# Gloria Mazzone

List of Publications by Year
in descending order

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|---|---|---|---|
| 75 papers | 2,019 citations | 236833 25 h-index | 265120 42 g-index |
| 81 all docs | 81 docs citations | 81 times ranked | 2308 citing authors |

| # | Article | IF | Citations |
|---|---|---|---|
| 1 | Food Antioxidants: Chemical Insights at the Molecular Level. Annual Review of Food Science and Technology, 2016, 7, 335-352. | 5.1 | 294 |
| 2 | Antioxidant properties of several coumarinâ€“chalcone hybrids from theoretical insights. RSC Advances, 2015, 5, 565-575. | 1.7 | 79 |
| 3 | Spinâ€“Orbit Charge Recombination Intersystem Crossing in Phenothiazineâ€“Anthracene Compact Dyads: Effect of Molecular Conformation on Electronic Coupling, Electronic Transitions, and Electron Spin Polarizations of the Triplet States. Journal of Physical Chemistry C, 2018, 122, 27850-27865. | 1.5 | 76 |
| 4 | Spinâ€“Orbit Chargeâ€Transfer Intersystem Crossing (ISC) in Compact Electron Donorâ€“Acceptor Dyads: ISC Mechanism and Application as Novel and Potent Photodynamic Therapy Reagents. Chemistry - A European Journal, 2020, 26, 1091-1102. | 1.7 | 76 |
| 5 | Understanding Zinc(II) Chelation with Quercetin and Luteolin: A Combined NMR and Theoretical Study. Journal of Physical Chemistry B, 2015, 119, 83-95. | 1.2 | 68 |
| 6 | 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. Chemical Communications, 2019, 55, 1510-1513. | 2.2 | 60 |
| 7 | Density functional study of the antioxidant activity of some recently synthesized resveratrol analogues. Food Chemistry, 2013, 141, 2017-2024. | 4.2 | 57 |
| 8 | The heavy atom effect on Zn(<scp>ii</scp>) phthalocyanine derivatives: a theoretical exploration of the photophysical properties. Physical Chemistry Chemical Physics, 2015, 17, 23595-23601. | 1.3 | 57 |
| 9 | Theoretical Determination of Electronic Spectra and Intersystem Spinâ€“Orbit Coupling: The Case of Isoindole-BODIPY Dyes. Journal of Chemical Theory and Computation, 2014, 10, 4006-4013. | 2.3 | 55 |
| 10 | Halogen atom effect on the photophysical properties of substituted aza-BODIPY derivatives. Physical Chemistry Chemical Physics, 2017, 19, 2530-2536. | 1.3 | 53 |
| 11 | Antioxidant properties comparative study of natural hydroxycinnamic acids and structurally modified derivatives: Computational insights. Computational and Theoretical Chemistry, 2016, 1077, 39-47. | 1.1 | 48 |
| 12 | Density Functional Predictions of Antioxidant Activity and UV Spectral Features of Nasutin A, Isonasutin, Ellagic Acid, and One of Its Possible Derivatives. Journal of Agricultural and Food Chemistry, 2013, 61, 9650-9657. | 2.4 | 44 |
| 13 | 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. Molecules, 2017, 22, 1093. | 1.7 | 44 |
| 14 | Photophysical properties of free and metallated meso-substituted tetrabenzotriazaporphyrin from density functional theory investigation. Dyes and Pigments, 2015, 120, 335-339. | 2.0 | 42 |
| 15 | PDT-correlated photophysical properties of thienopyrrole BODIPY derivatives. Theoretical insights. Dyes and Pigments, 2016, 130, 9-15. | 2.0 | 41 |
| 16 | Coumarinâ€“Chalcone Hybrids as Peroxyl Radical Scavengers: Kinetics and Mechanisms. Journal of Chemical Information and Modeling, 2016, 56, 662-670. | 2.5 | 41 |
| 17 | Homogeneous Gold Catalysis: Hydration of 1,2-Diphenylacetylene with Methanol in Aqueous Media. A Theoretical Viewpoint. Organometallics, 2012, 31, 3074-3080. | 1.1 | 40 |
| 18 | The mutual influence of non-covalent interactions in Ï€-electron deficient cavities: the case of anion recognition by tetraoxacalix[2]arene[2]triazine. Chemical Communications, 2010, 46, 5894. | 2.2 | 37 |

