Gloria I Cardenas-Jiron

List of Publications by Year
in descending order

101 papers	2,048 citations	257101 24 h-index	288905 40 g-index
101 all docs	101 docs citations	101 times ranked	1895 citing authors

#	Article	IF	Citations
1	A new sterically hindered asymmetric zinc phthalocyanine as an efficient sensitizer for dye-sensitized solar cells. New Journal of Chemistry, 2022, 46, 714-725.	1.4	16
2	Fullerene binding effects in Al(III)/Zn(II) Porphyrin/Phthalocyanine photophysical properties and charge transport. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2022, 269, 120740.	2.0	9
3	Insight into the effects of the anchoring groups on the photovoltaic performance of unsymmetrical phthalocyanine based dye-sensitized solar cells. Dalton Transactions, 2021, 50, 2981-2996.	1.6	13
4	Assessment of New Expanded Porpholactones as UV/Vis/NIR Chromophores for Dye-Sensitized Solar Cell Applications. Journal of Physical Chemistry A, 2021, 125, 2267-2275.	1.1	4
5	Near-Infrared Optical Properties and Charge Transport in Expanded Porphyrins. ECS Meeting Abstracts, 2021, MA2021-01, 761-761.	0.0	0
6	The bimetallic and the anchoring group effects on both optical and charge transport properties of hexaphyrin amethyrin. New Journal of Chemistry, 2021, 45, 6521-6534.	1.4	4
7	A photo-induced spin crossover based molecular switch and spin filter operating at room temperature. Dalton Transactions, 2021, 50, 6578-6587.	1.6	4
8	Zinc phthalocyanine absorbance in the near-infrared with application for transparent and colorless dye-sensitized solar cells. Comptes Rendus Chimie, 2021, 24, 157-170.	0.2	2
9	B12N12 cluster as a collector of noble gases: A quantum chemical study. Physica E: Low-Dimensional Systems and Nanostructures, 2020, 115, 113697.	1.3	32
10	Influence of cyano substituents on the electron density and catalytic activity towards the oxygen reduction reaction for iron phthalocyanine. The case for Fe(II) 2,3,9,10,16,17,23,24-octa(cyano)phthalocyanine. Electrochemistry Communications, 2020, 118, 106784.	2.3	20
11	Effects of the methylammonium ion substitution by 5-ammoniumvaleric acid in lead trihalide perovskite solar cells: a combined experimental and theoretical investigation. New Journal of Chemistry, 2020, 44, 14642-14649.	1.4	4
12	Local and macrocyclic (anti)aromaticity of porphyrinoids revealed by the topology of the induced magnetic field. Physical Chemistry Chemical Physics, 2020, 22, 21267-21274.	1.3	8
13	The boron nitride (B116N124) fullerene: Stability and electronic properties from DFT simulations. Chemical Physics Letters, 2020, 741, 137097.	1.2	19
14	Zn(II)-Porphyrinâ€“Squaraine Dyads as Potential Components for Dye-Sensitized Solar Cells: A Quantum Chemical Study of Optical and Charge Transport Properties. Journal of Physical Chemistry C, 2020, 124, 12968-12981.	1.5	9
15	Assessment of BODIPYâ€“Oxasmaragdyrin Dyads for Dye-Sensitized Solar Cells: Aromaticity, Photosensitization Capability, and Charge Transport. Journal of Physical Chemistry C, 2019, 123, 19362-19375.	1.5	15
16	Elucidating the Electronic Structure and Magnetic and Conducting Properties of Î¼-Oxo Mn-phthalocyanine [MnPc(CN)]₂O Complex. Journal of Physical Chemistry C, 2019, 123, 28359-28369.	1.5	1
17	Effect of the meso/beta halogenation in the photoelectronic properties and aromaticity of expanded porphyrins. Journal of Photochemistry and Photobiology A: Chemistry, 2019, 385, 112052.	2.0	6
