

Antonio Frances Monerris

List of Publications by Citations

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

56

papers

643

citations

16

h-index

22

g-index

63

ext. papers

883

ext. citations

5.2

avg, IF

4.29

L-index

#	Paper	IF	Citations
56	NHC-Based Iron Sensitizers for DSSCs. <i>Inorganics</i> , 2018 , 6, 63	2.9	55
55	Molecular Basis of SARS-CoV-2 Infection and Rational Design of Potential Antiviral Agents: Modeling and Simulation Approaches. <i>Journal of Proteome Research</i> , 2020 , 19, 4291-4315	5.6	36
54	Thermochromic Fluorescence from B18H20(NC5H5)2: An Inorganic/Organic Composite Luminescent Compound with an Unusual Molecular Geometry. <i>Advanced Optical Materials</i> , 2017 , 5, 1600694	8.1	33
53	Mechanism of activated chemiluminescence of cyclic peroxides: 1,2-dioxetanes and 1,2-dioxetanones. <i>Physical Chemistry Chemical Physics</i> , 2017 , 19, 3955-3962	3.6	25
52	Synthesis and Computational Study of a Pyridylcarbene Fe(II) Complex: Unexpected Effects of fac/mer Isomerism in Metal-to-Ligand Triplet Potential Energy Surfaces. <i>Inorganic Chemistry</i> , 2018 , 57, 10437-10441	5.1	25
51	Dynamics of the excited-state hydrogen transfer in a (dG) _n (dC) _n homopolymer: intrinsic photostability of DNA. <i>Chemical Science</i> , 2018 , 9, 7902-7911	9.4	24
50	Iron(II) complexes with diazanyl-NHC ligands: impact of efficiency of the azine core on photophysical properties. <i>Dalton Transactions</i> , 2019 , 48, 10915-10926	4.3	23
49	Photodissociation Mechanisms of Major Mercury(II) Species in the Atmospheric Chemical Cycle of Mercury. <i>Angewandte Chemie - International Edition</i> , 2020 , 59, 7605-7610	16.4	23
48	Assessment of the Potential Energy Hypersurfaces in Thymine within Multiconfigurational Theory: CASSCF vs. CASPT2. <i>Molecules</i> , 2016 , 21,	4.8	23
47	Impact of the fac/mer Isomerism on the Excited-State Dynamics of Pyridyl-carbene Fe(II) Complexes. <i>Inorganic Chemistry</i> , 2019 , 58, 5069-5081	5.1	22
46	Theoretical study of the hydroxyl radical addition to uracil and photochemistry of the formed U6OH adduct. <i>Journal of Physical Chemistry B</i> , 2014 , 118, 2932-9	3.4	21
45	Substitution of the laser borane anti-BH with pyridine: a structural and photophysical study of some unusually structured macropolyhedral boron hydrides. <i>Dalton Transactions</i> , 2018 , 47, 1709-1725	4.3	20
44	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. <i>Journal of Physical Chemistry Letters</i> , 2020 , 11, 9272-9281	6.4	18
43	Role of RNA Guanine Quadruplexes in Favoring the Dimerization of SARS Unique Domain in Coronaviruses. <i>Journal of Physical Chemistry Letters</i> , 2020 , 11, 5661-5667	6.4	17
42	Mechanism of the OH Radical Addition to Adenine from Quantum-Chemistry Determinations of Reaction Paths and Spectroscopic Tracking of the Intermediates. <i>Journal of Organic Chemistry</i> , 2017 , 82, 276-288	4.2	16
41	Theoretical study on the excited-state π -stacking versus intermolecular hydrogen-transfer processes in the guanine/cytosine/cytosine trimer. <i>Theoretical Chemistry Accounts</i> , 2016 , 135, 1	1.9	16
40	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). <i>Journal of Chemical Physics</i> , 2015 , 143, 215101	3.9	16

