Patrik R Callis

List of Publications by Year
in descending order

105	6,009	66234	71532
papers	citations	42 h-index	76 g-index

108	108	108	5190
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Local Electric Field Controls Fluorescence Quantum Yield of Red and Far-Red Fluorescent Proteins. Frontiers in Molecular Biosciences, 2021, 8, 633217.	1.6	18
2	Water as an Essential Cofactor for All Enzymes. Biophysical Journal, 2020, 118, 535a.	0.2	1
3	Buried Liquid Interfaces as a Form of Chemistry in Confinement: The Case of 4-Dimethylaminobenzonitrile at the Silicaâ€"Aqueous Interface. Journal of the American Chemical Society, 2020, 142, 2375-2385.	6.6	7
4	Two-photon absorption spectra of fluorescent isomorphic DNA base analogs. Biomedical Optics Express, 2018, 9, 447.	1.5	19
5	Femtosecond two-photon absorption spectra and permanent electric dipole moment change of tryptophan, 2-aminopurine and related intrinsic and synthetic fluorophores. , 2017, , .		0
6	TD-DFT calculations of one- and two-photon absorption in Coumarin C153 and Prodan: attuning theory to experiment. Physical Chemistry Chemical Physics, 2017, 19, 28824-28833.	1.3	10
7	Picosecond Fluorescence Dynamics of Tryptophan and 5-Fluorotryptophan in Monellin: Slow Waterâ€"Protein Relaxation Unmasked. Journal of Physical Chemistry B, 2015, 119, 4230-4239.	1.2	20
8	Adsorption and Aggregation at Silica/Methanol Interfaces: The Role of Solute Structure. Journal of Physical Chemistry C, 2015, 119, 14230-14238.	1.5	11
9	Simulating electrostatic effects on electronic transitions in proteins. Molecular Simulation, 2015, 41, 190-204.	0.9	7
10	Charge Invariant Proteinâ€"Water Relaxation in GB1 via Ultrafast Tryptophan Fluorescence. Journal of the American Chemical Society, 2014, 136, 2739-2747.	6.6	17
11	Binding phenomena and fluorescence quenching. II: Photophysics of aromatic residues and dependence of fluorescence spectra on protein conformation. Journal of Molecular Structure, 2014, 1077, 22-29.	1.8	58
12	Binding phenomena and fluorescence quenching. I: Descriptive quantum principles of fluorescence quenching using a supermolecule approach. Journal of Molecular Structure, 2014, 1077, 14-21.	1.8	35
13	MD + QM Correlations with Tryptophan Fluorescence Spectral Shifts and Lifetimes. Methods in Molecular Biology, 2014, 1076, 171-214.	0.4	9
14	Femtosecond Fluorescence Dynamics of Tryptophan and 5-Fluorotryptophan in Monellin: Slow Water Relaxation Unmasked. Biophysical Journal, 2013, 104, 681a.	0.2	5
15	Trp Fluorescence in GB1: Nanosecond Dynamics Strongly Depend on pH While 30Ps Relaxation is Constant. Biophysical Journal, 2013, 104, 344a-345a.	0.2	1
16	Insensitivity of Tryptophan Fluorescence to Local Charge Mutations. Journal of Physical Chemistry B, 2013, 117, 9598-9605.	1.2	21
17	Primary Role of the Chromophore Bond Length Alternation in Reversible Photoconversion of Red Fluorescence Proteins. Scientific Reports, 2012, 2, 688.	1.6	30
18	Computational Predictions of Exponential and Non-Exponential Tryptophan Fluorescence Decay in NATA, the Villin Headpiece Subdomain, and other Proteins. Biophysical Journal, 2012, 102, 217a.	0.2	2