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|---|---|---|---|
| 19 | Can Expanded Bacteriochlorins Act as Photosensitizers in Photodynamic Therapy? Good News from Density Functional Theory Computations. Molecules, 2016, 21, 288. | 1.7 | 37 |
| 20 | Interaction of CO with PdAu(111) and PdAu(100) Bimetallic Surfaces:â€‰ A Theoretical Cluster Model Study. Journal of Physical Chemistry C, 2008, 112, 6073-6081. | 1.5 | 36 |
| 21 | Mechanistic Aspects of the Reaction of Th<sup>+</sup> and Th<sup>2+</sup> with Water in the Gas Phase. Inorganic Chemistry, 2008, 47, 2083-2088. | 1.9 | 35 |
| 22 | Investigation of the Inertness to Hydrolysis of Platinum(IV) Prodrugs. Inorganic Chemistry, 2016, 55, 1580-1586. | 1.9 | 35 |
| 23 | Photophysical Properties of S, Se and Te-Substituted Deoxyguanosines: Insight into Their Ability To Act as Chemotherapeutic Agents. Journal of Chemical Information and Modeling, 2017, 57, 234-242. | 2.5 | 35 |
| 24 | Electronic spectra and intersystem spinâ€orbit coupling in 1,2â€and 1,3â€squaraines. Journal of Computational Chemistry, 2014, 35, 2107-2113. | 1.5 | 31 |
| 25 | Adsorption of Ethylene, Vinyl, Acetic Acid, and Acetate Species on PdAu(111) and PdAu(100) Surface Alloys: A Cluster Model Study. Journal of Chemical Theory and Computation, 2009, 5, 1350-1360. | 2.3 | 28 |
| 26 | A Review on Coordination Properties of Al(III) and Fe(III) toward Natural Antioxidant Molecules: Experimental and Theoretical Insights. Molecules, 2021, 26, 2603. | 1.7 | 27 |
| 27 | Excitation energies, singletâ€“triplet energy gaps, spinâ€“orbit matrix elements and heavy atom effects in BOIMPYs as possible photosensitizers for photodynamic therapy: a computational investigation. Physical Chemistry Chemical Physics, 2018, 20, 2656-2661. | 1.3 | 26 |
| 28 | Theoretical investigation of the absorption spectra and singlet-triplet energy gap of positively charged tetraphenylporphyrins as potential photodynamic therapy photosensitizers. Canadian Journal of Chemistry, 2013, 91, 902-906. | 0.6 | 25 |
| 29 | Dimethylplatinum(II) Complexes: Computational Insights into Ptâ€“C Bond Protonolysis. Inorganic Chemistry, 2011, 50, 10091-10101. | 1.9 | 24 |
| 30 | Antioxidant properties and free radical scavenging mechanisms of cyclocurcumin. New Journal of Chemistry, 2018, 42, 12698-12705. | 1.4 | 23 |
| 31 | Complexation of Al<sup>3+</sup> and Ni<sup>2+</sup> by <scp>l</scp>-Ascorbic Acid: An Experimental and Theoretical Investigation. Journal of Physical Chemistry A, 2017, 121, 9773-9781. | 1.1 | 21 |
| 32 | On the Inhibition of Hydroxyl Radical Formation by Hydroxycinnamic Acids: The Case of Caffeic Acid as a Promising Chelating Ligand of a Ferrous Ion. Journal of Physical Chemistry A, 2019, 123, 9560-9566. | 1.1 | 21 |
| 33 | Torsion-Induced Nonradiative Relaxation of the Singlet Excited State of meso-Thienyl Bodipy and Charge Separation, Charge Recombination-Induced Intersystem Crossing in Its Compact Electron Donor/Acceptor Dyads. Journal of Physical Chemistry B, 2021, 125, 4779-4793. | 1.2 | 19 |
| 34 | The ability of a zinc pyrrolidine complex to catalyze the synthesis of cyclic carbonates from carbon dioxide and epoxides: a mechanistic theoretical investigation. Dalton Transactions, 2017, 46, 9030-9035. | 1.6 | 17 |
| 35 | Gold(I)-Catalyzed Hydration of 1,2-Diphenylacetylene: Computational Insights. Journal of Chemical Theory and Computation, 2010, 6, 2782-2789. | 2.3 | 16 |
| 36 | Ab initio calculations on the<sup>1</sup>O<sub>2</sub>quenching mechanism by trans-resveratrol. Physical Chemistry Chemical Physics, 2014, 16, 12773-12781. | 1.3 | 16 |

