Daniel Roca-SanjuÃ¡n

List of Publications by Year
in descending order

101 papers	3,509 citations	136950 32 h-index	155660 55 g-index
105 all docs	105 docs citations	105 times ranked	3335 citing authors

#	Article	IF	Citations
1	Quantum-chemistry study of the ground and excited state absorption of distyrylbenzene: Multi vs single reference methods. Journal of Chemical Physics, 2022, 156, 044102.	3.0	3
2	Photoswitching activation of a ferrocenyl-stilbene analogue by its covalent grafting to gold. Physical Chemistry Chemical Physics, 2022, 24, 6185-6192.	2.8	4
3	Reconstruction of Nuclear Ensemble Approach Electronic Spectra Using Probabilistic Machine Learning. Journal of Chemical Theory and Computation, 2022, 18, 3052-3064.	5.3	5
4	Reaction of SO₃ with HONO₂ and Implications for Sulfur Partitioning in the Atmosphere. Journal of the American Chemical Society, 2022, 144, 9172-9177.	13.7	8
5	Luminescence in Crystalline Organic Materials: From Molecules to Molecular Solids. Advanced Optical Materials, 2021, 9, 2002251.	7.3	146
6	Theoretical Study on the Photo-Oxidation and Photoreduction of an Azetidine Derivative as a Model of DNA Repair. Molecules, 2021, 26, 2911.	3.8	5
7	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.	5.3	11
8	Photochemistry and Non-adiabatic Photodynamics of the HOSO Radical. Journal of the American Chemical Society, 2021, 143, 10836-10841.	13.7	16
9	Building a Functionalizable, Potent Chemiluminescent Agent: A Rational Design Study on 6,8-Substituted Luminol Derivatives. Journal of Organic Chemistry, 2021, 86, 11388-11398.	3.2	14
10	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.	13.8	11
11	Photochemistry of HOSO₂ and SO₃ and Implications for the Production of Sulfuric Acid. Journal of the American Chemical Society, 2021, 143, 18794-18802.	13.7	10
12	Photodissociation Mechanisms of Major Mercury(II) Species in the Atmospheric Chemical Cycle of Mercury. Angewandte Chemie, 2020, 132, 7675-7680.	2.0	4
13	Photodissociation Mechanisms of Major Mercury(II) Species in the Atmospheric Chemical Cycle of Mercury. Angewandte Chemie - International Edition, 2020, 59, 7605-7610.	13.8	45
14	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.	5.5	16
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.	7.1	50
16	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.	2.8	6
17	A Series of Ultra-Efficient Blue Borane Fluorophores. Inorganic Chemistry, 2020, 59, 17058-17070.	4.0	13
18	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.	2.8	6

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19	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.	3.3	13
20	Effect of Iodination on the Photophysics of the Laser Borane anti-B18H22: Generation of Efficient Photosensitizers of Oxygen. Inorganic Chemistry, 2019, 58, 10248-10259.	4.0	18
21	Induced Night Vision by Singlet-Oxygen-Mediated Activation of Rhodopsin. Journal of Physical Chemistry Letters, 2019, 10, 7133-7140.	4.6	14
22	Photochromic System among Boron Hydrides: The Hawthorne Rearrangement. Journal of Physical Chemistry Letters, 2019, 10, 6202-6207.	4.6	13
23	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.	2.8	25
24	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.	2.8	5
25	Gas-Phase Photolysis of Hg(I) Radical Species: A New Atmospheric Mercury Reduction Process. Journal of the American Chemical Society, 2019, 141, 8698-8702.	13.7	40
26	Hydroxyl Radical Addition to Thymine and Cytosine and Photochemistry of the Adducts at the C6 Position. ChemPhotoChem, 2019, 3, 889-896.	3.0	7
27	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.	4.5	40
28	Molecular Basis of the Chemiluminescence Mechanism of Luminol. Chemistry - A European Journal, 2019, 25, 5202-5213.	3.3	45
29	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.	2.8	18
30	Chemi- and Bioluminescence of Cyclic Peroxides. Chemical Reviews, 2018, 118, 6927-6974.	47.7	265
31	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.	3.3	29
32	Photoreduction of gaseous oxidized mercury changes global atmospheric mercury speciation, transport and deposition. Nature Communications, 2018, 9, 4796.	12.8	107
33	Dynamics of the excited-state hydrogen transfer in a (dC)Â·(dC) homopolymer: intrinsic photostability of DNA. Chemical Science, 2018, 9, 7902-7911.	7.4	29
34	Experimental and Theoretical Study on the Cycloreversion of a Nucleobaseâ€Derived Azetidine by Photoinduced Electron Transfer. Chemistry - A European Journal, 2018, 24, 15346-15354.	3.3	7
35	Quantum chemistry of the excited state: recent trends in methods developments and applications. Photochemistry, 2018, , 28-77.	0.2	5
36	Thermochromic Fluorescence from B₁₈H₂₀(NC₅H₅)₂: An Inorganicâ€“Organic Composite Luminescent Compound with an Unusual Molecular Geometry. Advanced Optical Materials, 2017, 5, 1600694.	7.3	45

