Daniel Roca-SanjuÃ¡n

List of Publications by Year
in descending order

101 papers	3,509 citations	136885 32 h-index	155592 55 g-index
105 all docs	105 docs citations	105 times ranked	3335 citing authors

#	Article	IF	Citations
1	Chemi- and Bioluminescence of Cyclic Peroxides. Chemical Reviews, 2018, 118, 6927-6974.	23.0	265
2	Peptide Metalâ€“Organic Frameworks for Enantioselective Separation of Chiral Drugs. Journal of the American Chemical Society, 2017, 139, 4294-4297.	6.6	247
3	Multiconfiguration secondâ€order perturbation theory approach to strong electron correlation in chemistry and photochemistry. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2012, 2, 585-603.	6.2	166
4	Solid State Luminescence Enhancement in Ï€-Conjugated Materials: Unraveling the Mechanism beyond the Framework of AIE/AIEE. Journal of Physical Chemistry C, 2017, 121, 23166-23183.	1.5	157
5	Luminescence in Crystalline Organic Materials: From Molecules to Molecular Solids. Advanced Optical Materials, 2021, 9, 2002251.	3.6	146
6	Ab initiodetermination of the ionization potentials of DNA and RNA nucleobases. Journal of Chemical Physics, 2006, 125, 084302.	1.2	139
7	Photoreduction of gaseous oxidized mercury changes global atmospheric mercury speciation, transport and deposition. Nature Communications, 2018, 9, 4796.	5.8	107
8	The Chemistry of Bioluminescence: An Analysis of Chemical Functionalities. ChemPhysChem, 2011, 12, 3064-3076.	1.0	105
9	Molecular Basis of DNA Photodimerization: Intrinsic Production of Cyclobutane Cytosine Dimers. Journal of the American Chemical Society, 2008, 130, 10768-10779.	6.6	100
10	Benzophenone Ultrafast Triplet Population: Revisiting the Kinetic Model by Surface-Hopping Dynamics. Journal of Physical Chemistry Letters, 2016, 7, 622-626.	2.1	89
11	Ab initio determination of the electron affinities of DNA and RNA nucleobases. Journal of Chemical Physics, 2008, 129, 095104.	1.2	83
12	Excitation of Nucleobases from a Computational Perspective I: Reaction Paths. Topics in Current Chemistry, 2013, 355, 57-97.	4.0	66
13	Toward the understanding of DNA fluorescence: The singlet excimer of cytosine. Journal of Chemical Physics, 2006, 125, 231102.	1.2	59
14	Essential on the Photophysics and Photochemistry of the Indole Chromophore by Using a Totally Unconstrained Theoretical Approach. Journal of Chemical Theory and Computation, 2011, 7, 4088-4096.	2.3	51
15	Photochemistry of oxidized Hg(I) and Hg(II) species suggests missing mercury oxidation in the troposphere. Proceedings of the National Academy of Sciences of the United States of America, 2020, 117, 30949-30956.	3.3	50
16	Chemiluminescence and Fluorescence States of a Small Model for Coelenteramide and Cypridina Oxyluciferin: A CASSCF/CASPT2 Study. Journal of Chemical Theory and Computation, 2011, 7, 4060-4069.	2.3	49
17	On the photoproduction of DNA/RNA cyclobutane pyrimidine dimers. Theoretical Chemistry Accounts, 2011, 128, 705-711.	0.5	48
18	Are the Bioâ€•and Chemiluminescence States of the Firefly Oxyluciferin the Same as the Fluorescence State?. Photochemistry and Photobiology, 2013, 89, 319-325.	1.3	48

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19	Resolving the Benzophenone DNA-Photosensitization Mechanism at QM/MM Level. Journal of Physical Chemistry Letters, 2015, 6, 576-580.	2.1	48
20	Photoinduced Formation Mechanism of the Thymineâ€“Thymine (6â€“4) Adduct. Journal of Physical Chemistry B, 2013, 117, 1999-2004.	1.2	46
