Patrik R Callis

List of Publications by Year
in descending order

105 papers	6,009 citations	66234 42 h-index	71532 76 g-index
108 all docs	108 docs citations	108 times ranked	5190 citing authors

#	Article	IF	Citations
1	Mechanisms of Tryptophan Fluorescence Shifts in Proteins. Biophysical Journal, 2001, 80, 2093-2109.	0.2	1,186
2	Fluorometric determination of the neutral lipid content of microalgal cells using Nile Red. Journal of Microbiological Methods, 1987, 6, 333-345.	0.7	296
3	[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
4	Quantitative Prediction of Fluorescence Quantum Yields for Tryptophan in Proteins. Journal of Physical Chemistry B, 2004, 108, 4248-4259.	1.2	214
5	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
6	Tryptophan Fluorescence Shifts in Proteins from Hybrid Simulations:Â An Electrostatic Approach. Journal of Physical Chemistry B, 1997, 101, 9429-9432.	1.2	145
7	Molecular orbital theory of the1Lband1Lastates of indole. Journal of Chemical Physics, 1991, 95, 4230-4240.	1.2	128
8	Advances in calculating Raman excitation profiles by means of the transform theory. Journal of Chemical Physics, 1983, 78, 712-722.	1.2	126
9	Hybrid simulations of solvation effects on electronic spectra: Indoles in water. Journal of Chemical Physics, 1994, 100, 4093-4109.	1.2	126
10	Perturbation selection rules for multiphoton electronic spectroscopy of neutral alternant	1.2	122
11	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
12	On the theory of twoâ€photon induced fluorescence anisotropy with application to indoles. Journal of Chemical Physics, 1993, 99, 27-37.	1.2	100
13	TWO-PHOTONâ€"INDUCED FLUORESCENCE. Annual Review of Physical Chemistry, 1997, 48, 271-297.	4.8	94
14	Two-photon fluorescence excitation spectra of aromatic amino acids. Chemical Physics Letters, 1993, 208, 276-282.	1.2	92
15	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
16	Mechanism of the Highly Efficient Quenching of Tryptophan Fluorescence in Human Î³D-Crystallinâ€. Biochemistry, 2006, 45, 11552-11563.	1.2	86
17	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
18	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

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19	Ab initio calculations of vibronic spectra for indole. Chemical Physics Letters, 1995, 244, 53-58.	1.2	82
20	FLUORESCENT TAUTOMERS AND THE APPARENT PHOTOPHYSICS OF ADENINE AND GUANINE. Photochemistry and Photobiology, 1980, 31, 323-327.	1.3	80
21	Resolution of La and Lb bands in methyl indoles by two-photon spectroscopy. Chemical Physics Letters, 1987, 140, 83-89.	1.2	76
22	Experimental and Theoretical Investigations of Environmentally Sensitive Single-Molecule Fluorophoresâ€. Journal of Physical Chemistry B, 2004, 108, 10465-10473.	1.2	76
23	Fluorescence of reduced nicotinamides using one- and two-photon excitation. Biophysical Chemistry, 1996, 62, 1-13.	1.5	72
24	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
25	Polarized fluorescence and estimated lifetimes of the DNA bases at room temperature. Chemical Physics Letters, 1979, 61, 568-570.	1.2	65
26	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
27	Site selective photoselection study of indole in argon matrix: location of the 1La origin. Chemical Physics Letters, 1995, 239, 31-37.	1.2	61
28	Ultrafast Fluorescence Dynamics of Tryptophan in the Proteins Monellin and IIAGlc. Journal of the American Chemical Society, 2006, 128, 1214-1221.	6.6	61
29	Search For Accidental Degeneracy in Purines. Journal of the American Chemical Society, 1964, 86, 2292-2294.	6.6	60
30	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
31	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
32	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
33	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
34	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
35	Resonance Raman studies of guanidinium and substituted guanidinium ions. The Journal of Physical Chemistry, 1990, 94, 4015-4025.	2.9	48
36	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

