

# Carlos E Crespo-Hernández

## List of Publications by Year in descending order

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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	Intramolecular Charge Transfer in the Azathioprine Prodrug Quenches Intersystem Crossing to the Reactive Triplet State in 6-Mercaptopurine. <i>Photochemistry and Photobiology</i> , 2022, 98, 617-632.	1.3	3
2	Photostability of 2,6-diaminopurine and its 2-deoxyribose investigated by femtosecond transient absorption spectroscopy. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 4204-4211.	1.3	4
3	On the Photostability of Cyanuric Acid and Its Candidature as a Prebiotic Nucleobase. <i>Molecules</i> , 2022, 27, 1184.	1.7	1
4	Increased Photostability of the Integral mRNA Vaccine Component N <sup>1</sup> -Methylpseudouridine Compared to Uridine. <i>Chemistry - A European Journal</i> , 2022, 28, .	1.7	4
5	Excited state dynamics of 2-deoxyisoguanosine and isoguanosine in aqueous solution. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 6769-6781.	1.3	2
6	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. <i>Journal of Physical Chemistry Letters</i> , 2022, 13, 2000-2006.	2.1	2
7	2-Oxopurine Riboside: A Dual Fluorescent Analog and Photosensitizer for RNA/DNA Research. <i>Journal of Physical Chemistry B</i> , 2022, 126, 4483-4490.	1.2	3
8	Excited state dynamics of 7-deazaguanosine and guanosine 5-monophosphate. <i>Journal of Chemical Physics</i> , 2021, 154, 075103.	1.2	9
9	Electronic Relaxation Pathways in Heavy-Atom-Free Photosensitizers Absorbing Near-Infrared Radiation and Exhibiting High Yields of Singlet Oxygen Generation. <i>Journal of the American Chemical Society</i> , 2021, 143, 2676-2681.	6.6	38
10	The kinetic landscape of an RNA-binding protein in cells. <i>Nature</i> , 2021, 591, 152-156.	13.7	50
11	Femtosecond intersystem crossing to the reactive triplet state of the 2,6-dithiopurine skin cancer photosensitizer. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 25048-25055.	1.3	3
12	Thionated organic compounds as emerging heavy-atom-free photodynamic therapy agents. <i>Chemical Science</i> , 2020, 11, 11113-11123.	3.7	49
13	Detection of the thietane precursor in the UVA formation of the DNA 6-4 photoadduct. <i>Nature Communications</i> , 2020, 11, 3599.	5.8	17
14	On the Origin of the Photostability of DNA and RNA Monomers: Excited State Relaxation Mechanism of the Pyrimidine Chromophore. <i>Journal of Physical Chemistry Letters</i> , 2020, 11, 5156-5161.	2.1	10
15	Excited State Lifetimes of Sulfur-Substituted DNA and RNA Monomers Probed Using the Femtosecond Fluorescence Up-Conversion Technique. <i>Molecules</i> , 2020, 25, 584.	1.7	8
16	Photochemical and Photodynamical Properties of Sulfur-Substituted Nucleic Acid Bases. <i>Photochemistry and Photobiology</i> , 2019, 95, 33-58.	1.3	89
17	Photo-protection/photo-damage in natural systems: general discussion. <i>Faraday Discussions</i> , 2019, 216, 538-563.	1.6	4
18	Photovoltaics and bio-inspired light harvesting: general discussion. <i>Faraday Discussions</i> , 2019, 216, 269-300.	1.6	0

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19	Tracking the origin of photostability in purine nucleobases: the photophysics of 2-oxopurine. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 13467-13473.	1.3	9
20	Excited-State Dynamics in the RNA Nucleotide Uridine 5'-Monophosphate Investigated Using Femtosecond Broadband Transient Absorption Spectroscopy. <i>Journal of Physical Chemistry Letters</i> , 2019, 10, 2156-2161.	2.1	34
21	Light induced damage and repair in nucleic acids and proteins: general discussion. <i>Faraday Discussions</i> , 2018, 207, 389-408.	1.6	0