21	Thermochromic Fluorescence from B₁₈H₂₀(NC₅H₅)₂: An Inorganicâ€“Organic Composite Luminescent Compound with an Unusual Molecular Geometry. Advanced Optical Materials, 2017, 5, 1600694.	3.6	45
22	Molecular Basis of the Chemiluminescence Mechanism of Luminol. Chemistry - A European Journal, 2019, 25, 5202-5213.	1.7	45
23	Photodissociation Mechanisms of Major Mercury(II) Species in the Atmospheric Chemical Cycle of Mercury. Angewandte Chemie - International Edition, 2020, 59, 7605-7610.	7.2	45
24	Chemiluminescence of Coelenterazine and Fluorescence of Coelenteramide: A Systematic Theoretical Study. Journal of Chemical Theory and Computation, 2012, 8, 2796-2807.	2.3	42
25	Proton/Hydrogen Transfer Mechanisms in the Guanineâ€“Cytosine Base Pair: Photostability and Tautomerism. Journal of Chemical Theory and Computation, 2013, 9, 481-496.	2.3	42
26	Computational determination of the dominant triplet population mechanism in photoexcited benzophenone. Physical Chemistry Chemical Physics, 2014, 16, 25393-25403.	1.3	42
27	Gas-Phase Photolysis of Hg(I) Radical Species: A New Atmospheric Mercury Reduction Process. Journal of the American Chemical Society, 2019, 141, 8698-8702.	6.6	40
28	Inverted energy gap law for the nonradiative decay in fluorescent floppy molecules: larger fluorescence quantum yields for smaller energy gaps. Organic Chemistry Frontiers, 2019, 6, 1948-1954.	2.3	40
29	Revisiting the Nonadiabatic Process in 1,2-Dioxetane. Journal of Chemical Theory and Computation, 2013, 9, 5404-5411.	2.3	38
30	On the Deactivation Mechanisms of Adenineâ€“Thymine Base Pair. Journal of Physical Chemistry B, 2012, 116, 4089-4097.	1.2	37
31	Mechanism of activated chemiluminescence of cyclic peroxides: 1,2-dioxetanes and 1,2-dioxetanones. Physical Chemistry Chemical Physics, 2017, 19, 3955-3962.	1.3	37
32	Ab initio determination of the ionization potentials of water clusters (H2O)n (n =) Tj ETQq0 0 0 rgBT /Overlock 10 T	1.2	36
33	Can the Closed-Shell DFT Methods Describe the Thermolysis of 1,2-Dioxetanone?. Journal of Chemical Theory and Computation, 2012, 8, 4359-4363.	2.3	31
34	Multiple Decay Mechanisms and 2Dâ€“UV Spectroscopic Fingerprints of Singlet Excited Solvated Adenineâ€“Uracil Monophosphate. Chemistry - A European Journal, 2016, 22, 7497-7507.	1.7	31
35	Toward Understanding the Photochemistry of Photoactive Yellow Protein: A CASPT2/CASSCF and Quantum Theory of Atoms in Molecules Combined Study of a Model Chromophore in Vacuo. Journal of Chemical Theory and Computation, 2009, 5, 3032-3038.	2.3	30
36	Substitution of the laser borane anti-B18H22 with pyridine: a structural and photophysical study of some unusually structured macropolyhedral boron hydrides. Dalton Transactions, 2018, 47, 1709-1725.	1.6	29

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37	Dynamics of the excited-state hydrogen transfer in a (dG)Â·(dC) homopolymer: intrinsic photostability of DNA. Chemical Science, 2018, 9, 7902-7911.	3.7	29
38	Determination of the Lowest-Energy Oxidation Site in Nucleotides:Â 2â€˜-Deoxythymidine 5â€˜-Monophosphate Anion. Journal of Physical Chemistry B, 2006, 110, 10234-10235.	1.2	28
39	Ultrafast Twisting of the Indoline Donor Unit Utilized in Solar Cell Dyes: Experimental and Theoretical Studies. Journal of Physical Chemistry C, 2015, 119, 2249-2259.	1.5	28
40	Assessment of the Potential Energy Hypersurfaces in Thymine within Multiconfigurational Theory: CASSCF vs. CASPT2. Molecules, 2016, 21, 1666.	1.7	28