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|---|---|---|---|
| 37 | Catalytic Role of Dinuclear Ïƒ,Ï€-Acetylide Gold(I) Complexes in the Hydroamination of Terminal Alkynes: Theoretical Insights. Journal of Chemical Theory and Computation, 2015, 11, 581-590. | 2.3 | 16 |
| 38 | Computational Investigation of the Influence of Halogen Atoms on the Photophysical Properties of Tetraphenylporphyrin and Its Zinc(II) Complexes. Journal of Physical Chemistry A, 2018, 122, 2809-2815. | 1.1 | 16 |
| 39 | Anticancer Activity, DNA Binding, and Photodynamic Properties of a Nâˆ§Câˆ§N-Coordinated Pt(II) Complex. Inorganic Chemistry, 2021, 60, 10350-10360. | 1.9 | 16 |
| 40 | The geometric effect in palladiumâ€“gold catalysis. Is the coupling the rate-determining step in the vinyl-acetate synthesis?. Chemical Communications, 2009, , 1852. | 2.2 | 15 |
| 41 | Chemical Insights into the Antioxidant Mechanisms of Alkylseleno and Alkyltelluro Phenols: Periodic Relatives Behaving Differently. Chemistry - A European Journal, 2018, 24, 8686-8691. | 1.7 | 15 |
| 42 | Experimental and theoretical study on the coordination properties of quercetin towards aluminum(III), iron(III) and copper(II) in aqueous solution. Journal of Molecular Liquids, 2021, 325, 115171. | 2.3 | 15 |
| 43 | Theoretical Insights into the Switching Off/On of <sup>1</sup>O<sub>2</sub> Photosensitization in Chemicontrolled Photodynamic Therapy. Chemistry - A European Journal, 2018, 24, 3512-3519. | 1.7 | 14 |
| 44 | BODIPY for photodynamic therapy applications: computational study of the effect of bromine substitution on 1O2 photosensitization. Journal of Molecular Modeling, 2018, 24, 183. | 0.8 | 14 |
| 45 | Spectrophotometric determination of choline in pharmaceutical formulations via host-guest complexation with a biomimetic calixarene receptor. Microchemical Journal, 2019, 146, 735-741. | 2.3 | 14 |
| 46 | Anion-Ï€ weak interactions in a heteroaromatic calixarene receptor. A theoretical investigation. Inorganica Chimica Acta, 2018, 470, 379-384. | 1.2 | 13 |
| 47 | Bodipy-squaraine triads: Preparation and study of the intramolecular energy transfer, charge separation and intersystem crossing. Dyes and Pigments, 2017, 147, 560-572. | 2.0 | 12 |
| 48 | Novel choline selective electrochemical membrane sensor with application in milk powders and infant formulas. Talanta, 2021, 221, 121409. | 2.9 | 12 |
| 49 | The influence of surface oxygen and hydroxyl groups on the dehydrogenation of ethylene on PdAu surface alloys. A theoretical cluster model study. Chemical Physics Letters, 2010, 493, 87-93. | 1.2 | 11 |
| 50 | Quantum mechanical DFT elucidation of CO<sub>2</sub> catalytic conversion mechanisms: Three examples. International Journal of Quantum Chemistry, 2018, 118, e25572. | 1.0 | 10 |
| 51 | Theoretical exploration of the photophysical properties of two-component Ru<sup>II</sup>â€“porphyrin dyes as promising assemblies for a combined antitumor effect. Dalton Transactions, 2020, 49, 12653-12661. | 1.6 | 10 |
| 52 | Theoretical mechanistic study of the formic acid decomposition assisted by a Ru(II)-phosphine catalyst. Journal of Molecular Modeling, 2014, 20, 2250. | 0.8 | 9 |
| 53 | A Boron-Containing Compound Acting on Multiple Targets Against Alzheimerâ€™s Disease. Insights from Ab Initio and Molecular Dynamics Simulations. Journal of Chemical Information and Modeling, 2021, 61, 3397-3410. | 2.5 | 9 |
| 54 | Trimethylphosphate and Dimethylphosphate Hydrolysis by Binuclear Cd<sup>II</sup>, Mn<sup>II</sup>, and Zn<sup>II</sup>â€“Fe<sup>II</sup> Promiscuous Organophosphateâ€Đegrading Enzyme: Reaction Mechanisms. Chemistry - A European Journal, 2017, 23, 13742-13753. | 1.7 | 8 |

