

Gloria Mazzone

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.

70
papers

1,454
citations

23
h-index

35
g-index

81
ext. papers

1,768
ext. citations

4.4
avg, IF

5.04
L-index

#	Paper	IF	Citations
70	Food Antioxidants: Chemical Insights at the Molecular Level. <i>Annual Review of Food Science and Technology</i> , 2016 , 7, 335-52	14.7	222
69	Antioxidant properties of several coumarin-chalcone hybrids from theoretical insights. <i>RSC Advances</i> , 2015 , 5, 565-575	3.7	61
68	Spin-Orbit Charge Recombination Intersystem Crossing in Phenothiazine-Anthracene Compact Dyads: Effect of Molecular Conformation on Electronic Coupling, Electronic Transitions, and Electron Spin Polarizations of the Triplet States. <i>Journal of Physical Chemistry C</i> , 2018 , 122, 27850-27865	3.8	56
67	Understanding zinc(II) chelation with quercetin and luteolin: a combined NMR and theoretical study. <i>Journal of Physical Chemistry B</i> , 2015 , 119, 83-95	3.4	50
66	Density functional study of the antioxidant activity of some recently synthesized resveratrol analogues. <i>Food Chemistry</i> , 2013 , 141, 2017-24	8.5	46
65	Theoretical Determination of Electronic Spectra and Intersystem Spin-Orbit Coupling: The Case of Isoindole-BODIPY Dyes. <i>Journal of Chemical Theory and Computation</i> , 2014 , 10, 4006-13	6.4	45
64	Spin-Orbit Charge-Transfer Intersystem Crossing (ISC) in Compact Electron Donor-Acceptor Dyads: ISC Mechanism and Application as Novel and Potent Photodynamic Therapy Reagents. <i>Chemistry - A European Journal</i> , 2020 , 26, 1091-1102	4.8	44
63	Halogen atom effect on the photophysical properties of substituted aza-BODIPY derivatives. <i>Physical Chemistry Chemical Physics</i> , 2017 , 19, 2530-2536	3.6	42
62	The heavy atom effect on Zn(II) phthalocyanine derivatives: a theoretical exploration of the photophysical properties. <i>Physical Chemistry Chemical Physics</i> , 2015 , 17, 23595-601	3.6	41
61	Increasing the anti-Stokes shift in TTA upconversion with photosensitizers showing red-shifted spin-allowed charge transfer absorption but a non-compromised triplet state energy level. <i>Chemical Communications</i> , 2019 , 55, 1510-1513	5.8	39
60	Homogeneous Gold Catalysis: Hydration of 1,2-Diphenylacetylene with Methanol in Aqueous Media. A Theoretical Viewpoint. <i>Organometallics</i> , 2012 , 31, 3074-3080	3.8	39
59	The mutual influence of non-covalent interactions in pi-electron deficient cavities: the case of anion recognition by tetraoxacalix[2]arene[2]triazine. <i>Chemical Communications</i> , 2010 , 46, 5894-6	5.8	37
58	PDT-correlated photophysical properties of thienopyrrole BODIPY derivatives. Theoretical insights. <i>Dyes and Pigments</i> , 2016 , 130, 9-15	4.6	37
57	Photophysical properties of free and metallated meso-substituted tetrabenzotriazaporphyrin from density functional theory investigation. <i>Dyes and Pigments</i> , 2015 , 120, 335-339	4.6	36
56	Density functional predictions of antioxidant activity and UV spectral features of nasutin A, isonasutin, ellagic acid, and one of its possible derivatives. <i>Journal of Agricultural and Food Chemistry</i> , 2013 , 61, 9650-7	5.7	36
55	Interaction of CO with PdAu(111) and PdAu(100) Bimetallic Surfaces: A Theoretical Cluster Model Study. <i>Journal of Physical Chemistry C</i> , 2008 , 112, 6073-6081	3.8	35
54	Antioxidant properties comparative study of natural hydroxycinnamic acids and structurally modified derivatives: Computational insights. <i>Computational and Theoretical Chemistry</i> , 2016 , 1077, 39-47		34