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37	Polarized twoâ€photon fluorescence excitation studies of pyrimidine. Journal of Chemical Physics, 1981, 75, 5640-5646.	1.2	44
38	Dependence of Tryptophan Emission Wavelength on Conformation in Cyclic Hexapeptides. Journal of Physical Chemistry B, 2006, 110, 7009-7016.	1.2	44
39	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
40	Hydrodynamic relaxation times of DNA from decay of flow dichroism measurements. Biopolymers, 1969, 8, 379-390.	1.2	43
41	Polarization of electronic transitions in cytosine. Journal of the American Chemical Society, 1970, 92, 3593-3599.	6.6	42
42	Polarized two-photon fluorescence excitation spectra of indole and benzimidazole. Chemical Physics Letters, 1986, 125, 106-112.	1.2	42
43	Lowest Triplet State of Indole:Â An ab Initio Study. Journal of Physical Chemistry A, 1997, 101, 2686-2691.	1.1	42
44	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
45	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
46	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
47	The Emitting State of Tryptophan in Proteins with Highly Blue-Shifted Fluorescence. Angewandte Chemie - International Edition, 2007, 46, 5137-5139.	7.2	37
48	Effects of the crystal field on transition moments in 9-ethylguanine. Journal of the American Chemical Society, 1991, 113, 3260-3267.	6.6	36
49	Fluorescence anisotropy of tyrosine using one-and two-photon excitation. Biophysical Chemistry, 1995, 56, 263-271.	1.5	36
50	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
51	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
52	Reduction pathways of organohalogen compounds. Journal of Electroanalytical Chemistry and Interfacial Electrochemistry, 1977, 78, 145-159.	0.3	33
53	Flow dichroism of DNA: A new apparatus and further studies. Biopolymers, 1969, 7, 335-352.	1.2	30
54	Primary Role of the Chromophore Bond Length Alternation in Reversible Photoconversion of Red Fluorescence Proteins. Scientific Reports, 2012, 2, 688.	1.6	30

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55	The Photophysical Properties of 6-Azaindole. Journal of Physical Chemistry B, 2003, 107, 637-645.	1.2	29
56	Polarization of electronic transitions in 9-ethylguanine. Journal of the American Chemical Society, 1971, 93, 6679-6680.	6.6	27
57	Alternant hydrocarbon selection rules in the two-photon spectroscopy of perturbed benzene. Chemical Physics Letters, 1982, 93, 111-114.	1.2	27
58	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
59	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
60	Vibrational assignments for indole with the aid of ultrasharp phosphorescence spectra. International Journal of Quantum Chemistry, 1999, 72, 347-356.	1.0	24
61	1La origin locations of methyl indoles in argon matrices. Chemical Physics Letters, 1996, 262, 343-348.	1.2	23
62	A THEORETICAL STUDY OF THE CYTOSINE EXCIMER STATE: THE ROLE OF GEOMETRY OPTIMIZATION. Photochemistry and Photobiology, 1994, 59, 125-129.	1.3	22
63	Rapid internal conversion by nucleic acid components in solution. Chemical Physics Letters, 1975, 36, 618-623.	1.2	21
64	Insensitivity of Tryptophan Fluorescence to Local Charge Mutations. Journal of Physical Chemistry B, 2013, 117, 9598-9605.	1.2	21
65	Two-photon spectra of inductively perturbed naphthalenes. Chemical Physics Letters, 1988, 144, 158-164.	1.2	20
66	Methyl rotor effects in 3- and 5-methylindole. The Journal of Physical Chemistry, 1992, 96, 5771-5778.	2.9	20
67	One- and two-photon spectra of jet-cooled 2,3-dimethylindole: 1Lb and 1La assignments. Chemical Physics, 2002, 283, 269-278.	0.9	20
68	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
69	Fluorescence from adenine cations. The Journal of Physical Chemistry, 1982, 86, 49-55.	2.9	19
70	Two-photon absorption spectra of fluorescent isomorphic DNA base analogs. Biomedical Optics Express, 2018, 9, 447.	1.5	19
71	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
72	Simulations of Tryptophan Fluorescence Dynamics during Folding of the Villin Headpiece. Journal of Physical Chemistry B, 2012, 116, 2586-2594.	1.2	18

