Carlos E Crespo-HernÃ¡ndez

List of Publications by Year
in descending order

105 papers	6,754 citations	76196 40 h-index	60497 81 g-index
119 all docs	119 docs citations	119 times ranked	3775 citing authors

#	Article	IF	Citations
1	Ultrafast Excited-State Dynamics in Nucleic Acids. Chemical Reviews, 2004, 104, 1977-2020.	23.0	1,157
2	DNA Excited-State Dynamics: From Single Bases to the Double Helix. Annual Review of Physical Chemistry, 2009, 60, 217-239.	4.8	737
3	Thymine Dimerization in DNA Is an Ultrafast Photoreaction. Science, 2007, 315, 625-629.	6.0	496
4	Base stacking controls excited-state dynamics in AÂ·T DNA. Nature, 2005, 436, 1141-1144.	13.7	424
5	Internal conversion to the electronic ground state occurs via two distinct pathways for pyrimidine bases in aqueous solution. Proceedings of the National Academy of Sciences of the United States of America, 2007, 104, 435-440.	3.3	283
6	UV excitation of single DNA and RNA strands produces high yields of exciplex states between two stacked bases. Proceedings of the National Academy of Sciences of the United States of America, 2008, 105, 10285-10290.	3.3	172
7	The origin of efficient triplet state population in sulfur-substituted nucleobases. Nature Communications, 2016, 7, 13077.	5.8	149
8	Determination of Redox Potentials for the Watsonâ˘Crick Base Pairs, DNA Nucleosides, and Relevant Nucleoside Analogues. Journal of Physical Chemistry B, 2007, 111, 5386-5395.	1.2	140
9	2,4-Dithiothymine as a Potent UVA Chemotherapeutic Agent. Journal of the American Chemical Society, 2014, 136, 17930-17933.	6.6	126
10	Ab Initio Ionization Energy Thresholds of DNA and RNA Bases in Gas Phase and in Aqueous Solution. Journal of Physical Chemistry A, 2004, 108, 6373-6377.	1.1	119
11	Solvent-Dependent Photophysics of 1-Cyclohexyluracil:Â Ultrafast Branching in the Initial Bright State Leads Nonradiatively to the Electronic Ground State and a Long-Lived1nÏ€* State. Journal of Physical Chemistry B, 2006, 110, 18641-18650.	1.2	112
12	Influence of Secondary Structure on Electronic Energy Relaxation in Adenine Homopolymers. Journal of Physical Chemistry B, 2004, 108, 11182-11188.	1.2	110
13	On the origin of ultrafast nonradiative transitions in nitro-polycyclic aromatic hydrocarbons: Excited-state dynamics in 1-nitronaphthalene. Journal of Chemical Physics, 2009, 131, 224518.	1.2	110
14	Excited-State Dynamics in 6-Thioguanosine from the Femtosecond to Microsecond Time Scale. Journal of Physical Chemistry B, 2011, 115, 3263-3270.	1.2	97
15	Increase in the photoreactivity of uracil derivatives by doubling thionation. Physical Chemistry Chemical Physics, 2015, 17, 27851-27861.	1.3	96
16	Predicting Thymine Dimerization Yields from Molecular Dynamics Simulations. Biophysical Journal, 2008, 94, 3590-3600.	0.2	90
17	Environmental Photochemistry of Nitro-PAHs: Direct Observation of Ultrafast Intersystem Crossing in 1-Nitropyrene. Journal of Physical Chemistry A, 2008, 112, 6313-6319.	1.1	89
18	Photochemical and Photodynamical Properties of Sulfurâ€Substituted Nucleic Acid Bases,. Photochemistry and Photobiology, 2019, 95, 33-58.	1.3	89

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19	Stricklerâ€"Berg analysis of excited singlet state dynamics in DNA and RNA nucleosides. Faraday Discussions, 2004, 127, 137-147.	1.6	87
20	Communication: The dark singlet state as a doorway state in the ultrafast and efficient intersystem crossing dynamics in 2-thiothymine and 2-thiouracil. Journal of Chemical Physics, 2014, 140, 071101.	1.2	86
21	Photochemistry of Pyrene on Unactivated and Activated Silica Surfaces. Environmental Science & Technology, 2000, 34, 415-421.	4.6	82