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| 55 | Mechanism of action of the curcumin cis-diammineplatinum(<scp>ii</scp>) complex as a photocytotoxic agent. Inorganic Chemistry Frontiers, 2020, 7, 2759-2769. | 3.0 | 8 |
| 56 | A combined Monte Carlo/<scp>DFT</scp> approach to simulate <scp>UV</scp>â€vis spectra of molecules and aggregates: Merocyanine dyes as a case study. Journal of Computational Chemistry, 2021, 42, 1054-1063. | 1.5 | 8 |
| 57 | Theoretical insight into joint photodynamic action of a gold(<scp>i</scp>) complex and a BODIPY chromophore for singlet oxygen generation. Physical Chemistry Chemical Physics, 2019, 21, 3446-3452. | 1.3 | 7 |
| 58 | Experimental and theoretical study of the complexation of Fe3+ and Cu2+ by lâ€ascorbic acid in aqueous solution. Journal of Molecular Liquids, 2022, 355, 118973. | 2.3 | 7 |
| 59 | Cytotoxicity of Alizarine versus Tetrabromocathecol Cyclometalated Pt(II) Theranostic Agents: A Combined Experimental and Computational Investigation. Inorganic Chemistry, 2022, 61, 7188-7200. | 1.9 | 7 |
| 60 | Porphyrins and Metalloporphyrins Combined with N-Heterocyclic Carbene (NHC) Gold(I) Complexes for Photodynamic Therapy Application: What Is the Weight of the Heavy Atom Effect?. Molecules, 2022, 27, 4046. | 1.7 | 7 |
| 61 | Photophysical Properties of Nitrated and Halogenated Phosphorus Tritolylcorrole Complexes: Insights from Theory. Molecules, 2018, 23, 2779. | 1.7 | 6 |
| 62 | The combined use of deuterium NMR and computer simulations for conformational investigation of flexible molecules in nematic solutions. Computational and Theoretical Chemistry, 2005, 728, 209-214. | 1.5 | 5 |
| 63 | Direct and cluster-assisted dehydrogenation of methane by Nb<sup>+</sup> and Ta<sup>+</sup>: a theoretical investigation. Physical Chemistry Chemical Physics, 2017, 19, 16178-16188. | 1.3 | 5 |
| 64 | Time-Dependent Density Functional Computations of the Spectrochemical Properties of Dithiolodithiole and Thiophene Electrochromic Systems. Materials, 2017, 10, 981. | 1.3 | 5 |
| 65 | Heteroleptic Cu(<scp>ii</scp>) saccharin complexes: intriguing coordination modes and properties. Inorganic Chemistry Frontiers, 2021, 8, 3342-3353. | 3.0 | 5 |
| 66 | Computational Analysis of Photophysical Properties and Reactivity of a New Phototherapeutic Cyclometalated Au(III)â€Hydride Complex. Chemistry - A European Journal, 2021, 27, 15528-15535. | 1.7 | 5 |
| 67 | Theoretical determination of the aquation reaction mechanism of cyclometalated benzimidazole Ru(II) and Ir(III) anticancer complexes. Inorganica Chimica Acta, 2018, 470, 325-330. | 1.2 | 5 |
| 68 | Theoretical investigation on bisarylselanylbenzo-2,1,3-selenadiazoles as potential photosensitizers in photodynamic therapy. Journal of Chemical Physics, 2021, 154, 084113. | 1.2 | 4 |
| 69 | Cyclopentadienoneâ€“NHC iron(0) complexes as low valent electrocatalysts for water oxidation. Catalysis Science and Technology, 2021, 11, 1407-1418. | 2.1 | 4 |
| 70 | Dinuclear Ruthenium(II)â€Pyrrolide Complexes Linked by Different Organic Units as PDT Photosensitizers: Computational Study of the Linker Influence on the Photophysical Properties*. ChemPhotoChem, 2022, 6, . | 1.5 | 4 |
| 71 | Theoretical investigation of the action mechanisms of N,N-di-alkylated diarylamine antioxidants. Theoretical Chemistry Accounts, 2017, 136, 1. | 0.5 | 3 |
| 72 | On the Electrochromic Properties of Borepins: A Computational Prediction. ACS Omega, 2018, 3, 9556-9563. | 1.6 | 3 |

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|---|---|---|---|
| 73 | A comparative computational mechanistic study on derivatives of pyriplatin, modified with the â€“CH2Ph3P+ group, as anticancer complexes targeting mitochondria. Inorganica Chimica Acta, 2020, 512, 119863. | 1.2 | 3 |
| 74 | Activation by Glutathione in Hypoxic Environment of an Azoâ€based Rhodamine Activatable Photosensitizer. A Computational Elucidation. Chemistry - A European Journal, 2022, 28, . | 1.7 | 3 |
| 75 | Computational Studies of the Photogeneration from Dihydrosanguinarine and the Probable Cytotoxicity Mechanism of Sanguinarine. Applied Sciences (Switzerland), 2022, 12, 1095. | 1.3 | 2 |