41	DNA nucleobase properties and photoreactivity: Modeling environmental effects. Pure and Applied Chemistry, 2009, 81, 743-754.	0.9	25
42	Theoretical Study of the Hydroxyl Radical Addition to Uracil and Photochemistry of the Formed U6OH^{â€¢} Adduct. Journal of Physical Chemistry B, 2014, 118, 2932-2939.	1.2	25
43	Ab initio quantum-chemical computations of the absorption cross sections of HgX2 and HgXY (X, Y =) Tj ETQq1 1 0.784314 rgBT /Ov 2019, 21, 455-467.	1.3	25
44	On the photophysics and photochemistry of the water dimer. Journal of Chemical Physics, 2012, 137, 244309.	1.2	24
45	Hydrogen abstraction by photoexcited benzophenone: consequences for DNA photosensitization. Physical Chemistry Chemical Physics, 2016, 18, 7829-7836.	1.3	24
46	Theoretical study of the dark photochemistry of 1,3-butadiene via the chemiexcitation of Dewar dioxetane. Physical Chemistry Chemical Physics, 2015, 17, 18653-18664.	1.3	23
47	Determination of the Electron-Detachment Energies of 2â€²-Deoxyguanosine 5â€²-Monophosphate Anion: Influence of the Conformation. Journal of Physical Chemistry B, 2009, 113, 2451-2457.	1.2	22
48	On the N₁â€“H and N₃â€“H Bond Dissociation in Uracil by Low Energy Electrons: A CASSCF/CASPT2 Study. Journal of Chemical Theory and Computation, 2012, 8, 2769-2776.	2.3	22
49	Modeling hole transfer in DNA: Low-lying excited states of oxidized cytosine homodimer and cytosineâ€“adenine heterodimer. Chemical Physics, 2008, 349, 188-196.	0.9	21
50	Theoretical study on the excited-state Ï€-stacking versus intermolecular hydrogen-transfer processes in the guanineâ€“cytosine/cytosine trimer. Theoretical Chemistry Accounts, 2016, 135, 1.	0.5	20
51	Mechanism of the OH Radical Addition to Adenine from Quantum-Chemistry Determinations of Reaction Paths and Spectroscopic Tracking of the Intermediates. Journal of Organic Chemistry, 2017, 82, 276-288.	1.7	20
52	Complete-active-space second-order perturbation theory (CASPT2//CASSCF) study of the dissociative electron attachment in canonical DNA nucleobases caused by low-energy electrons (0-3 eV). Journal of Chemical Physics, 2015, 143, 215101.	1.2	19
53	Investigations on the synthesis and chemiluminescence of novel 2-coumaranones - II. Arkivoc, 2015, 2015, 44-59.	0.3	19
54	Investigations on the synthesis and chemiluminescence of novel 2-coumaranones. Arkivoc, 2013, 2013, 174-188.	0.3	18

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55	Ab initio quantumâ€“chemical computations of the electronic states in HgBr2 and IBr: Molecules of interest on the Earthâ€™s atmosphere. Journal of Chemical Physics, 2016, 145, 244304.	1.2	18
56	Effect of Iodination on the Photophysics of the Laser Borane anti-B18H22: Generation of Efficient Photosensitizers of Oxygen. Inorganic Chemistry, 2019, 58, 10248-10259.	1.9	18
57	Excited-state non-radiative decay in stilbenoid compounds: an ab initio quantum-chemistry study on size and substituent effects. Physical Chemistry Chemical Physics, 2019, 21, 22429-22439.	1.3	18
58	Unveiling the role of upper excited electronic states in the photochemistry and laser performance of anti-B18H22. Journal of Materials Chemistry C, 2020, 8, 12806-12818.	2.7	16
59	Photochemistry and Non-adiabatic Photodynamics of the HOSO Radical. Journal of the American Chemical Society, 2021, 143, 10836-10841.	6.6	16
60	Communication: Electronic UV-Vis transient spectra of the Â·OH reaction products of uracil, thymine, cytosine, and 5,6-dihydrouracil by using the complete active space self-consistent field second-order perturbation (CASPT2//CASSCF) theory. Journal of Chemical Physics, 2013, 139, 071101.	1.2	15
