents with Different Viscosity, Polarity and Proticity. ChemPhysChem, 2015, 16, 3500-3510.	2.1	11
146	Organic photovoltaics without pâ€“n junctions: a computational study of ferroelectric columnar molecular clusters. Physical Chemistry Chemical Physics, 2015, 17, 20580-20587.	2.8	11
147	Highly Polarized Coumarin Derivatives Revisited: Solventâ€Controlled Competition Between Protonâ€Coupled Electron Transfer and Twisted Intramolecular Charge Transfer. Chemistry - A European Journal, 2020, 26, 7281-7291.	3.3	11
148	Computational studies of the photophysics of neutral and zwitterionic glycine in an aqueous environment: The glycineâ€“(H2O)2 cluster. Chemical Physics Letters, 2008, 457, 404-407.	2.6	10
149	Photocatalytic water splitting with acridine dyes: Guidelines from computational chemistry. Chemical Physics, 2016, 464, 78-85.	1.9	10
150	Evidence for competing proton-transfer and hydrogen-transfer reactions in the S1 state of indigo. Chemical Physics, 2018, 515, 535-542.	1.9	10
151	Photoinduced hydrogen-transfer reactions in pyridine-water clusters: Insights from excited-state electronic-structure calculations. Chemical Physics, 2018, 515, 550-556.	1.9	10
152	Theoretical investigations of the proton transfer reaction in hydrogen-bonded complexes of cytosine with HNO. Chemical Physics Letters, 1995, 234, 94-100.	2.6	9
153	Theoretical investigations of the excited-state intramolecular proton transfer reaction in N-substituted-3-hydroxypyridinones. Chemical Physics, 1995, 193, 67-78.	1.9	9
154	Photochemistry of the water dimer: Time-dependent quantum wave-packet description of the dynamics at the S1-S0 conical intersection. Journal of Chemical Physics, 2009, 131, 134307.	3.0	9
155	Mechanisms of photoreactivity in hydrogen-bonded adenineâ€“H₂O complexes. Physical Chemistry Chemical Physics, 2019, 21, 14238-14249.	2.8	9
156	Thioperoxy Derivative Generated by UV-Induced Transformation of N-Hydroxypyridine-2(1H)-thione Isolated in Low-Temperature Matrixes. Journal of Physical Chemistry A, 2008, 112, 238-248.	2.5	8
157	Theoretical study of the photophysics of SF5CF3. Chemical Physics, 2005, 313, 169-176.	1.9	7
158	Multipeak negative differential resistance from interplay between nonlinear stark effect and double-branch current flow. RSC Advances, 2014, 4, 52933-52939.	3.6	7
159	Titanyl Phthalocyanine as a Water Photooxidation Agent. Journal of Physical Chemistry C, 2015, , 150611081346002.	3.1	7
160	Ferroelectric molecular field-switch based on double proton transfer process: Static and dynamical simulations. Journal of Chemical Physics, 2016, 144, 134303.	3.0	7
161	Ferrimagnetism in 2D networks of porphyrin-X and -XO (X=Sc,...,Zn) with acetylene bridges. Journal of Magnetism and Magnetic Materials, 2016, 401, 304-309.	2.3	7
162	The synthesis and photophysical properties of tris-coumarins. Physical Chemistry Chemical Physics, 2019, 21, 8314-8325.	2.8	7

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163	Mechanism of photoinduced intramolecular charge transfer in aminobenzethynes: an ab initio study. Journal of Photochemistry and Photobiology A: Chemistry, 1997, 105, 325-328.	3.9	6
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