53	Metal Atom Effect on the Photophysical Properties of Mg(II), Zn(II), Cd(II), and Pd(II) Tetraphenylporphyrin Complexes Proposed as Possible Drugs in Photodynamic Therapy. <i>Molecules</i> , 2017 , 22,	4.8	34
52	Coumarin-Chalcone Hybrids as Peroxyl Radical Scavengers: Kinetics and Mechanisms. <i>Journal of Chemical Information and Modeling</i> , 2016 , 56, 662-70	6.1	32
51	Electronic spectra and intersystem spin-orbit coupling in 1,2- and 1,3-squaraines. <i>Journal of Computational Chemistry</i> , 2014 , 35, 2107-13	3.5	30
50	Mechanistic aspects of the reaction of Th ⁺ and Th ²⁺ with water in the gas phase. <i>Inorganic Chemistry</i> , 2008 , 47, 2083-8	5.1	30
49	Can Expanded Bacteriochlorins Act as Photosensitizers in Photodynamic Therapy? Good News from Density Functional Theory Computations. <i>Molecules</i> , 2016 , 21, 288	4.8	29
48	Investigation of the Inertness to Hydrolysis of Platinum(IV) Prodrugs. <i>Inorganic Chemistry</i> , 2016 , 55, 1580-6	6.6	24
47	Adsorption of Ethylene, Vinyl, Acetic Acid, and Acetate Species on PdAu(111) and PdAu(100) Surface Alloys: A Cluster Model Study. <i>Journal of Chemical Theory and Computation</i> , 2009 , 5, 1350-60	6.4	23
46	Photophysical Properties of S, Se and Te-Substituted Deoxyguanosines: Insight into Their Ability To Act as Chemotherapeutic Agents. <i>Journal of Chemical Information and Modeling</i> , 2017 , 57, 234-242	6.1	22
45	Dimethylplatinum(II) complexes: computational insights into Pt-C bond protonolysis. <i>Inorganic Chemistry</i> , 2011 , 50, 10091-101	5.1	21
44	Theoretical investigation of the absorption spectra and singlet-triplet energy gap of positively charged tetraphenylporphyrins as potential photodynamic therapy photosensitizers. <i>Canadian Journal of Chemistry</i> , 2013 , 91, 902-906	0.9	20
43	Catalytic role of dinuclear μ -acetylide gold(I) complexes in the hydroamination of terminal alkynes: theoretical insights. <i>Journal of Chemical Theory and Computation</i> , 2015 , 11, 581-90	6.4	16
42	Gold(I)-Catalyzed Hydration of 1,2-Diphenylacetylene: Computational Insights. <i>Journal of Chemical Theory and Computation</i> , 2010 , 6, 2782-9	6.4	16
41	Excitation energies, singlet-triplet energy gaps, spin-orbit matrix elements and heavy atom effects in BOIMPYs as possible photosensitizers for photodynamic therapy: a computational investigation. <i>Physical Chemistry Chemical Physics</i> , 2018 , 20, 2656-2661	3.6	15
40	On the Inhibition of Hydroxyl Radical Formation by Hydroxycinnamic Acids: The Case of Caffeic Acid as a Promising Chelating Ligand of a Ferrous Ion. <i>Journal of Physical Chemistry A</i> , 2019 , 123, 9560-9566	2.8	15
39	The ability of a zinc pyrrolidine complex to catalyze the synthesis of cyclic carbonates from carbon dioxide and epoxides: a mechanistic theoretical investigation. <i>Dalton Transactions</i> , 2017 , 46, 9030-9035	4.3	14
38	The geometric effect in palladium-gold catalysis. Is the coupling the rate-determining step in the vinyl-acetate synthesis?. <i>Chemical Communications</i> , 2009 , 1852-4	5.8	14
37	Complexation of Al and Ni by L-Ascorbic Acid: An Experimental and Theoretical Investigation. <i>Journal of Physical Chemistry A</i> , 2017 , 121, 9773-9781	2.8	13
36	Computational Investigation of the Influence of Halogen Atoms on the Photophysical Properties of Tetraphenylporphyrin and Its Zinc(II) Complexes. <i>Journal of Physical Chemistry A</i> , 2018 , 122, 2809-2815	2.8	11