22	Photochemistry of Nucleic Acid Bases and Their Thio- and Aza-Analogues in Solution. Topics in Current Chemistry, 2014, 355, 245-327.	4.0	82
23	Room-Temperature Phosphorescence of the DNA Monomer Analogue 4-Thiothymidine in Aqueous Solutions after UVA Excitation. Journal of Physical Chemistry Letters, 2010, 1, 2239-2243.	2.1	81
24	Electronic and Structural Elements That Regulate the Excited-State Dynamics in Purine Nucleobase Derivatives. Journal of the American Chemical Society, 2015, 137, 4368-4381.	6.6	72
25	Excited-State Dynamics in Nitro-Naphthalene Derivatives: Intersystem Crossing to the Triplet Manifold in Hundreds of Femtoseconds. Journal of Physical Chemistry A, 2013, 117, 6580-6588.	1.1	68
26	Internal conversion and intersystem crossing pathways in UV excited, isolated uracils and their implications in prebiotic chemistry. Physical Chemistry Chemical Physics, 2016, 18, 20168-20176.	1.3	65
27	Subpicosecond Intersystem Crossing in Mono- and Di(organophosphine)gold(I) Naphthalene Derivatives in Solution. Journal of the American Chemical Society, 2012, 134, 14808-14817.	6.6	58
28	2-Thiouracil intersystem crossing photodynamics studied by wavelength-dependent photoelectron and transient absorption spectroscopies. Physical Chemistry Chemical Physics, 2017, 19, 19756-19766.	1.3	58
29	Complexity of excited-state dynamics in DNA (Reply). Nature, 2006, 441, E8-E8.	13.7	56
30	Ultrafast spin crossover in 4-thiothymidine in an ionic liquid. Chemical Communications, 2010, 46, 5963.	2.2	56
31	HnRNP A1 Alters the Structure of a Conserved Enterovirus IRES Domain to Stimulate Viral Translation. Journal of Molecular Biology, 2017, 429, 2841-2858.	2.0	56
32	Ground-State Recovery Following UV Excitation is Much Slower in GÂ·Câˆ'DNA Duplexes and Hairpins Than in Mononucleotides. Journal of the American Chemical Society, 2008, 130, 10844-10845.	6.6	53
33	The kinetic landscape of an RNA-binding protein in cells. Nature, 2021, 591, 152-156.	13.7	50
34	Decoding the Molecular Basis for the Population Mechanism of the Triplet Phototoxic Precursors in UVA Lightâ€Activated Pyrimidine Anticancer Drugs. Chemistry - A European Journal, 2017, 23, 2619-2627.	1.7	49
35	Thionated organic compounds as emerging heavy-atom-free photodynamic therapy agents. Chemical Science, 2020, 11, 11113-11123.	3.7	49
36	Deuterium Isotope Effect on Excited-State Dynamics in an Alternating GC Oligonucleotide. Journal of the American Chemical Society, 2009, 131, 17557-17559.	6.6	48

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37	Role of intersystem crossing in the fluorescence quenching of 2-aminopurine 2â€™-deoxyriboside in solution. Photochemical and Photobiological Sciences, 2013, 12, 1341-1350.	1.6	48
38	Heavy-Atom-Substituted Nucleobases in Photodynamic Applications: Substitution of Sulfur with Selenium in 6-Thioguanine Induces a Remarkable Increase in the Rate of Triplet Decay in 6-Selenoguanine. Journal of the American Chemical Society, 2018, 140, 11214-11218.	6.6	48
39	Excited-State Dynamics of the Thiopurine Prodrug 6-Thioguanine: Can N9-Glycosylation Affect Its Phototoxic Activity?. Molecules, 2017, 22, 379.	1.7	43
40	Conformational Control in the Population of the Triplet State and Photoreactivity of Nitronaphthalene Derivatives. Journal of Physical Chemistry A, 2013, 117, 14100-14108.	1.1	41
41	Electronic Relaxation Pathways in Heavy-Atom-Free Photosensitizers Absorbing Near-Infrared Radiation and Exhibiting High Yields of Singlet Oxygen Generation. Journal of the American Chemical Society, 2021, 143, 2676-2681.	6.6	38