22	Photodynamics in Metal-Chelating Tetraphenylazadipyrromethene Complexes: Implications for Their Potential Use as Photovoltaic Materials. <i>Journal of Physical Chemistry C</i> , 2018, 122, 13579-13589.	1.5	3
23	Photocrosslinking between nucleic acids and proteins: general discussion. <i>Faraday Discussions</i> , 2018, 207, 283-306.	1.6	5
24	Light induced charge and energy transport in nucleic acids and proteins: general discussion. <i>Faraday Discussions</i> , 2018, 207, 153-180.	1.6	1
25	Dithionated Nucleobases as Effective Photodynamic Agents against Human Epidermoid Carcinoma Cells. <i>ChemMedChem</i> , 2018, 13, 1044-1050.	1.6	27
26	Photochemical relaxation pathways of S <sup>6</sup> -methylthioinosine and O <sup>6</sup> -methylguanosine in solution. <i>Faraday Discussions</i> , 2018, 207, 351-374.	1.6	9
27	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. <i>Journal of the American Chemical Society</i> , 2018, 140, 11214-11218.	6.6	48
28	Electronic relaxation pathways of the biologically relevant pterin chromophore. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 12720-12729.	1.3	11
29	Photochemical Reactivity of dTPT3: A Crucial Nucleobase Derivative in the Development of Semisynthetic Organisms. <i>Journal of Physical Chemistry Letters</i> , 2017, 8, 2387-2392.	2.1	12
30	Solvatochromic Effects on the Absorption Spectrum of 2-Thiocytosine. <i>Journal of Physical Chemistry B</i> , 2017, 121, 5187-5196.	1.2	31
31	Decoding the Molecular Basis for the Population Mechanism of the Triplet Phototoxic Precursors in UVA Light-Activated Pyrimidine Anticancer Drugs. <i>Chemistry - A European Journal</i> , 2017, 23, 2619-2627.	1.7	49
32	HnRNP A1 Alters the Structure of a Conserved Enterovirus IRES Domain to Stimulate Viral Translation. <i>Journal of Molecular Biology</i> , 2017, 429, 2841-2858.	2.0	56
33	2-Thiouracil intersystem crossing photodynamics studied by wavelength-dependent photoelectron and transient absorption spectroscopies. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 19756-19766.	1.3	58
34	Photochemical Relaxation Pathways in Dinitropyrene Isomer Pollutants. <i>Journal of Physical Chemistry A</i> , 2017, 121, 8197-8206.	1.1	11
35	Excited-State Dynamics in O <sup>6</sup> -Methylguanosine: Impact of O <sup>6</sup> -Methylation on the Relaxation Mechanism of Guanine Monomers. <i>Journal of Physical Chemistry Letters</i> , 2017, 8, 4380-4385.	2.1	11
36	Ultrafast Excited-State Dynamics in Cyclometalated Ir(III) Complexes Coordinated with Perylenebisimide and Its $\dot{\text{C}}$ -Radical Anion Ligands. <i>Journal of Physical Chemistry C</i> , 2017, 121, 21184-21198.	1.5	11

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37	Excited-State Dynamics of the Thiopurine Prodrug 6-Thioguanine: Can N9-Glycosylation Affect Its Phototoxic Activity?. <i>Molecules</i> , 2017, 22, 379.	1.7	43
38	Photorelaxation and Photorepair Processes in Nucleic and Amino Acid Derivatives. <i>Molecules</i> , 2017, 22, 2203.	1.7	3
39	Correction: Photochemical etiology of promising ancestors of the RNA nucleobases. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 22731-22731.	1.3	2
40	The Triplet State of 6- <i>thio</i> -2'-deoxyguanosine: Intrinsic Properties and Reactivity Toward Molecular Oxygen. <i>Photochemistry and Photobiology</i> , 2016, 92, 286-292.	1.3	35
41	Internal conversion and intersystem crossing pathways in UV excited, isolated uracils and their implications in prebiotic chemistry. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 20168-20176.	1.3	65