39	Photochemistry of oxidized Hg(I) and Hg(II) species suggests missing mercury oxidation in the troposphere. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2020 , 117, 30949-30956	11.5	16
38	Photophysical properties of bichromophoric Fe(II) complexes bearing an aromatic electron acceptor. <i>Theoretical Chemistry Accounts</i> , 2019 , 138, 1	1.9	13
37	Communication: Electronic UV-Vis transient spectra of the DH 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. <i>Journal of Chemical Physics</i> , 2013 , 139, 071101	3.9	13
36	Effect of Iodination on the Photophysics of the Laser Borane -BH: Generation of Efficient Photosensitizers of Oxygen. <i>Inorganic Chemistry</i> , 2019 , 58, 10248-10259	5.1	11
35	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. <i>Physical Chemistry Chemical Physics</i> , 2019 , 21, 16981-16988	3.6	11
34	Hypoxia-Selective Dissociation Mechanism of a Nitroimidazole Nucleoside in a DNA Environment. <i>Journal of Physical Chemistry Letters</i> , 2019 , 10, 6750-6754	6.4	11
33	Triplet photosensitization mechanism of thymine by an oxidized nucleobase: from a dimeric model to DNA environment. <i>Physical Chemistry Chemical Physics</i> , 2018 , 20, 25666-25675	3.6	11
32	Toward Luminescent Iron Complexes: Unravelling the Photophysics by Computing Potential Energy Surfaces. <i>ChemPhotoChem</i> , 2019 , 3, 666-683	3.3	10
31	Photoinduced intersystem crossing in DNA oxidative lesions and epigenetic intermediates. <i>Chemical Communications</i> , 2020 , 56, 4404-4407	5.8	10
30	Regioselectivity of the OH Radical Addition to Uracil in Nucleic Acids. A Theoretical Approach Based on QM/MM Simulations. <i>Journal of Chemical Theory and Computation</i> , 2017 , 13, 5089-5096	6.4	10
29	Trans-to-cis photoisomerization of cyclocurcumin in different environments rationalized by computational photochemistry. <i>Physical Chemistry Chemical Physics</i> , 2020 , 22, 4749-4757	3.6	8
28	Mechanism of excited state deactivation of indan-1-ylidene and fluoren-9-ylidene malononitriles. <i>Physical Chemistry Chemical Physics</i> , 2016 , 18, 32786-32795	3.6	8
27	Photophysical Investigation of Iron(II) Complexes Bearing Bidentate Annulated Isomeric Pyridine-NHC Ligands. <i>Journal of Physical Chemistry C</i> , 2020 , 124, 18379-18389	3.8	8
26	Triplet versus singlet chemiexcitation mechanism in dioxetanone: a CASSCF/CASPT2 study. <i>Theoretical Chemistry Accounts</i> , 2017 , 136, 1	1.9	7
25	Photochromic System among Boron Hydrides: The Hawthorne Rearrangement. <i>Journal of Physical Chemistry Letters</i> , 2019 , 10, 6202-6207	6.4	7
24	Unveiling the role of upper excited electronic states in the photochemistry and laser performance of anti-B18H22. <i>Journal of Materials Chemistry C</i> , 2020 , 8, 12806-12818	7.1	6
23	Towards Iron(II) Complexes with Octahedral Geometry: Synthesis, Structure and Photophysical Properties. <i>Molecules</i> , 2020 , 25,	4.8	5
22	Experimental and Theoretical Study on the Cycloreversion of a Nucleobase-Derived Azetidone by Photoinduced Electron Transfer. <i>Chemistry - A European Journal</i> , 2018 , 24, 15346-15354	4.8	5

