

# Angelo Giussani

## List of Publications by Year in descending order

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Version: 2024-02-01

30  
papers

2,632  
citations

516710

16  
h-index

477307

29  
g-index

34  
all docs

34  
docs citations

34  
times ranked

3098  
citing authors

#	ARTICLE	IF	CITATIONS
1	<scp>Molcas</scp> 8: New capabilities for multiconfigurational quantum chemical calculations across the periodic table. <i>Journal of Computational Chemistry</i> , 2016, 37, 506-541.	3.3	1,317
2	OpenMolcas: From Source Code to Insight. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 5925-5964.	5.3	661
3	Excitation of Nucleobases from a Computational Perspective I: Reaction Paths. <i>Topics in Current Chemistry</i> , 2013, 355, 57-97.	4.0	66
4	Essential on the Photophysics and Photochemistry of the Indole Chromophore by Using a Totally Unconstrained Theoretical Approach. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 4088-4096.	5.3	51
5	Photoinduced Formation Mechanism of the Thymineâ€“Thymine (6â€“4) Adduct. <i>Journal of Physical Chemistry B</i> , 2013, 117, 1999-2004.	2.6	46
6	Molecular Basis of the Chemiluminescence Mechanism of Luminol. <i>Chemistry - A European Journal</i> , 2019, 25, 5202-5213.	3.3	45
7	Modeling the high-energy electronic state manifold of adenine: Calibration for nonlinear electronic spectroscopy. <i>Journal of Chemical Physics</i> , 2015, 142, 212443.	3.0	44
8	Spectral lineshapes in nonlinear electronic spectroscopy. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 30925-30936.	2.8	39
9	Pyrene, a Test Case for Deep-Ultraviolet Molecular Photophysics. <i>Journal of Physical Chemistry Letters</i> , 2019, 10, 3481-3487.	4.6	35
10	Insights into the Complex Photophysics and Photochemistry of the Simplest Nitroaromatic Compound: A CASPT2//CASSCF Study on Nitrobenzene. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 2777-2788.	5.3	34
11	Multiple Decay Mechanisms and 2Dâ€“UV Spectroscopic Fingerprints of Singlet Excited Solvated Adenineâ€“Uracil Monophosphate. <i>Chemistry - A European Journal</i> , 2016, 22, 7497-7507.	3.3	31
12	Probing deactivation pathways of DNA nucleobases by two-dimensional electronic spectroscopy: first principles simulations. <i>Faraday Discussions</i> , 2015, 177, 345-362.	3.2	29
13	Spectroscopic fingerprints of DNA/RNA pyrimidine nucleobases in third-order nonlinear electronic spectra. <i>Theoretical Chemistry Accounts</i> , 2016, 135, 1.	1.4	28
14	Toward the Understanding of the Photophysics and Photochemistry of 1-Nitronaphthalene under Solar Radiation: The First Theoretical Evidence of a Photodegradation Intramolecular Rearrangement Mechanism Involving the Triplet States. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 3987-3995.	5.3	24
15	Relaxation Mechanisms of 5-Azacytosine. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 3915-3924.	5.3	24
16	Photoinduced formation mechanism of the thymineâ€“thymine (6â€“4) adduct in DNA; a QM(CASPT2//CASSCF):MM(AMBER) study. <i>Faraday Discussions</i> , 2018, 207, 375-387.	3.2	20
17	Photophysics of 1-Aminonaphthalene: A Theoretical and Time-Resolved Experimental Study. <i>Journal of Physical Chemistry A</i> , 2009, 113, 13509-13518.	2.5	14
18	Two-dimensional electronic spectroscopy as a tool for tracking molecular conformations in DNA/RNA aggregates. <i>Faraday Discussions</i> , 2018, 207, 233-250.	3.2	14

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19	Induced Night Vision by Singlet-Oxygen-Mediated Activation of Rhodopsin. <i>Journal of Physical Chemistry Letters</i> , 2019, 10, 7133-7140.	4.6	14
20	Building a Functionalizable, Potent Chemiluminescent Agent: A Rational Design Study on 6,8-Substituted Luminol Derivatives. <i>Journal of Organic Chemistry</i> , 2021, 86, 11388-11398.	3.2	14
21	On the Simulation of Two-dimensional Electronic Spectroscopy of Indole-containing Peptides. <i>Photochemistry and Photobiology</i> , 2017, 93, 1368-1380.	2.5	13
22	How important is roaming in the photodegradation of nitrobenzene?. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 15945-15952.	2.8	12
23	Combined Theoretical and Experimental Study of the Photophysics of Asulam. <i>Journal of Physical Chemistry A</i> , 2013, 117, 2125-2137.	2.5	11
24	Similar chemical structures, dissimilar triplet quantum yields: a CASPT2 model rationalizing the trend of triplet quantum yields in nitroaromatic systems. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 10514-10522.	2.8	10
25	On the Intrinsically Low Quantum Yields of Pyrimidine DNA Photodamages: Evaluating the Reactivity of the Corresponding Minimum Energy Crossing Points. <i>Journal of Physical Chemistry Letters</i> , 2020, 11, 4984-4989.	4.6	8
26	On the Importance of Ligand-Centered Excited States in the Emission of Cyclometalated Ir(III) Complexes. <i>Inorganic Chemistry</i> , 2021, 60, 13222-13232.	4.0	7
27	On the chemiluminescence emission of luminol: protic and aprotic solvents and encapsulation to improve the properties in aqueous solution. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 27617-27625.	2.8	6
28	Regiochemical memory in the adiabatic photolysis of thymine-derived oxetanes. A combined ultrafast spectroscopic and CASSCF/CASPT2 computational study. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 20037-20042.	2.8	6
29	Azole-containing cationic bis-cyclometallated iridium( $\text{III}$ ) isocyanide complexes: a theoretical insight into the emission energy and emission efficiency. <i>Dalton Transactions</i> , 2019, 48, 9725-9733.	3.3	5
30	Light induced damage and repair in nucleic acids and proteins: general discussion. <i>Faraday Discussions</i> , 2018, 207, 389-408.	3.2	0