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37	Peptide Metalâ€“Organic Frameworks for Enantioselective Separation of Chiral Drugs. Journal of the American Chemical Society, 2017, 139, 4294-4297.	13.7	247
38	Triplet versus singlet chemiexcitation mechanism in dioxetanone: a CASSCF/CASPT2 study. Theoretical Chemistry Accounts, 2017, 136, 1.	1.4	8
39	Mechanism of activated chemiluminescence of cyclic peroxides: 1,2-dioxetanes and 1,2-dioxetanones. Physical Chemistry Chemical Physics, 2017, 19, 3955-3962.	2.8	37
40	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.	3.2	20
41	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.	3.1	157
42	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.	5.3	13
43	Assessment of the Potential Energy Hypersurfaces in Thymine within Multiconfigurational Theory: CASSCF vs. CASPT2. Molecules, 2016, 21, 1666.	3.8	28
44	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.	3.0	18
45	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.	3.2	3
46	Mechanism of excited state deactivation of indan-1-ylidene and fluoren-9-ylidene malononitriles. Physical Chemistry Chemical Physics, 2016, 18, 32786-32795.	2.8	13
47	Multiple Decay Mechanisms and 2Dâ€UV Spectroscopic Fingerprints of Singlet Excited Solvated Adenineâ€Uracil Monophosphate. Chemistry - A European Journal, 2016, 22, 7497-7507.	3.3	31
48	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.	1.4	20
49	Hydrogen abstraction by photoexcited benzophenone: consequences for DNA photosensitization. Physical Chemistry Chemical Physics, 2016, 18, 7829-7836.	2.8	24
50	Benzophenone Ultrafast Triplet Population: Revisiting the Kinetic Model by Surface-Hopping Dynamics. Journal of Physical Chemistry Letters, 2016, 7, 622-626.	4.6	89
51	Advances in computational photochemistry and chemiluminescence of biological and nanotechnological molecules. Photochemistry, 2016, , 16-60.	0.2	4
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.	3.0	19
53	Quantum Chemistry of Excited States in Polyhedral Boranes. Challenges and Advances in Computational Chemistry and Physics, 2015, , 97-119.	0.6	3
54	A surface hopping algorithm for nonadiabatic minimum energy path calculations. Journal of Computational Chemistry, 2015, 36, 312-320.	3.3	7

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55	Resolving the Benzophenone DNA-Photosensitization Mechanism at QM/MM Level. Journal of Physical Chemistry Letters, 2015, 6, 576-580.	4.6	48
56	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.	3.1	28
57	Theoretical study of the dark photochemistry of 1,3-butadiene via the chemiexcitation of Dewar dioxetane. Physical Chemistry Chemical Physics, 2015, 17, 18653-18664.	2.8	23
58	Investigations on the synthesis and chemiluminescence of novel 2-coumaranones - II. Arkivoc, 2015, 2015, 44-59.	0.5	19
59	Chapter 2. Recent method developments and applications in computational photochemistry, chemiluminescene and bioluminescence. Photochemistry, 2014, , 11-42.	0.2	3
60	Can the Hexagonal Ice-like Model Render the Spectroscopic Fingerprints of Structured Water? Feedback from Quantum-Chemical Computations. Entropy, 2014, 16, 4101-4120.	2.2	12
61	A twoâ€scale approach to electron correlation in multiconfigurational perturbation theory. Journal of Computational Chemistry, 2014, 35, 1609-1617.	3.3	4
62	A theoretical analysis of the intrinsic light-harvesting properties of xanthopterin. Computational and Theoretical Chemistry, 2014, 1040-1041, 230-236.	2.5	1
63	Computational determination of the dominant triplet population mechanism in photoexcited benzophenone. Physical Chemistry Chemical Physics, 2014, 16, 25393-25403.	2.8	42
64	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.	2.6	25
65	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.	2.5	3
66	Revisiting the Nonadiabatic Process in 1,2-Dioxetane. Journal of Chemical Theory and Computation, 2013, 9, 5404-5411.	5.3	38
67	Excitation of Nucleobases from a Computational Perspective I: Reaction Paths. Topics in Current Chemistry, 2013, 355, 57-97.	4.0	66
68	Ketorolac beats ketoprofen: lower photodecarboxylation, photohemolysis and phototoxicity. MedChemComm, 2013, 4, 1619.	3.4	2
69	Are the Bioâ€•and Chemiluminescence States of the Firefly Oxyluciferin the Same as the Fluorescence State?. Photochemistry and Photobiology, 2013, 89, 319-325.	2.5	48
70	Photoinduced Formation Mechanism of the Thymineâ€“Thymine (6â€“4) Adduct. Journal of Physical Chemistry B, 2013, 117, 1999-2004.	2.6	46
71	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.	1.7	10
72	Toward an Understanding of the Hydrogenation Reaction of MO₂ Gas-Phase Clusters (M =) Tj ETQq0 0 0 rgBT /Overlock 10	2.5	12