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19	Simulations of Tryptophan Fluorescence Dynamics during Folding of the Villin Headpiece. Journal of Physical Chemistry B, 2012, 116, 2586-2594.	1.2	18
20	Correlation of Tryptophan Fluorescence Spectral Shifts and Lifetimes Arising Directly from Heterogeneous Environment. Journal of Physical Chemistry B, 2011, 115, 3245-3253.	1.2	62
21	Predicting Fluorescence Lifetimes and Spectra of Biopolymers. Methods in Enzymology, 2011, 487, 1-38.	0.4	14
22	Electrochromism and Solvatochromism in Fluorescence Response of Organic Dyes: A Nanoscopic View. Springer Series on Fluorescence, 2010, , 309-330.	0.8	6
23	Understanding Wavelength Dependence of Tryptophan Fluorescence Decays. Biophysical Journal, 2010, 98, 583a.	0.2	1
24	Exploring the Electrostatic Landscape of Proteins with Tryptophan Fluorescence. Reviews in Fluorescence, 2009, , 199-248.	0.5	14
25	Mechanism of the Very Efficient Quenching of Tryptophan Fluorescence in Human Î³D- and Î³S-Crystallins: The Î³-Crystallin Fold May Have Evolved To Protect Tryptophan Residues from Ultraviolet Photodamage. Biochemistry, 2009, 48, 3708-3716.	1.2	84
26	Femtosecond Fluorescence Spectra of Tryptophan in Human Î³-Crystallin Mutants: Site-Dependent Ultrafast Quenching. Journal of the American Chemical Society, 2009, 131, 16751-16757.	6.6	44
27	Solvent Effects on the Fluorescence Quenching of Tryptophan by Amides via Electron Transfer. Experimental and Computational Studies. Journal of Physical Chemistry B, 2009, 113, 2572-2577.	1.2	66
28	Constraints on the conformation of the cytoplasmic face of dark-adapted and light-excited rhodopsin inferred from antirhodopsin antibody imprints. Protein Science, 2009, 12, 2453-2475.	3.1	13
29	Molecular Dynamics Simulations of Perylene and Tetracene Librations: Comparison With Femtosecond Upconversion Data. Journal of Physical Chemistry A, 2008, 112, 5593-5597.	1.1	7
30	Ab Initio Prediction of Tryptophan Fluorescence Quenching by Protein Electric Field Enabled Electron Transfer. Journal of Physical Chemistry B, 2007, 111, 10335-10339.	1.2	59
31	The Emitting State of Tryptophan in Proteins with Highly Blue-Shifted Fluorescence. Angewandte Chemie - International Edition, 2007, 46, 5137-5139.	7.2	37
32	Mechanism of the Highly Efficient Quenching of Tryptophan Fluorescence in Human Î³D-Crystallinâ€. Biochemistry, 2006, 45, 11552-11563.	1.2	86
33	Ultrafast Fluorescence Dynamics of Tryptophan in the Proteins Monellin and IIAGlc. Journal of the American Chemical Society, 2006, 128, 1214-1221.	6.6	61
34	Dependence of Tryptophan Emission Wavelength on Conformation in Cyclic Hexapeptides. Journal of Physical Chemistry B, 2006, 110, 7009-7016.	1.2	44
35	Short range photoinduced electron transfer in proteins: QM-MM simulations of tryptophan and flavin fluorescence quenching in proteins. Chemical Physics, 2006, 326, 230-239.	0.9	47
36	Ionization Potentials of Fluoroindoles and the Origin of Nonexponential Tryptophan Fluorescence Decay in ProteinsâŠ¥. Journal of the American Chemical Society, 2005, 127, 4104-4113.	6.6	85

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37	Photophysics of Tryptophan Fluorescence:â€‰ Link with the Catalytic Strategy of the Citrate Synthase from Thermoplasma acidophilum. Biochemistry, 2005, 44, 1394-1413.	1.2	38
38	Experimental and Theoretical Investigations of Environmentally Sensitive Single-Molecule Fluorophoresâ€. Journal of Physical Chemistry B, 2004, 108, 10465-10473.	1.2	76
39	Quantitative Prediction of Fluorescence Quantum Yields for Tryptophan in Proteins. Journal of Physical Chemistry B, 2004, 108, 4248-4259.	1.2	214
40	Understanding the variable fluorescence quantum yield of tryptophan in proteins using QM-MM simulations. Quenching by charge transfer to the peptide backbone. Chemical Physics Letters, 2003, 369, 409-414.	1.2	110
41	The Photophysical Properties of 6-Azaindole. Journal of Physical Chemistry B, 2003, 107, 637-645.	1.2	29
42	The Theory of Two-Photon-Induced Fluorescence Anisotropy. , 2002, , 1-42.		10
43	One- and two-photon spectra of jet-cooled 2,3-dimethylindole: 1Lb and 1La assignments. Chemical Physics, 2002, 283, 269-278.	0.9	20
44	Mechanisms of Tryptophan Fluorescence Shifts in Proteins. Biophysical Journal, 2001, 80, 2093-2109.	0.2	1,186
45	Electronic structure and hyperfine interactions in thioether-substituted tyrosyl radicals. Chemical Physics Letters, 2000, 331, 108-114.	1.2	6
46	Evidence for [sup 1]L[sub a] fluorescence from jet-cooled 3-methylindole-polar solvent complexes. Journal of Chemical Physics, 2000, 113, 5235.	1.2	40
47	Fluorescence Properties of Benz[f]indole, a Wavelength and Quenching Selective Tryptophan Analog. Journal of Physical Chemistry B, 2000, 104, 1837-1843.	1.2	14
48	Vibrational assignments for indole with the aid of ultrasharp phosphorescence spectra. International Journal of Quantum Chemistry, 1999, 72, 347-356.	1.0	24
49	Evidence of pure 1Lb fluorescence from redshifted indole-polar solvent complexes in a supersonic jet. Journal of Chemical Physics, 1998, 108, 10189-10196.	1.2	38
50	TWO-PHOTONâ€“INDUCED FLUORESCENCE. Annual Review of Physical Chemistry, 1997, 48, 271-297.	4.8	94
51	Lowest Triplet State of Indole:Â An ab Initio Study. Journal of Physical Chemistry A, 1997, 101, 2686-2691.	1.1	42
52	Tryptophan Fluorescence Shifts in Proteins from Hybrid Simulations:Â An Electrostatic Approach. Journal of Physical Chemistry B, 1997, 101, 9429-9432.	1.2	145
53	[7] 1La and 1Lb transitions of tryptophan: Applications of theory and experimental observations to fluorescence of proteins. Methods in Enzymology, 1997, 278, 113-150.	0.4	268
54	1La origin locations of methyl indoles in argon matrices. Chemical Physics Letters, 1996, 262, 343-348.	1.2	23