42	Unintended Consequences of Expanding the Genetic Alphabet. <i>Journal of the American Chemical Society</i> , 2016, 138, 11457-11460.	6.6	36
43	The Photochemical Branching Ratio in 1,6-Dinitropyrene Depends on the Excitation Energy. <i>Journal of Physical Chemistry Letters</i> , 2016, 7, 5086-5092.	2.1	18
44	Can a Six-Letter Alphabet Increase the Likelihood of Photochemical Assault to the Genetic Code?. <i>Chemistry - A European Journal</i> , 2016, 22, 16648-16656.	1.7	17
45	The origin of efficient triplet state population in sulfur-substituted nucleobases. <i>Nature Communications</i> , 2016, 7, 13077.	5.8	149
46	Photochemical etiology of promising ancestors of the RNA nucleobases. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 20097-20103.	1.3	19
47	Increase in the photoreactivity of uracil derivatives by doubling thionation. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 27851-27861.	1.3	96
48	Electronic and Structural Elements That Regulate the Excited-State Dynamics in Purine Nucleobase Derivatives. <i>Journal of the American Chemical Society</i> , 2015, 137, 4368-4381.	6.6	72
49	Direct Observation of Triplet-State Population Dynamics in the RNA Uracil Derivative 1-Cyclohexyluracil. <i>Journal of Physical Chemistry Letters</i> , 2015, 6, 4404-4409.	2.1	30
50	Photochemistry of Nucleic Acid Bases and Their Thio- and Aza-Analogues in Solution. <i>Topics in Current Chemistry</i> , 2014, 355, 245-327.	4.0	82
51	2,4-Dithiothymine as a Potent UVA Chemotherapeutic Agent. <i>Journal of the American Chemical Society</i> , 2014, 136, 17930-17933.	6.6	126
52	Communication: The dark singlet state as a doorway state in the ultrafast and efficient intersystem crossing dynamics in 2-thiothymine and 2-thiouracil. <i>Journal of Chemical Physics</i> , 2014, 140, 071101.	1.2	86
53	Excited-State Dynamics in Nitro-Naphthalene Derivatives: Intersystem Crossing to the Triplet Manifold in Hundreds of Femtoseconds. <i>Journal of Physical Chemistry A</i> , 2013, 117, 6580-6588.	1.1	68
54	Electronic spectra and excited-state dynamics of 4-fluoro-N,N-dimethylaniline. <i>Chemical Physics Letters</i> , 2013, 586, 70-75.	1.2	11

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55	Role of intersystem crossing in the fluorescence quenching of 2-aminopurine 2'-deoxyriboside in solution. <i>Photochemical and Photobiological Sciences</i> , 2013, 12, 1341-1350.	1.6	48
56	Conformational Control in the Population of the Triplet State and Photoreactivity of Nitronaphthalene Derivatives. <i>Journal of Physical Chemistry A</i> , 2013, 117, 14100-14108.	1.1	41
57	On the Primary Reaction Pathways in the Photochemistry of Nitro-Polycyclic Aromatic Hydrocarbons. <i>Modern Chemistry &amp; Applications</i> , 2013, 01, .	0.2	14
58	Subpicosecond Intersystem Crossing in Mono- and Di(organophosphine)gold(I) Naphthalene Derivatives in Solution. <i>Journal of the American Chemical Society</i> , 2012, 134, 14808-14817.	6.6	58
59	<i>In silico</i> structure-function analysis of <i>E. cloacae</i> nitroreductase. <i>Proteins: Structure, Function and Bioinformatics</i> , 2012, 80, 2728-2741.	1.5	15
60	Synthesis, Optical Characterization, and Electrochemical Properties of Isomeric Tetraphenylbenzodifurans Containing Electron Acceptor Groups. <i>Journal of Physical Chemistry A</i> , 2011, 115, 4157-4168.	1.1	17
61	Excited-State Dynamics in 6-Thioguanosine from the Femtosecond to Microsecond Time Scale. <i>Journal of Physical Chemistry B</i> , 2011, 115, 3263-3270.	1.2	97
62	Quenching Enhancement of the Singlet Excited State of Pheophorbide $\text{a}^{\text{a}}$ by DNA in the Presence of the Quinone Carboquone. <i>Photochemistry and Photobiology</i> , 2011, 87, 275-283.	1.3	4