18	Effect of new asymmetrical Zn(<scp>ii</scp>) phthalocyanines on the photovoltaic performance of a dye-sensitized solar cell. New Journal of Chemistry, 2019, 43, 14390-14401.	1.4	28

#	Article	IF	Citations
19	The influence of antenna and anchoring moieties on the improvement of photoelectronic properties in Zn(<scp>ii</scp>)â€“porphyrinâ€“TiO₂ as potential dye-sensitized solar cells. Physical Chemistry Chemical Physics, 2019, 21, 4339-4348.	1.3	17
20	Spin-filter transport and magnetic properties in a binuclear Cu(ii) expanded porphyrin based molecular junction. Dalton Transactions, 2019, 48, 8418-8426.	1.6	12
21	Interpreting Aromaticity and Antiaromaticity through Bifurcation Analysis of the Induced Magnetic Field. ChemistryOpen, 2019, 8, 321-326.	0.9	9
22	Stability, electronic and optical properties of the boron nitride cage (B47N53) from quantum mechanical calculations. Physica E: Low-Dimensional Systems and Nanostructures, 2019, 111, 118-126.	1.3	23
23	Orbital-Weighted Dual Descriptor for the Study of Local Reactivity of Systems with (Quasi-) Degenerate States. Journal of Physical Chemistry A, 2019, 123, 10556-10562.	1.1	89
24	Quantum chemical studies of porphyrinâ€•and expanded porphyrinâ€‹based systems and their potential applications in nanoscience.Latin America research review. International Journal of Quantum Chemistry, 2019, 119, e25821.	1.0	7
25	Atypical antioxidant activity of non-phenolic amino-coumarins. RSC Advances, 2018, 8, 1927-1933.	1.7	9
26	Theoretical rationalisation of the photophysics of a TICT excited state of cinnamoylâ€“coumarin derivatives in homogeneous and biological membrane models. Physical Chemistry Chemical Physics, 2018, 20, 27621-27629.	1.3	10
27	Excited States of Light-Harvesting Systems Based on Fullerene/Graphene Oxide and Porphyrin/Smaragdyrin. Journal of Physical Chemistry C, 2017, 121, 4859-4872.	1.5	23
28	Insights on the Reactivity of Terminal Phosphanido Metal Complexes toward Activated Alkynes from Theoretical Computations. Inorganic Chemistry, 2017, 56, 6652-6661.	1.9	2
29	Reaction Kinetics of Phenolic Antioxidants toward Photoinduced Pyranine Free Radicals in Biological Models. Journal of Physical Chemistry B, 2017, 121, 6331-6340.	1.2	7
30	Theoretical assessment of TD-DFT applied to a ferrocene-based complex. Computational and Theoretical Chemistry, 2017, 1118, 65-74.	1.1	10
31	Covalent functionalization of octagraphene with magnetic octahedral B6â^’ and non-planar C6â^’ clusters. Physica E: Low-Dimensional Systems and Nanostructures, 2017, 94, 196-203.	1.3	12
32	MECHANISTIC STUDY OF A RUTHENIUM HYDRIDE COMPLEX OF TYPE [RuH(CO)(N-N)(PR3)2]+ AS CATALYST PRECURSOR FOR THE HYDROFORMYLATION REACTION OF 1-HEXENE. Journal of the Chilean Chemical Society, 2016, 61, 3281-3286.	0.5	3
33	Tautomerization mechanism and spectral properties of porphyrinâ€“glucose complexes as models of antibacterial material. Theoretical Chemistry Accounts, 2016, 135, 1.	0.5	10
34	Excited Electronic States of Porphyrin-Based Assemblies Using Density Functional Theory. , 2016, , 233-289.		1
35	Doping Effects in the Charge Transport of Grapheneâ€“Porphyrins. Journal of Physical Chemistry C, 2016, 120, 2013-2026.	1.5	12
36	Understanding the Hydrolysis Mechanism of Ethyl Acetate Catalyzed by an Aqueous Molybdocene: A Computational Chemistry Investigation. Inorganic Chemistry, 2015, 54, 1223-1231.	1.9	13