21	A theoretical analysis of the structure and properties of BH isomers. Consequences to the laser and semiconductor doping capabilities of large borane clusters. <i>Physical Chemistry Chemical Physics</i> , 2019 , 21, 12916-12923	3.6	4
20	Hydroxyl Radical Addition to Thymine and Cytosine and Photochemistry of the Adducts at the C6 Position. <i>ChemPhotoChem</i> , 2019 , 3, 889-896	3.3	4
19	Microscopic interactions between ivermectin and key human and viral proteins involved in SARS-CoV-2 infection. <i>Physical Chemistry Chemical Physics</i> , 2021 , 23, 22957-22971	3.6	4
18	Experimental and theoretical studies on thymine photodimerization mediated by oxidatively generated DNA lesions and epigenetic intermediates. <i>Physical Chemistry Chemical Physics</i> , 2020 , 22, 25661-25668	3.6	4
17	A Series of Ultra-Efficient Blue Borane Fluorophores. <i>Inorganic Chemistry</i> , 2020 , 59, 17058-17070	5.1	4
16	Photochemistry and Non-adiabatic Photodynamics of the HOSO Radical. <i>Journal of the American Chemical Society</i> , 2021 , 143, 10836-10841	16.4	4
15	Photoinduced DNA Lesions in Dormant Bacteria: The Peculiar Route Leading to Spore Photoproducts Characterized by Multiscale Molecular Dynamics*. <i>Chemistry - A European Journal</i> , 2020 , 26, 14236-14241	4.8	3
14	Iron@ Wake: The Performance of Quantum Mechanical-Derived Versus General-Purpose Force Fields Tested on a Luminescent Iron Complex. <i>Molecules</i> , 2020 , 25,	4.8	3
13	Quantum Chemistry of Excited States in Polyhedral Boranes. <i>Challenges and Advances in Computational Chemistry and Physics</i> , 2015 , 97-119	0.7	3
12	Multiconfigurational Quantum Chemistry Determinations of Absorption Cross Sections (σ) in the Gas Phase and Molar Extinction Coefficients (ϵ) in Aqueous Solution and Air-Water Interface. <i>Journal of Chemical Theory and Computation</i> , 2021 , 17, 3571-3582	6.4	3
11	A Combined Experimental and Theoretical Approach to the Photogeneration of 5,6-Dihydropyrimidin-5-yl Radicals in Nonaqueous Media. <i>Journal of Organic Chemistry</i> , 2016 , 81, 4031-8	4.2	3
10	Conical intersection properties unraveled by the position spread tensor. <i>Theoretical Chemistry Accounts</i> , 2018 , 137, 1	1.9	3
9	Photochemistry of HOSO and SO and Implications for the Production of Sulfuric Acid. <i>Journal of the American Chemical Society</i> , 2021 , 143, 18794-18802	16.4	2
8	Advances in computational photochemistry and chemiluminescence of biological and nanotechnological molecules. <i>Photochemistry</i> , 2016 , 16-60	1.8	2
7	Quantum chemistry of the excited state: recent trends in methods developments and applications. <i>Photochemistry</i> , 2018 , 28-77	1.8	2
6	Triplet stabilization for enhanced drug photorelease from sunscreen-based photocages. <i>Organic and Biomolecular Chemistry</i> , 2021 , 19, 1752-1759	3.9	2
5	Light-Induced On/Off Switching of the Surfactant Character of the o-Cobaltabis(dicarbollide) Anion with No Covalent Bond Alteration. <i>Angewandte Chemie - International Edition</i> , 2021 , 60, 25753-25757	16.4	2
4	Photodissociation Mechanisms of Major Mercury(II) Species in the Atmospheric Chemical Cycle of Mercury. <i>Angewandte Chemie</i> , 2020 , 132, 7675-7680	3.6	1

3	Theoretical Study on the Photo-Oxidation and Photoreduction of an Azetidine Derivative as a Model of DNA Repair. <i>Molecules</i> , 2021 , 26,	4.8	1
2	DNA Photodamage and Repair: Computational Photobiology in Action. <i>Challenges and Advances in Computational Chemistry and Physics</i> , 2021 , 293-332	0.7	0
1	Bidentate pyridyl-NHC ligands: synthesis, ground and excited state properties of their iron(II) complexes and role of the fac/mer isomerism. <i>European Journal of Inorganic Chemistry</i> ,	2.3	0