63	Photophysical and photochemical properties of the pharmaceutical compound salbutamol in aqueous solutions. <i>Chemosphere</i> , 2011, 83, 1513-1523.	4.2	25
64	Room-Temperature Phosphorescence of the DNA Monomer Analogue 4-Thiothymidine in Aqueous Solutions after UVA Excitation. <i>Journal of Physical Chemistry Letters</i> , 2010, 1, 2239-2243.	2.1	81
65	Excited-State Dynamics of (Organophosphine)gold(I) Pyrenyl Isomers. <i>Journal of Physical Chemistry Letters</i> , 2010, 1, 1205-1211.	2.1	31
66	Ultrafast spin crossover in 4-thiothymidine in an ionic liquid. <i>Chemical Communications</i> , 2010, 46, 5963.	2.2	56
67	On the origin of ultrafast nonradiative transitions in nitro-polycyclic aromatic hydrocarbons: Excited-state dynamics in 1-nitronaphthalene. <i>Journal of Chemical Physics</i> , 2009, 131, 224518.	1.2	110
68	The Excited-State Lifetimes in a G $\cdot$ ...C DNA Duplex are Nearly Independent of Helix Conformation and Base-Pairing Motif. <i>ChemPhysChem</i> , 2009, 10, 1421-1425.	1.0	24
69	Deuterium Isotope Effect on Excited-State Dynamics in an Alternating GC Oligonucleotide. <i>Journal of the American Chemical Society</i> , 2009, 131, 17557-17559.	6.6	48
70	DNA Excited-State Dynamics: From Single Bases to the Double Helix. <i>Annual Review of Physical Chemistry</i> , 2009, 60, 217-239.	4.8	737
71	Structure-Activity Relationships in Nitro-Aromatic Compounds. , 2009, , 217-240.		2
72	Predicting Thymine Dimerization Yields from Molecular Dynamics Simulations. <i>Biophysical Journal</i> , 2008, 94, 3590-3600.	0.2	90

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73	Environmental Photochemistry of Nitro-PAHs: Direct Observation of Ultrafast Intersystem Crossing in 1-Nitropyrene. <i>Journal of Physical Chemistry A</i> , 2008, 112, 6313-6319.	1.1	89
74	Ionization Energy Thresholds of Microhydrated Adenine and Its Tautomers. <i>Journal of Physical Chemistry A</i> , 2008, 112, 12702-12706.	1.1	20
75	Theoretical Elucidation of Conflicting Experimental Data on Vertical Ionization Potentials of Microhydrated Thymine. <i>Journal of Physical Chemistry A</i> , 2008, 112, 4405-4409.	1.1	16
76	Ground-State Recovery Following UV Excitation is Much Slower in G $\hat{C}$ -C $\hat{A}$ DNA Duplexes and Hairpins Than in Mononucleotides. <i>Journal of the American Chemical Society</i> , 2008, 130, 10844-10845.	6.6	53
77	UV excitation of single DNA and RNA strands produces high yields of exciplex states between two stacked bases. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2008, 105, 10285-10290.	3.3	172
78	Internal conversion to the electronic ground state occurs via two distinct pathways for pyrimidine bases in aqueous solution. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2007, 104, 435-440.	3.3	283
79	Thymine Dimerization in DNA Is an Ultrafast Photoreaction. <i>Science</i> , 2007, 315, 625-629.	6.0	496
80	Determination of Redox Potentials for the Watson-Crick Base Pairs, DNA Nucleosides, and Relevant Nucleoside Analogues. <i>Journal of Physical Chemistry B</i> , 2007, 111, 5386-5395.	1.2	140
81	Vertical Singlet Excitations on Adenine Dimer: A Time Dependent Density Functional Study. <i>AIP Conference Proceedings</i> , 2007, , .	0.3	0
82	Excited State Dynamics in Single and Double-Stranded DNA Constructs: Ultrafast Formation of the Major Radiation Product in DNA. , 2007, , .		0
83	Influence of Microhydration on the Ionization Energy Thresholds of Thymine: Comparisons of Theoretical Calculations with Experimental Values. <i>Journal of Physical Chemistry A</i> , 2006, 110, 7485-7490.	1.1	32