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73	Proton/Hydrogen Transfer Mechanisms in the Guanineâ€“Cytosine Base Pair: Photostability and Tautomerism. Journal of Chemical Theory and Computation, 2013, 9, 481-496.	5.3	42
74	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.	3.0	15
75	Investigations on the synthesis and chemiluminescence of novel 2-coumaranones. Arkivoc, 2013, 2013, 174-188.	0.5	18
76	Can the Closed-Shell DFT Methods Describe the Thermolysis of 1,2-Dioxetanone?. Journal of Chemical Theory and Computation, 2012, 8, 4359-4363.	5.3	31
77	Chemiluminescence of Coelenterazine and Fluorescence of Coelenteramide: A Systematic Theoretical Study. Journal of Chemical Theory and Computation, 2012, 8, 2796-2807.	5.3	42
78	Computational Photochemistry and Photophysics: the state of the art. Photochemistry, 2012, , 42-72.	0.2	11
79	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.	5.3	22
80	On the photophysics and photochemistry of the water dimer. Journal of Chemical Physics, 2012, 137, 244309.	3.0	24
81	Multiconfiguration secondâ€•order perturbation theory approach to strong electron correlation in chemistry and photochemistry. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2012, 2, 585-603.	14.6	166
82	On the Deactivation Mechanisms of Adenineâ€“Thymine Base Pair. Journal of Physical Chemistry B, 2012, 116, 4089-4097.	2.6	37
83	Comment on â€œDensity functional theory study of 1,2-dioxetanone decomposition in condensed phaseâ€• Journal of Computational Chemistry, 2012, 33, 2124-2126.	3.3	13
84	Ab initio determination of the ionization potentials of water clusters (H2O)n (n =) Tj ETQq0 0 0 rgBT /Overlock 10	3.0	36
85	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.	5.3	51
86	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.	5.3	49
87	On the photoproduction of DNA/RNA cyclobutane pyrimidine dimers. Theoretical Chemistry Accounts, 2011, 128, 705-711.	1.4	48
88	The Chemistry of Bioluminescence: An Analysis of Chemical Functionalities. ChemPhysChem, 2011, 12, 3064-3076.	2.1	105
89	Modeling hole transfer in DNA. II. Molecular basis of charge transport in the DNA chain. Theoretical Chemistry Accounts, 2010, 126, 177-183.	1.4	9
90	Recent trends in computational photochemistry. Photochemistry, 2010, , 10-36.	0.2	7

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91	DNA nucleobase properties and photoreactivity: Modeling environmental effects. Pure and Applied Chemistry, 2009, 81, 743-754.	1.9	25
92	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.	2.6	22
93	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.	5.3	30
94	Modeling hole transfer in DNA: Low-lying excited states of oxidized cytosine homodimer and cytosineâ€“adenine heterodimer. Chemical Physics, 2008, 349, 188-196.	1.9	21
95	Ab initio determination of the electron affinities of DNA and RNA nucleobases. Journal of Chemical Physics, 2008, 129, 095104.	3.0	83
96	Molecular Basis of DNA Photodimerization: Intrinsic Production of Cyclobutane Cytosine Dimers. Journal of the American Chemical Society, 2008, 130, 10768-10779.	13.7	100
97	Bioexcimers as Precursors of Charge Transfer and Reactivity in Photobiology. AIP Conference Proceedings, 2007, , .	0.4	4
98	Determination of the Lowest-Energy Oxidation Site in Nucleotides:Â 2â€˜-Deoxythymidine 5â€˜-Monophosphate Anion. Journal of Physical Chemistry B, 2006, 110, 10234-10235.	2.6	28
99	Toward the understanding of DNA fluorescence: The singlet excimer of cytosine. Journal of Chemical Physics, 2006, 125, 231102.	3.0	59
100	Ab initiodetermination of the ionization potentials of DNA and RNA nucleobases. Journal of Chemical Physics, 2006, 125, 084302.	3.0	139
101	Lightâ€induced On/Off Switching of the Surfactant Character of the oâ€Cobaltabis(dicarbollide) Anion with No Covalent Bond Alteration. Angewandte Chemie, 0, , .	2.0	2