35	Ab initio calculations on the (1)O ₂ quenching mechanism by trans-resveratrol. <i>Physical Chemistry Chemical Physics</i> , 2014 , 16, 12773-81	3.6	11
34	Theoretical Insights into the Switching Off/On of O Photosensitization in Chemically Controlled Photodynamic Therapy. <i>Chemistry - A European Journal</i> , 2018 , 24, 3512-3519	4.8	10
33	Anion- π interactions in a heteroaromatic calixarene receptor. A theoretical investigation. <i>Inorganica Chimica Acta</i> , 2018 , 470, 379-384	2.7	10
32	Chemical Insights into the Antioxidant Mechanisms of Alkylseleno and Alkyltelluro Phenols: Periodic Relatives Behaving Differently. <i>Chemistry - A European Journal</i> , 2018 , 24, 8686-8691	4.8	9
31	Quantum mechanical DFT elucidation of CO ₂ catalytic conversion mechanisms: Three examples. <i>International Journal of Quantum Chemistry</i> , 2018 , 118, e25572	2.1	9
30	Theoretical mechanistic study of the formic acid decomposition assisted by a Ru(II)-phosphine catalyst. <i>Journal of Molecular Modeling</i> , 2014 , 20, 2250	2	9
29	A Review on Coordination Properties of Al(III) and Fe(III) toward Natural Antioxidant Molecules: Experimental and Theoretical Insights. <i>Molecules</i> , 2021 , 26,	4.8	9
28	BODIPY for photodynamic therapy applications: computational study of the effect of bromine substitution on O photosensitization. <i>Journal of Molecular Modeling</i> , 2018 , 24, 183	2	8
27	Antioxidant properties and free radical scavenging mechanisms of cyclocurcumin. <i>New Journal of Chemistry</i> , 2018 , 42, 12698-12705	3.6	8
26	Bodipy-squaraine triads: Preparation and study of the intramolecular energy transfer, charge separation and intersystem crossing. <i>Dyes and Pigments</i> , 2017 , 147, 560-572	4.6	8
25	Novel choline selective electrochemical membrane sensor with application in milk powders and infant formulas. <i>Talanta</i> , 2021 , 221, 121409	6.2	8
24	Spectrophotometric determination of choline in pharmaceutical formulations via host-guest complexation with a biomimetic calixarene receptor. <i>Microchemical Journal</i> , 2019 , 146, 735-741	4.8	7
23	Trimethylphosphate and Dimethylphosphate Hydrolysis by Binuclear Cd, Mn, and Zn-Fe Promiscuous Organophosphate-Degrading Enzyme: Reaction Mechanisms. <i>Chemistry - A European Journal</i> , 2017 , 23, 13742-13753	4.8	6
22	A Boron-Containing Compound Acting on Multiple Targets Against Alzheimer's Disease. Insights from Ab Initio and Molecular Dynamics Simulations. <i>Journal of Chemical Information and Modeling</i> , 2021 , 61, 3397-3410	6.1	6
21	Direct and cluster-assisted dehydrogenation of methane by Nb and Ta: a theoretical investigation. <i>Physical Chemistry Chemical Physics</i> , 2017 , 19, 16178-16188	3.6	5
20	The influence of surface oxygen and hydroxyl groups on the dehydrogenation of ethylene on PdAu surface alloys. A theoretical cluster model study. <i>Chemical Physics Letters</i> , 2010 , 493, 87-93	2.5	5
19	The combined use of deuterium NMR and computer simulations for conformational investigation of flexible molecules in nematic solutions. <i>Computational and Theoretical Chemistry</i> , 2005 , 728, 209-214		5
18	Experimental and theoretical study on the coordination properties of quercetin towards aluminum(III), iron(III) and copper(II) in aqueous solution. <i>Journal of Molecular Liquids</i> , 2021 , 325, 115171 ⁶		5