84	Solvent-Dependent Photophysics of 1-Cyclohexyluracil: Ultrafast Branching in the Initial Bright State Leads Nonradiatively to the Electronic Ground State and a Long-Lived $1n\pi^*$ State. <i>Journal of Physical Chemistry B</i> , 2006, 110, 18641-18650.	1.2	112
85	Role of Sequence and Conformation on the Photochemistry and the Photophysics of A-T DNA Dimers: An Experimental and Computational Approach. <i>Journal of Physical Chemistry B</i> , 2006, 110, 15589-15596.	1.2	11
86	Complexity of excited-state dynamics in DNA (Reply). <i>Nature</i> , 2006, 441, E8-E8.	13.7	56
87	Base stacking controls excited-state dynamics in A-T DNA. <i>Nature</i> , 2005, 436, 1141-1144.	13.7	424
88	The Influence of Microhydration on the Ionization Energy Thresholds of Uracil and Thymine. <i>Journal of Physical Chemistry A</i> , 2005, 109, 9279-9283.	1.1	34
89	Ultrafast Excited-State Dynamics in Nucleic Acids. <i>Chemical Reviews</i> , 2004, 104, 1977-2020.	23.0	1,157
90	Formamidopyrimidines as major products in the low- and high-intensity UV irradiation of guanine derivatives. <i>Journal of Photochemistry and Photobiology B: Biology</i> , 2004, 73, 167-175.	1.7	14

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91	Ultrafast Excited-State Dynamics in Nucleic Acids. <i>ChemInform</i> , 2004, 35, no.	0.1	0
92	Strickler-Berg analysis of excited singlet state dynamics in DNA and RNA nucleosides. <i>Faraday Discussions</i> , 2004, 127, 137-147.	1.6	87
93	Influence of Secondary Structure on Electronic Energy Relaxation in Adenine Homopolymers. <i>Journal of Physical Chemistry B</i> , 2004, 108, 11182-11188.	1.2	110
94	Ab Initio Ionization Energy Thresholds of DNA and RNA Bases in Gas Phase and in Aqueous Solution. <i>Journal of Physical Chemistry A</i> , 2004, 108, 6373-6377.	1.1	119
95	Magnetic field-enhanced photoinization of 6-methylpurine. <i>Chemical Physics Letters</i> , 2003, 382, 661-664.	1.2	0
96	Near Threshold Photo-Oxidation of Dinucleotides Containing Purines upon 266 nm Nanosecond Laser Excitation. The Role of Base Stacking, Conformation, and Sequence. <i>Journal of Physical Chemistry B</i> , 2003, 107, 1062-1070.	1.2	21
97	The 254 nm low intensity and 266 nm laser photochemistry of adenosine.. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2002, 152, 123-133.	2.0	12
98	Photoionization of DNA and RNA Bases, Nucleosides and Nucleotides Through a Combination of One- and Two-photon Pathways upon 266 nm Nanosecond Laser Excitation. <i>Photochemistry and Photobiology</i> , 2002, 76, 259-267.	1.3	3
99	Photoionization of DNA and RNA Bases, Nucleosides and Nucleotides Through a Combination of One- and Two-photon Pathways upon 266 nm Nanosecond Laser Excitation. <i>Photochemistry and Photobiology</i> , 2002, 76, 259.	1.3	23
100	Mechanism of formation of the MV <sup>+</sup> radical during the UV excitation of methylviologen. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2001, 142, 19-24.	2.0	12
101	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. <i>Photochemistry and Photobiology</i> , 2000, 71, 544.	1.3	12
102	Photochemistry of Pyrene on Unactivated and Activated Silica Surfaces. <i>Environmental Science &amp; Technology</i> , 2000, 34, 415-421.	4.6	82
103	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. <i>Photochemistry and Photobiology</i> , 2000, 71, 534-543.	1.3	3
104	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. <i>Photochemistry and Photobiology</i> , 2000, 71, 544-550.	1.3	2
105	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. <i>Photochemistry and Photobiology</i> , 2000, 71, 534.	1.3	18