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73	Local Electric Field Controls Fluorescence Quantum Yield of Red and Far-Red Fluorescent Proteins. Frontiers in Molecular Biosciences, 2021, 8, 633217.	1.6	18
74	Fluorescence excitation spectrum of indoleâ€"D2O in supersonic jet. Chemical Physics Letters, 1994, 222, 156-160.	1.2	17
75	Charge Invariant Proteinâ€"Water Relaxation in GB1 via Ultrafast Tryptophan Fluorescence. Journal of the American Chemical Society, 2014, 136, 2739-2747.	6.6	17
76	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
77	The polarization of excimer fluorescence from a dinucleotide. Chemical Physics Letters, 1973, 19, 551-555.	1.2	14
78	POLARIZED FLUORESCENCE OF 5-METHYLCYTOSINE SPECIES IN SOLUTION AT ROOM TEMPERATURE. Photochemistry and Photobiology, 1980, 32, 1-7.	1.3	14
79	Vibronic band shapes for indole from scaled bond order changes. Chemical Physics Letters, 1994, 229, 153-160.	1.2	14
80	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
81	Exploring the Electrostatic Landscape of Proteins with Tryptophan Fluorescence. Reviews in Fluorescence, 2009, , 199-248.	0.5	14
82	Predicting Fluorescence Lifetimes and Spectra of Biopolymers. Methods in Enzymology, 2011, 487, 1-38.	0.4	14
83	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
84	Adsorption and Aggregation at Silica/Methanol Interfaces: The Role of Solute Structure. Journal of Physical Chemistry C, 2015, 119, 14230-14238.	1.5	11
85	The Theory of Two-Photon-Induced Fluorescence Anisotropy. , 2002, , 1-42.		10
86	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
87	MD + QM Correlations with Tryptophan Fluorescence Spectral Shifts and Lifetimes. Methods in Molecular Biology, 2014, 1076, 171-214.	0.4	9
88	PHOTOCHEMISTRY AND PHOTOPHYSICS OF GUANINEâ€CONTAINING DINUCLEOSIDES. Photochemistry and Photobiology, 1979, 29, 1107-1113.	1.3	8
89	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
90	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

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91	Simulating electrostatic effects on electronic transitions in proteins. Molecular Simulation, 2015, 41, 190-204.	0.9	7
92	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
93	Electronic structure and hyperfine interactions in thioether-substituted tyrosyl radicals. Chemical Physics Letters, 2000, 331, 108-114.	1.2	6
94	Electrochromism and Solvatochromism in Fluorescence Response of Organic Dyes: A Nanoscopic View. Springer Series on Fluorescence, 2010, , 309-330.	0.8	6
95	A theoretical study of the cytosine excimer state. Chemical Physics Letters, 1993, 209, 519-524.	1.2	5
96	Femtosecond Fluorescence Dynamics of Tryptophan and 5-Fluorotryptophan in Monellin: Slow Water Relaxation Unmasked. Biophysical Journal, 2013, 104, 681a.	0.2	5
97	Tonoplast ATPase proton pumps in wheat roots. Plant Science, 1989, 65, 153-160.	1.7	4
98	<title>Simulation of solvent dynamics effects on the fluorescence of 3-methylindole in water</title>. , 1992, , .		3
99	<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
100	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
101	Two-photon electronic spectra of nucleotides. , 1990, , .		1
102	Understanding Wavelength Dependence of Tryptophan Fluorescence Decays. Biophysical Journal, 2010, 98, 583a.	0.2	1
103	Trp Fluorescence in GB1: Nanosecond Dynamics Strongly Depend on pH While 30Ps Relaxation is Constant. Biophysical Journal, 2013, 104, 344a-345a.	0.2	1
104	Water as an Essential Cofactor for All Enzymes. Biophysical Journal, 2020, 118, 535a.	0.2	1
105	Femtosecond two-photon absorption spectra and permanent electric dipole moment change of tryptophan, 2-aminopurine and related intrinsic and synthetic fluorophores. , 2017, , .		0