61	Induced Night Vision by Singlet-Oxygen-Mediated Activation of Rhodopsin. Journal of Physical Chemistry Letters, 2019, 10, 7133-7140.	2.1	14
62	Building a Functionalizable, Potent Chemiluminescent Agent: A Rational Design Study on 6,8-Substituted Luminol Derivatives. Journal of Organic Chemistry, 2021, 86, 11388-11398.	1.7	14
63	Comment on â€œDensity functional theory study of 1,2-dioxetanone decomposition in condensed phaseâ€• Journal of Computational Chemistry, 2012, 33, 2124-2126.	1.5	13
64	Mechanism of excited state deactivation of indan-1-ylidene and fluoren-9-ylidene malononitriles. Physical Chemistry Chemical Physics, 2016, 18, 32786-32795.	1.3	13
65	Regioselectivity of the OH Radical Addition to Uracil in Nucleic Acids. A Theoretical Approach Based on QM/MM Simulations. Journal of Chemical Theory and Computation, 2017, 13, 5089-5096.	2.3	13
66	Photochromic System among Boron Hydrides: The Hawthorne Rearrangement. Journal of Physical Chemistry Letters, 2019, 10, 6202-6207.	2.1	13
67	A Series of Ultra-Efficient Blue Borane Fluorophores. Inorganic Chemistry, 2020, 59, 17058-17070.	1.9	13
68	Characterization of Locally Excited and Chargeâ€Transfer States of the Anticancer Drug Lapatinib by Ultrafast Spectroscopy and Computational Studies. Chemistry - A European Journal, 2020, 26, 15922-15930.	1.7	13
69	Toward an Understanding of the Hydrogenation Reaction of MO₂ Gas-Phase Clusters (M =) Tj ETQq1 1 0.784314 rgBT /O	1.1	12
70	Can the Hexagonal Ice-like Model Render the Spectroscopic Fingerprints of Structured Water? Feedback from Quantum-Chemical Computations. Entropy, 2014, 16, 4101-4120.	1.1	12
71	Computational Photochemistry and Photophysics: the state of the art. Photochemistry, 2012, , 42-72.	0.2	11
72	Multiconfigurational Quantum Chemistry Determinations of Absorption Cross Sections (Ïƒ) in the Gas Phase and Molar Extinction Coefficients (Îµ) in Aqueous Solution and Airâ€“Water Interface. Journal of Chemical Theory and Computation, 2021, 17, 3571-3582.	2.3	11

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73	Lightâ€Induced On/Off Switching of the Surfactant Character of the oâ€Cobaltabis(dicarbollide) Anion with No Covalent Bond Alteration. Angewandte Chemie - International Edition, 2021, 60, 25753-25757.	7.2	11
74	Towards the understanding at the molecular level of the structured-water absorption and fluorescence spectra: a fingerprint of Ï€-stacked water. Molecular Physics, 2013, 111, 1308-1315.	0.8	10
75	Photochemistry of HOSO₂ and SO₃ and Implications for the Production of Sulfuric Acid. Journal of the American Chemical Society, 2021, 143, 18794-18802.	6.6	10
76	Modeling hole transfer in DNA. II. Molecular basis of charge transport in the DNA chain. Theoretical Chemistry Accounts, 2010, 126, 177-183.	0.5	9
77	Triplet versus singlet chemiexcitation mechanism in dioxetanone: a CASSCF/CASPT2 study. Theoretical Chemistry Accounts, 2017, 136, 1.	0.5	8
78	Reaction of SO₃ with HONO₂ and Implications for Sulfur Partitioning in the Atmosphere. Journal of the American Chemical Society, 2022, 144, 9172-9177.	6.6	8
79	Recent trends in computational photochemistry. Photochemistry, 2010, , 10-36.	0.2	7
80	A surface hopping algorithm for nonadiabatic minimum energy path calculations. Journal of Computational Chemistry, 2015, 36, 312-320.	1.5	7
81	Experimental and Theoretical Study on the Cycloreversion of a Nucleobaseâ€Derived Azetidine by Photoinduced Electron Transfer. Chemistry - A European Journal, 2018, 24, 15346-15354.	1.7	7