17	Torsion-Induced Nonradiative Relaxation of the Singlet Excited State of π -Thienyl Bodipy and Charge Separation, Charge Recombination-Induced Intersystem Crossing in Its Compact Electron Donor/Acceptor Dyads. <i>Journal of Physical Chemistry B</i> , 2021 , 125, 4779-4793	3.4	5
16	Anticancer Activity, DNA Binding, and Photodynamic Properties of a N π C π N-Coordinated Pt(II) Complex. <i>Inorganic Chemistry</i> , 2021 , 60, 10350-10360	5.1	5
15	Theoretical insight into joint photodynamic action of a gold(I) complex and a BODIPY chromophore for singlet oxygen generation. <i>Physical Chemistry Chemical Physics</i> , 2019 , 21, 3446-3452	3.6	5
14	Photophysical Properties of Nitrated and Halogenated Phosphorus Tritolylcorrole Complexes: Insights from Theory. <i>Molecules</i> , 2018 , 23,	4.8	4
13	Mechanism of action of the curcumin cis-diammineplatinum(II) complex as a photocytotoxic agent. <i>Inorganic Chemistry Frontiers</i> , 2020 , 7, 2759-2769	6.8	3
12	Theoretical investigation of the action mechanisms of N,N-di-alkylated diarylamine antioxidants. <i>Theoretical Chemistry Accounts</i> , 2017 , 136, 1	1.9	2
11	Time-Dependent Density Functional Computations of the Spectrochemical Properties of Dithiolodithiole and Thiophene Electrochromic Systems. <i>Materials</i> , 2017 , 10,	3.5	2
10	Theoretical determination of the aquation reaction mechanism of cyclometalated benzimidazole Ru(II) and Ir(III) anticancer complexes. <i>Inorganica Chimica Acta</i> , 2018 , 470, 325-330	2.7	2
9	Theoretical exploration of the photophysical properties of two-component Ru-porphyrin dyes as promising assemblies for a combined antitumor effect. <i>Dalton Transactions</i> , 2020 , 49, 12653-12661	4.3	2
8	A comparative computational mechanistic study on derivatives of pyriplatin, modified with the π H ₂ Ph ₃ P ⁺ group, as anticancer complexes targeting mitochondria. <i>Inorganica Chimica Acta</i> , 2020 , 512, 119863	2.7	1
7	On the Electrochromic Properties of Borepins: A Computational Prediction. <i>ACS Omega</i> , 2018 , 3, 9556-9563	3.6	1
6	Computational Analysis of Photophysical Properties and Reactivity of a New Phototherapeutic Cyclometalated Au(III)-Hydride Complex. <i>Chemistry - A European Journal</i> , 2021 , 27, 15528-15535	4.8	1
5	Cyclopentadienone π H ₂ C iron(0) complexes as low valent electrocatalysts for water oxidation. <i>Catalysis Science and Technology</i> , 2021 , 11, 1407-1418	5.5	1
4	A combined Monte Carlo/DFT approach to simulate UV-vis spectra of molecules and aggregates: Merocyanine dyes as a case study. <i>Journal of Computational Chemistry</i> , 2021 , 42, 1054-1063	3.5	0
3	Theoretical investigation on bisarylselanylbenzo-2,1,3-selenadiazoles as potential photosensitizers in photodynamic therapy. <i>Journal of Chemical Physics</i> , 2021 , 154, 084113	3.9	0
2	Experimental and theoretical study of the complexation of Fe ³⁺ and Cu ²⁺ by l-ascorbic acid in aqueous solution. <i>Journal of Molecular Liquids</i> , 2022 , 355, 118973	6	0
1	Computational Studies of the Photogeneration from Dihydrosanguinarine and the Probable Cytotoxicity Mechanism of Sanguinarine. <i>Applied Sciences (Switzerland)</i> , 2022 , 12, 1095	2.6	