#	Article	IF	Citations
37	Theoretical assessment of the photosensitization mechanisms of porphyrinâ€“ruthenium(II) complexes for the formation of reactive oxygen species. Journal of Photochemistry and Photobiology A: Chemistry, 2014, 294, 68-74.	2.0	10
38	Functionalized Graphene and Cobalt Phthalocyanine Based Materials with Potential Use for Electrical Conduction. Challenges and Advances in Computational Chemistry and Physics, 2014, , 185-215.	0.6	1
39	Electron Transport Properties through Graphene Oxideâ€“Cobalt Phthalocyanine Complexes. Journal of Physical Chemistry C, 2013, 117, 23664-23675.	1.5	22
40	A three-layer ONIOM model for the outside binding of cationic porphyrins and nucleotide pair DNA. Journal of Molecular Modeling, 2013, 19, 811-824.	0.8	2
41	Assessment of the photosensitization properties of cationic porphyrins in interaction with DNA nucleotide pairs. Journal of Molecular Modeling, 2013, 19, 2913-2924.	0.8	6
42	Nitric Oxide Oxidation Mediated by Substituted Nickel Phthalocyanines: A Theoretical Viewpoint. Journal of Physical Chemistry C, 2012, 116, 16979-16984.	1.5	11
43	Theoretical Study on the Electronic Excitations of a Porphyrin-Polypyridyl Ruthenium(II) Photosensitizer. Journal of Physical Chemistry A, 2011, 115, 11988-11997.	1.1	15
44	Electrical Characteristics of Cobalt Phthalocyanine Complexes Adsorbed on Graphene. Journal of Physical Chemistry C, 2011, 115, 16052-16062.	1.5	38
45	Quantitative structure property relationships to evaluate the photosensitizing capability in porphyrins and chlorins. International Journal of Quantum Chemistry, 2011, 111, 1570-1582.	1.0	7
46	Vibrational spectroscopy and density functional theory calculations of polyâ€‹scp›D‹/scp›â€mannuronate and heteropolymeric fractions from sodium alginate. Journal of Raman Spectroscopy, 2011, 42, 870-878.	1.2	45
47	A through-space charge transfer mechanism for explaining the oxidation of 2-chlorophenol on a tetrasulphonated nickel(III) phthalocyanine. Computational and Theoretical Chemistry, 2011, 963, 161-167.	1.1	6
48	A theoretical investigation on the spectroscopic properties and photosensitizing capability of 5, 10, 15, 20-tetraphenylsapphyrin and 5, 10, 15, 20-tetraphenyl-26,28-diheterosapphyrins with two O, S, or Se Atoms. Theoretical Chemistry Accounts, 2010, 127, 475-484.	0.5	15
49	A computational study on the stabilityâ€“aromaticity correlation of triply N-confused porphyrins: CMMSE-09. Journal of Mathematical Chemistry, 2010, 48, 137-144.	0.7	6
50	Inhibitory effect of aromatic geranyl derivatives isolated from Heliotropium filifolium on infectious pancreatic necrosis virus replication. Veterinary Microbiology, 2010, 141, 53-58.	0.8	22
51	Synthesis and reactivity of Î·5-tetramethylcyclopentadienyl-propenyl rhenium complexes: Molecular structure of [(Î·5:Î·2-C5Me4CH2CHCH2)Re(CO)2]. Journal of Organometallic Chemistry, 2010, 695, 346-351.	0.8	8
52	Flow-Induced Î²-Hairpin Folding of the Glycoprotein IbÎ± Î²-Switch. Biophysical Journal, 2010, 99, 1182-1191.	0.2	16
53	Experimental and theoretical characterization of Ru(II) complexes with polypyridine and phosphine ligands. Journal of Organometallic Chemistry, 2009, 694, 3781-3792.	0.8	10
54	Theoretical study of the binding nature of glassy carbon with nickel(II) phthalocyanine complexes. Chemical Physics, 2009, 365, 164-169.	0.9	9