42	Unintended Consequences of Expanding the Genetic Alphabet. Journal of the American Chemical Society, 2016, 138, 11457-11460.	6.6	36
43	The Triplet State of 6â€thioâ€²â€²â€deoxyguanosine: Intrinsic Properties and Reactivity Toward Molecular Oxygen. Photochemistry and Photobiology, 2016, 92, 286-292.	1.3	35
44	The Influence of Microhydration on the Ionization Energy Thresholds of Uracil and Thymine. Journal of Physical Chemistry A, 2005, 109, 9279-9283.	1.1	34
45	Excited-State Dynamics in the RNA Nucleotide Uridine 5â€²-Monophosphate Investigated Using Femtosecond Broadband Transient Absorption Spectroscopy. Journal of Physical Chemistry Letters, 2019, 10, 2156-2161.	2.1	34
46	Influence of Microhydration on the Ionization Energy Thresholds of Thymine:Â Comparisons of Theoretical Calculations with Experimental Values. Journal of Physical Chemistry A, 2006, 110, 7485-7490.	1.1	32
47	Excited-State Dynamics of (Organophosphine)gold(I) Pyrenyl Isomers. Journal of Physical Chemistry Letters, 2010, 1, 1205-1211.	2.1	31
48	Solvatochromic Effects on the Absorption Spectrum of 2-Thiocytosine. Journal of Physical Chemistry B, 2017, 121, 5187-5196.	1.2	31
49	Direct Observation of Triplet-State Population Dynamics in the RNA Uracil Derivative 1-Cyclohexyluracil. Journal of Physical Chemistry Letters, 2015, 6, 4404-4409.	2.1	30
50	Dithionated Nucleobases as Effective Photodynamic Agents against Human Epidermoid Carcinoma Cells. ChemMedChem, 2018, 13, 1044-1050.	1.6	27
51	Photophysical and photochemical properties of the pharmaceutical compound salbutamol in aqueous solutions. Chemosphere, 2011, 83, 1513-1523.	4.2	25
52	The Excitedâ€State Lifetimes in a Gâ‹…C DNA Duplex are Nearly Independent of Helix Conformation and Baseâ€Pairing Motif. ChemPhysChem, 2009, 10, 1421-1425.	1.0	24
53	Photoionization of DNA and RNA Bases, Nucleosides and Nucleotides Through a Combination of One- and Two-photon Pathways upon 266 nm Nanosecond Laser ExcitationÂ¶. Photochemistry and Photobiology, 2002, 76, 259.	1.3	23
54	Near Threshold Photo-Oxidation of Dinucleotides Containing Purines upon 266 nm Nanosecond Laser Excitation. The Role of Base Stacking, Conformation, and Sequenceâ€. Journal of Physical Chemistry B, 2003, 107, 1062-1070.	1.2	21

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55	Ionization Energy Thresholds of Microhydrated Adenine and Its Tautomers. Journal of Physical Chemistry A, 2008, 112, 12702-12706.	1.1	20
56	Photochemical etiology of promising ancestors of the RNA nucleobases. Physical Chemistry Chemical Physics, 2016, 18, 20097-20103.	1.3	19
57	The Photochemical Branching Ratio in 1,6-Dinitropyrene Depends on the Excitation Energy. Journal of Physical Chemistry Letters, 2016, 7, 5086-5092.	2.1	18
58	Part I. Photochemical and Photophysical Studies of Guanine Derivatives: Intermediates Contributing to its Photodestruction Mechanism in Aqueous Solution and the Participation of the Electron Adduct. Photochemistry and Photobiology, 2000, 71, 534.	1.3	18
59	Synthesis, Optical Characterization, and Electrochemical Properties of Isomeric Tetraphenylbenzodifurans Containing Electron Acceptor Groups. Journal of Physical Chemistry A, 2011, 115, 4157-4168.	1.1	17
60	Can a Sixâ€Letter Alphabet Increase the Likelihood of Photochemical Assault to the Genetic Code?. Chemistry - A European Journal, 2016, 22, 16648-16656.	1.7	17
61	Detection of the thietane precursor in the UVA formation of the DNA 6-4 photoadduct. Nature Communications, 2020, 11, 3599.	5.8	17
62	Theoretical Elucidation of Conflicting Experimental Data on Vertical Ionization Potentials of Microhydrated Thymine. Journal of Physical Chemistry A, 2008, 112, 4405-4409.	1.1	16
