Antonio Frances Monerris

List of Publications by Year
in descending order

59	1,128	393982 19	476904 29
papers	citations	h-index	g-index

63	63	63	1002
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	NHC-Based Iron Sensitizers for DSSCs. Inorganics, 2018, 6, 63.	1.2	76
2	Molecular Basis of SARS-CoV-2 Infection and Rational Design of Potential Antiviral Agents: Modeling and Simulation Approaches. Journal of Proteome Research, 2020, 19, 4291-4315.	1.8	68
3	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
4	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
5	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
6	Thermodynamics of the Interaction between the Spike Protein of Severe Acute Respiratory Syndrome Coronavirus-2 and the Receptor of Human Angiotensin-Converting Enzyme 2. Effects of Possible Ligands. Journal of Physical Chemistry Letters, 2020, 11, 9272-9281.	2.1	39
7	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
8	Synthesis and Computational Study of a Pyridylcarbene Fe(II) Complex: Unexpected Effects of fac/mer Isomerism in Metal-to-Ligand Triplet Potential Energy Surfaces. Inorganic Chemistry, 2018, 57, 10431-10441.	1.9	37
9	Iron(<scp>ii</scp>) complexes with diazinyl-NHC ligands: impact of Ï€-deficiency of the azine core on photophysical properties. Dalton Transactions, 2019, 48, 10915-10926.	1.6	37
10	Impact of the fac/mer Isomerism on the Excited-State Dynamics of Pyridyl-carbene Fe(II) Complexes. Inorganic Chemistry, 2019, 58, 5069-5081.	1.9	35
11	Role of RNA Guanine Quadruplexes in Favoring the Dimerization of SARS Unique Domain in Coronaviruses. Journal of Physical Chemistry Letters, 2020, 11, 5661-5667.	2.1	33
12	Intraligand Excited States Turn a Ruthenium Oligothiophene Complex into a Light-Triggered Ubertoxin with Anticancer Effects in Extreme Hypoxia. Journal of the American Chemical Society, 2022, 144, 8317-8336.	6.6	32
13	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
14	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
15	Assessment of the Potential Energy Hypersurfaces in Thymine within Multiconfigurational Theory: CASSCF vs. CASPT2. Molecules, 2016, 21, 1666.	1.7	28
16	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
17	Photoinduced intersystem crossing in DNA oxidative lesions and epigenetic intermediates. Chemical Communications, 2020, 56, 4404-4407.	2.2	25
18	Toward Luminescent Iron Complexes: Unravelling the Photophysics by Computing Potential Energy Surfaces. ChemPhotoChem, 2019, 3, 666-683.	1.5	21

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19	Towards Iron(II) Complexes with Octahedral Geometry: Synthesis, Structure and Photophysical Properties. Molecules, 2020, 25, 5991.	1.7	21
20	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
21	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
22	Triplet photosensitization mechanism of thymine by an oxidized nucleobase: from a dimeric model to DNA environment. Physical Chemistry Chemical Physics, 2018, 20, 25666-25675.	1.3	20
23	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
24	Hypoxia-Selective Dissociation Mechanism of a Nitroimidazole Nucleoside in a DNA Environment. Journal of Physical Chemistry Letters, 2019, 10, 6750-6754.	2.1	19
25	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
26	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
27	Photophysical Investigation of Iron(II) Complexes Bearing Bidentate Annulated Isomeric Pyridine-NHC Ligands. Journal of Physical Chemistry C, 2020, 124, 18379-18389.	1.5	16
28	Trans-to-cis photoisomerization of cyclocurcumin in different environments rationalized by computational photochemistry. Physical Chemistry Chemical Physics, 2020, 22, 4749-4757.	1.3	16
29	Photochemistry and Non-adiabatic Photodynamics of the HOSO Radical. Journal of the American Chemical Society, 2021, 143, 10836-10841.	6.6	16
30	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
31	Ultrafast dynamics in polycyclic aromatic hydrocarbons: the key case of conical intersections at higher excited states and their role in the photophysics of phenanthrene monomer. Physical Chemistry Chemical Physics, 2019, 21, 16981-16988.	1.3	15
32	Photophysical properties of bichromophoric Fe(II) complexes bearing an aromatic electron acceptor. Theoretical Chemistry Accounts, 2019, 138, 1.	0.5	14
33	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
34	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
35	Photochromic System among Boron Hydrides: The Hawthorne Rearrangement. Journal of Physical Chemistry Letters, 2019, 10, 6202-6207.	2.1	13
36	A Series of Ultra-Efficient Blue Borane Fluorophores. Inorganic Chemistry, 2020, 59, 17058-17070.	1.9	13

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37	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
38	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
39	Microscopic interactions between ivermectin and key human and viral proteins involved in SARS-CoV-2 infection. Physical Chemistry Chemical Physics, 2021, 23, 22957-22971.	1.3	11
40	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
41	Experimental and theoretical studies on thymine photodimerization mediated by oxidatively generated DNA lesions and epigenetic intermediates. Physical Chemistry Chemical Physics, 2020, 22, 25661-25668.	1.3	9
42	Triplet versus singlet chemiexcitation mechanism in dioxetanone: a CASSCF/CASPT2 study. Theoretical Chemistry Accounts, 2017, 136, 1.	0.5	8
43	Ironâ€™s Wake: The Performance of Quantum Mechanical-Derived Versus General-Purpose Force Fields Tested on a Luminescent Iron Complex. Molecules, 2020, 25, 3084.	1.7	8
44	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
45	Hydroxyl Radical Addition to Thymine and Cytosine and Photochemistry of the Adducts at the C6 Position. ChemPhotoChem, 2019, 3, 889-896.	1.5	7
46	Bidentate Pyridylâ€NHC Ligands: Synthesis, Ground and Excited State Properties of Their Iron(II) Complexes and the Role of the fac/mer Isomerism. European Journal of Inorganic Chemistry, 2022, 2022, .	1.0	7
47	Spatial and Temporal Resolution of the Oxygen-Independent Photoinduced DNA Interstrand Cross-Linking by a Nitroimidazole Derivative. Journal of Chemical Information and Modeling, 2022, 62, 3239-3252.	2.5	6
48	Conical intersection properties unraveled by the position spread tensor. Theoretical Chemistry Accounts, 2018, 137, 1.	0.5	5
49	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
50	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
51	Quantum chemistry of the excited state: recent trends in methods developments and applications. Photochemistry, 2018, , 28-77.	0.2	5
52	Photodissociation Mechanisms of Major Mercury(II) Species in the Atmospheric Chemical Cycle of Mercury. Angewandte Chemie, 2020, 132, 7675-7680.	1.6	4
53	Triplet stabilization for enhanced drug photorelease from sunscreen-based photocages. Organic and Biomolecular Chemistry, 2021, 19, 1752-1759.	1.5	4
54	Advances in computational photochemistry and chemiluminescence of biological and nanotechnological molecules. Photochemistry, 2016, , 16-60.	0.2	4

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55	Quantum Chemistry of Excited States in Polyhedral Boranes. Challenges and Advances in Computational Chemistry and Physics, 2015, , 97-119.	0.6	3
56	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
57	Photoinduced DNA Lesions in Dormant Bacteria: The Peculiar Route Leading to Spore Photoproducts Characterized by Multiscale Molecular Dynamics**. Chemistry - A European Journal, 2020, 26, 14236-14241.	1.7	3
58	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
59	Ultrafast excited state dynamics of NHC-Fe(II) complexes designed for light harvesting (Conference) Tj ETQq1 1 0.784314 rgBT /Overl		1