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55	Fluorescence of reduced nicotinamides using one- and two-photon excitation. Biophysical Chemistry, 1996, 62, 1-13.	1.5	72
56	Site selective photoselection study of indole in argon matrix: location of the 1La origin. Chemical Physics Letters, 1995, 239, 31-37.	1.2	61
57	Ab initio calculations of vibronic spectra for indole. Chemical Physics Letters, 1995, 244, 53-58.	1.2	82
58	Fluorescence anisotropy of tyrosine using one-and two-photon excitation. Biophysical Chemistry, 1995, 56, 263-271.	1.5	36
59	Molecular Orbital Theory of the 1La and 1Lb States of Indole. 2. An ab Initio Study. The Journal of Physical Chemistry, 1995, 99, 8572-8581.	2.9	87
60	Theoretical Study of the Crystal Field Effects on the Transition Dipole Moments in Methylated Adenines. The Journal of Physical Chemistry, 1994, 98, 10397-10407.	2.9	27
61	Fluorescence excitation spectrum of indoleâ€"D2O in supersonic jet. Chemical Physics Letters, 1994, 222, 156-160.	1.2	17
62	Vibronic band shapes for indole from scaled bond order changes. Chemical Physics Letters, 1994, 229, 153-160.	1.2	14
63	A THEORETICAL STUDY OF THE CYTOSINE EXCIMER STATE: THE ROLE OF GEOMETRY OPTIMIZATION. Photochemistry and Photobiology, 1994, 59, 125-129.	1.3	22
64	Hybrid simulations of solvation effects on electronic spectra: Indoles in water. Journal of Chemical Physics, 1994, 100, 4093-4109.	1.2	126
65	Fluorescence Lifetime Measurements of Fluoranthene, 1-Naphthol, and Napropamide in the Presence of Dissolved Humic Acid. Environmental Science & Technology, 1994, 28, 1582-1588.	4.6	59
66	<title><formula>^{<roman>1</roman>}</formula>L<formula><inf><roman>a</roman></inf></formula> transitions of jet-cooled indoles and complexes from two-photon fluorescence excitation</title>. , 1994, , .		3
67	A theoretical study of the cytosine excimer state. Chemical Physics Letters, 1993, 209, 519-524.	1.2	5
68	Two-photon fluorescence excitation spectra of aromatic amino acids. Chemical Physics Letters, 1993, 208, 276-282.	1.2	92
69	On the theory of twoâ€photon induced fluorescence anisotropy with application to indoles. Journal of Chemical Physics, 1993, 99, 27-37.	1.2	100
70	Methyl rotor effects in 3- and 5-methylindole. The Journal of Physical Chemistry, 1992, 96, 5771-5778.	2.9	20
71	<title>Simulation of solvent dynamics effects on the fluorescence of 3-methylindole in water</title>. , 1992, , .		3
72	Effects of the crystal field on transition moments in 9-ethylguanine. Journal of the American Chemical Society, 1991, 113, 3260-3267.	6.6	36