63	<i>In silico</i> structureâ€“function analysis of <i>E. cloacae</i> nitroreductase. Proteins: Structure, Function and Bioinformatics, 2012, 80, 2728-2741.	1.5	15
64	Formamidopyrimidines as major products in the low- and high-intensity UV irradiation of guanine derivatives. Journal of Photochemistry and Photobiology B: Biology, 2004, 73, 167-175.	1.7	14
65	On the Primary Reaction Pathways in the Photochemistry of Nitro-Polycyclic Aromatic Hydrocarbons. Modern Chemistry & Applications, 2013, 01, .	0.2	14
66	Part II. Mechanism of Formation of Guanine as one of the Major Products in the 254 nm Photolysis of Guanine Derivatives: Concentration and pH Effects. Photochemistry and Photobiology, 2000, 71, 544.	1.3	12
67	Mechanism of formation of the MV+ radical during the UV excitation of methylviologen. Journal of Photochemistry and Photobiology A: Chemistry, 2001, 142, 19-24.	2.0	12
68	The 254 nm low intensity and 266 nm laser photochemistry of adenosine.. Journal of Photochemistry and Photobiology A: Chemistry, 2002, 152, 123-133.	2.0	12
69	Photochemical Reactivity of dTPT3: A Crucial Nucleobase Derivative in the Development of Semisynthetic Organisms. Journal of Physical Chemistry Letters, 2017, 8, 2387-2392.	2.1	12
70	Role of Sequence and Conformation on the Photochemistry and the Photophysics of Aâˆ'T DNA Dimers:Â An Experimental and Computational Approach. Journal of Physical Chemistry B, 2006, 110, 15589-15596.	1.2	11
71	Electronic spectra and excited-state dynamics of 4-fluoro-N,N-dimethylaniline. Chemical Physics Letters, 2013, 586, 70-75.	1.2	11
72	Electronic relaxation pathways of the biologically relevant pterin chromophore. Physical Chemistry Chemical Physics, 2017, 19, 12720-12729.	1.3	11

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73	Photochemical Relaxation Pathways in Dinitropyrene Isomer Pollutants. Journal of Physical Chemistry A, 2017, 121, 8197-8206.	1.1	11
74	Excited-State Dynamics in O⁶-Methylguanosine: Impact of O⁶-Methylation on the Relaxation Mechanism of Guanine Monomers. Journal of Physical Chemistry Letters, 2017, 8, 4380-4385.	2.1	11
75	Ultrafast Excited-State Dynamics in Cyclometalated Ir(III) Complexes Coordinated with Perylenebisimide and Its Ï€-Radical Anion Ligands. Journal of Physical Chemistry C, 2017, 121, 21184-21198.	1.5	11
76	On the Origin of the Photostability of DNA and RNA Monomers: Excited State Relaxation Mechanism of the Pyrimidine Chromophore. Journal of Physical Chemistry Letters, 2020, 11, 5156-5161.	2.1	10
77	Photochemical relaxation pathways of S⁶-methylthioinosine and O⁶-methylguanosine in solution. Faraday Discussions, 2018, 207, 351-374.	1.6	9
78	Tracking the origin of photostability in purine nucleobases: the photophysics of 2-oxopurine. Physical Chemistry Chemical Physics, 2019, 21, 13467-13473.	1.3	9
79	Excited state dynamics of 7-deazaguanosine and guanosine 5â€²-monophosphate. Journal of Chemical Physics, 2021, 154, 075103.	1.2	9
80	Excited State Lifetimes of Sulfur-Substituted DNA and RNA Monomers Probed Using the Femtosecond Fluorescence Up-Conversion Technique. Molecules, 2020, 25, 584.	1.7	8
81	Photocrosslinking between nucleic acids and proteins: general discussion. Faraday Discussions, 2018, 207, 283-306.	1.6	5
82	Quenching Enhancement of the Singlet Excited State of Pheophorbideâ€a by DNA in the Presence of the Quinone Carboquone. Photochemistry and Photobiology, 2011, 87, 275-283.	1.3	4
83	Photo-protection/photo-damage in natural systems: general discussion. Faraday Discussions, 2019, 216, 538-563.	1.6	4