82	Hydroxyl Radical Addition to Thymine and Cytosine and Photochemistry of the Adducts at the C6 Position. ChemPhotoChem, 2019, 3, 889-896.	1.5	7
83	On the chemiluminescence emission of luminol: protic and aprotic solvents and encapsulation to improve the properties in aqueous solution. Physical Chemistry Chemical Physics, 2020, 22, 27617-27625.	1.3	6
84	Regiochemical memory in the adiabatic photolysis of thymine-derived oxetanes. A combined ultrafast spectroscopic and CASSCF/CASPT2 computational study. Physical Chemistry Chemical Physics, 2020, 22, 20037-20042.	1.3	6
85	A theoretical analysis of the structure and properties of B₂₆H₃₀ isomers. Consequences to the laser and semiconductor doping capabilities of large borane clusters. Physical Chemistry Chemical Physics, 2019, 21, 12916-12923.	1.3	5
86	Theoretical Study on the Photo-Oxidation and Photoreduction of an Azetidine Derivative as a Model of DNA Repair. Molecules, 2021, 26, 2911.	1.7	5
87	Quantum chemistry of the excited state: recent trends in methods developments and applications. Photochemistry, 2018, , 28-77.	0.2	5
88	Reconstruction of Nuclear Ensemble Approach Electronic Spectra Using Probabilistic Machine Learning. Journal of Chemical Theory and Computation, 2022, 18, 3052-3064.	2.3	5
89	Bioexcimers as Precursors of Charge Transfer and Reactivity in Photobiology. AIP Conference Proceedings, 2007, , .	0.3	4
90	A twoâ€scale approach to electron correlation in multiconfigurational perturbation theory. Journal of Computational Chemistry, 2014, 35, 1609-1617.	1.5	4

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91	Photodissociation Mechanisms of Major Mercury(II) Species in the Atmospheric Chemical Cycle of Mercury. Angewandte Chemie, 2020, 132, 7675-7680.	1.6	4
92	Advances in computational photochemistry and chemiluminescence of biological and nanotechnological molecules. Photochemistry, 2016, , 16-60.	0.2	4
93	Photoswitching activation of a ferrocenyl-stilbene analogue by its covalent grafting to gold. Physical Chemistry Chemical Physics, 2022, 24, 6185-6192.	1.3	4
94	Chapter 2. Recent method developments and applications in computational photochemistry, chemiluminescene and bioluminescence. Photochemistry, 2014, , 11-42.	0.2	3
95	On the hexagonal ice-like model of structured water: Theoretical analysis of the low-lying excited states. Computational and Theoretical Chemistry, 2014, 1040-1041, 266-273.	1.1	3
96	Quantum Chemistry of Excited States in Polyhedral Boranes. Challenges and Advances in Computational Chemistry and Physics, 2015, , 97-119.	0.6	3
97	A Combined Experimental and Theoretical Approach to the Photogeneration of 5,6-Dihydropyrimidin-5-yl Radicals in Nonaqueous Media. Journal of Organic Chemistry, 2016, 81, 4031-4038.	1.7	3
98	Quantum-chemistry study of the ground and excited state absorption of distyrylbenzene: Multi vs single reference methods. Journal of Chemical Physics, 2022, 156, 044102.	1.2	3
99	Ketorolac beats ketoprofen: lower photodecarboxylation, photohemolysis and phototoxicity. MedChemComm, 2013, 4, 1619.	3.5	2
100	Lightâ€Induced On/Off Switching of the Surfactant Character of the oâ€Cobaltabis(dicarbollide) Anion with No Covalent Bond Alteration. Angewandte Chemie, 0, , .	1.6	2
101	A theoretical analysis of the intrinsic light-harvesting properties of xanthopterin. Computational and Theoretical Chemistry, 2014, 1040-1041, 230-236.	1.1	1