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73	Molecular orbital theory of the1Lband1Lastates of indole. Journal of Chemical Physics, 1991, 95, 4230-4240.	1.2	128
74	Two-photon electronic spectra of nucleotides. , 1990, , .		1
75	Photophysics of indole derivatives: experimental resolution of La and Lb transitions and comparison with theory. The Journal of Physical Chemistry, 1990, 94, 3469-3479.	2.9	147
76	Resonance Raman studies of guanidinium and substituted guanidinium ions. The Journal of Physical Chemistry, 1990, 94, 4015-4025.	2.9	48
77	Two-photon fluorescence excitation spectra of indole in vapor and jet: 1La states. The Journal of Physical Chemistry, 1990, 94, 7340-7342.	2.9	59
78	Tonoplast ATPase proton pumps in wheat roots. Plant Science, 1989, 65, 153-160.	1.7	4
79	Two-photon spectra of inductively perturbed naphthalenes. Chemical Physics Letters, 1988, 144, 158-164.	1.2	20
80	A powerâ€squared sensor for twoâ€photon spectroscopy and dispersion of secondâ€order coherence. Journal of Applied Physics, 1988, 64, 4301-4305.	1.1	16
81	Fluorometric determination of the neutral lipid content of microalgal cells using Nile Red. Journal of Microbiological Methods, 1987, 6, 333-345.	0.7	296
82	A CNDO/S study of the importance of electron repulsion parameters and charge density changes on the weakness of the v8(e2g) vibronic activity in the benzene 260 nm band. Chemical Physics Letters, 1987, 133, 14-20.	1.2	8
83	Resolution of La and Lb bands in methyl indoles by two-photon spectroscopy. Chemical Physics Letters, 1987, 140, 83-89.	1.2	76
84	Polarized two-photon fluorescence excitation spectra of indole and benzimidazole. Chemical Physics Letters, 1986, 125, 106-112.	1.2	42
85	AN EXTENDED SEMIâ€EMPIRICAL MOLECULAR ORBITAL STUDY OF THE * EXCITED STATES OF NUCLEIC ACID BASES. Photochemistry and Photobiology, 1986, 44, 315-322.	1.3	34
86	Two-photon properties of the La and Lb bands of substituted benzenes computed from CNDO/S. Chemical Physics Letters, 1984, 107, 125-130.	1.2	18
87	Transition density topology of the La and Lb states in indoles and purines. International Journal of Quantum Chemistry, 1984, 26, 579-588.	1.0	26
88	Perturbation selection rules for multiphoton electronic spectroscopy of neutral alternant	1.2	122
89	Advances in calculating Raman excitation profiles by means of the transform theory. Journal of Chemical Physics, 1983, 78, 712-722.	1.2	126
90	Fluorescence from adenine cations. The Journal of Physical Chemistry, 1982, 86, 49-55.	2.9	19

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91	Alternant hydrocarbon selection rules in the two-photon spectroscopy of perturbed benzene. Chemical Physics Letters, 1982, 93, 111-114.	1.2	27
92	Polarized twoâ€photon fluorescence excitation studies of pyrimidine. Journal of Chemical Physics, 1981, 75, 5640-5646.	1.2	44
93	FLUORESCENT TAUTOMERS AND THE APPARENT PHOTOPHYSICS OF ADENINE AND GUANINE. Photochemistry and Photobiology, 1980, 31, 323-327.	1.3	80
94	POLARIZED FLUORESCENCE OF 5-METHYLCYTOSINE SPECIES IN SOLUTION AT ROOM TEMPERATURE. Photochemistry and Photobiology, 1980, 32, 1-7.	1.3	14
95	PHOTOCHEMISTRY AND PHOTOPHYSICS OF GUANINEâ€CONTAINING DINUCLEOSIDES. Photochemistry and Photobiology, 1979, 29, 1107-1113.	1.3	8
96	Polarized fluorescence and estimated lifetimes of the DNA bases at room temperature. Chemical Physics Letters, 1979, 61, 568-570.	1.2	65
97	Reduction pathways of organohalogen compounds. Journal of Electroanalytical Chemistry and Interfacial Electrochemistry, 1977, 78, 145-159.	0.3	33
98	Excitons, energy transfer, and charge resonance in excited dinucleotides and polynucleotides. A photoselection study. The Journal of Physical Chemistry, 1976, 80, 2280-2288.	2.9	53
99	Rapid internal conversion by nucleic acid components in solution. Chemical Physics Letters, 1975, 36, 618-623.	1.2	21
100	The polarization of excimer fluorescence from a dinucleotide. Chemical Physics Letters, 1973, 19, 551-555.	1.2	14
101	Polarization of electronic transitions in 9-ethylguanine. Journal of the American Chemical Society, 1971, 93, 6679-6680.	6.6	27
102	Polarization of electronic transitions in cytosine. Journal of the American Chemical Society, 1970, 92, 3593-3599.	6.6	42
103	Flow dichroism of DNA: A new apparatus and further studies. Biopolymers, 1969, 7, 335-352.	1.2	30
104	Hydrodynamic relaxation times of DNA from decay of flow dichroism measurements. Biopolymers, 1969, 8, 379-390.	1.2	43
105	Search For Accidental Degeneracy in Purines. Journal of the American Chemical Society, 1964, 86, 2292-2294.	6.6	60