84	Photostability of 2,6-diaminopurine and its 2â€²-deoxyriboside investigated by femtosecond transient absorption spectroscopy. Physical Chemistry Chemical Physics, 2022, 24, 4204-4211.	1.3	4
85	Increased Photostability of the Integral mRNA Vaccine Component N₁â€Methylpseudouridine Compared to Uridine. Chemistry - A European Journal, 2022, 28, .	1.7	4
86	Part I. Photochemical and Photophysical Studies of Guanine Derivatives: Intermediates Contributing to its Photodestruction Mechanism in Aqueous Solution and the Participation of the Electron Adduct. Photochemistry and Photobiology, 2000, 71, 534-543.	1.3	3
87	Photoionization of DNA and RNA Bases, Nucleosides and Nucleotides Through a Combination of One- and Two-photon Pathways upon 266 nm Nanosecond Laser ExcitationÂ¶. Photochemistry and Photobiology, 2002, 76, 259-267.	1.3	3
88	Photorelaxation and Photorepair Processes in Nucleic and Amino Acid Derivatives. Molecules, 2017, 22, 2203.	1.7	3
89	Photodynamics in Metal-Chelating Tetraphenylazadipyrromethene Complexes: Implications for Their Potential Use as Photovoltaic Materials. Journal of Physical Chemistry C, 2018, 122, 13579-13589.	1.5	3
90	Intramolecular Charge Transfer in the Azathioprine Prodrug Quenches Intersystem Crossing to the Reactive Triplet State in 6â€Mercaptopurine^{â€}. Photochemistry and Photobiology, 2022, 98, 617-632.	1.3	3

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91	Femtosecond intersystem crossing to the reactive triplet state of the 2,6-dithiopurine skin cancer photosensitizer. Physical Chemistry Chemical Physics, 2021, 23, 25048-25055.	1.3	3
92	2-Oxopurine Riboside: A Dual Fluorescent Analog and Photosensitizer for RNA/DNA Research. Journal of Physical Chemistry B, 2022, 126, 4483-4490.	1.2	3
93	Part II. Mechanism of Formation of Guanine as one of the Major Products in the 254 nm Photolysis of Guanine Derivatives: Concentration and pH Effects. Photochemistry and Photobiology, 2000, 71, 544-550.	1.3	2
94	Correction: Photochemical etiology of promising ancestors of the RNA nucleobases. Physical Chemistry Chemical Physics, 2016, 18, 22731-22731.	1.3	2
95	Structureâ€"Activity Relationships in Nitro-Aromatic Compounds. , 2009, , 217-240.		2
96	Excited state dynamics of 2â€²-deoxyisoguanosine and isoguanosine in aqueous solution. Physical Chemistry Chemical Physics, 2022, 24, 6769-6781.	1.3	2
97	Disclosing the Role of C4-Oxo Substitution in the Photochemistry of DNA and RNA Pyrimidine Monomers: Formation of Photoproducts from the Vibrationally Excited Ground State. Journal of Physical Chemistry Letters, 2022, 13, 2000-2006.	2.1	2
98	Light induced charge and energy transport in nucleic acids and proteins: general discussion. Faraday Discussions, 2018, 207, 153-180.	1.6	1
99	On the Photostability of Cyanuric Acid and Its Candidature as a Prebiotic Nucleobase. Molecules, 2022, 27, 1184.	1.7	1
100	Magnetic field-enhanced photoionization of 6-methylpurine. Chemical Physics Letters, 2003, 382, 661-664.	1.2	0
101	Ultrafast Excited-State Dynamics in Nucleic Acids. ChemInform, 2004, 35, no.	0.1	0
102	Vertical Singlet Excitations on Adenine Dimer: A Time Dependent Density Functional Study. AIP Conference Proceedings, 2007, , .	0.3	0
103	Light induced damage and repair in nucleic acids and proteins: general discussion. Faraday Discussions, 2018, 207, 389-408.	1.6	0
104	Photovoltaics and bio-inspired light harvesting: general discussion. Faraday Discussions, 2019, 216, 269-300.	1.6	0
105	Excited State Dynamics in Single and Double-Stranded DNA Constructs: Ultrafast Formation of the Major Radiation Product in DNAâ€. , 2007, , .		0