#	Article	IF	Citations
55	Theoretical evidence of the Ni(III) participation in the chlorophenol oxidation on tetrasulphonated nickel phthalocyanine. International Journal of Quantum Chemistry, 2008, 108, 2586-2594.	1.0	8
56	Effect of Chlorin Structure on Theoretical Electronic Absorption Spectra and on the Energy Released by Porphyrin-Based Photosensitizers. Journal of Physical Chemistry A, 2008, 112, 13574-13583.	1.1	29
57	Theoretical Insight into Pyrrole Inversion and Planarity in 5,10,15,20-Tetraphenylsapphyrin and 5,10,15,20-Tetraphenyl-26,28-Diheterosapphyrins with Two O, S, or Se Atoms. Journal of Physical Chemistry A, 2008, 112, 8100-8106.	1.1	11
58	Theoretical and Spectroscopic Study of Nickel(II) Porphyrin Derivatives. Journal of Physical Chemistry A, 2007, 111, 2706-2714.	1.1	65
59	Molecular magnetic properties of heteroporphyrins: a theoretical analysis. Physical Chemistry Chemical Physics, 2007, 9, 5644.	1.3	14
60	Theoretical Modeling of the Oxidation of Hydrazine by Iron(II) Phthalocyanine in the Gas Phase. Influence of the Metal Character. Journal of Physical Chemistry A, 2006, 110, 11870-11875.	1.1	18
61	Nickel(II) complexes with tetraaza macrocycles in the electrocatalytic oxidation of sulfite. Journal of Coordination Chemistry, 2006, 59, 1467-1475.	0.8	7
62	Electrocatalytic reduction of carbon dioxide induced by bis(N-R-2-hydroxy-1-naphthaldiminato)-copper(II) (R=n-octyl, n-dodecyl): Magnetic and theoretical studies and the X-ray structure of bis(N-n-octyl-2-hydroxy-1-naphthaldiminato)-copper(II). Inorganica Chimica Acta, 2006, 359, 3947-3953.	1.2	17
63	Influence of 5-chloro and 5-methyl benzotriazole on the corrosion of copper in acid solution: an experimental and a theoretical approach. Journal of Solid State Electrochemistry, 2006, 10, 894-904.	1.2	22
64	Inverted correlations between rate constants and redox potential of the catalyst for the electrooxidation of 2-aminoethanethiol mediated by surface confined substituted cobalt-phthalocyanines. Journal of Electroanalytical Chemistry, 2005, 580, 50-56.	1.9	30
65	Electropreparation and characterization of polyNiTSPc films. An EQCM study. Journal of Electroanalytical Chemistry, 2005, 580, 94-104.	1.9	43
66	The influence of aniline and its derivatives on the corrosion behaviour of copper in acid solution: a theoretical approach. Computational and Theoretical Chemistry, 2005, 757, 1-7.	1.5	36
67	Synthetic N-substituted metal aza-macrocyclic complexes: properties and applications. Journal of Coordination Chemistry, 2005, 58, 89-109.	0.8	16
68	Synthesis of Î²-Lactams by Ag+-Induced Ring Expansion of 1-Hydroxycyclopropylamines:Â A Theoretical Analysis. Journal of Physical Chemistry A, 2005, 109, 7822-7831.	1.1	2
69	Through-Space and Through-Bond Mixed Charge Transfer Mechanisms on the Hydrazine Oxidation by Cobalt(II) Phthalocyanine in the Gas Phase. Journal of Physical Chemistry A, 2005, 109, 1196-1204.	1.1	16
70	Experimental and Theoretical Study of the Activity of Substituted Metallophthalocyanines for Nitrite Electro-oxidation. Journal of the Electrochemical Society, 2004, 151, E32.	1.3	47
71	Solvent Effect on Density Functional Reactivity Indexes Applied to Substituted Nickel Phthalocyanines. Journal of Physical Chemistry A, 2004, 108, 6045-6051.	1.1	11
72	Fukui Indexes Applied to the Reduced and Nonreduced Species of the Nickel(II) Tetraazadinaphtho[14]annulene Complex and Its Protonated Derivative. Journal of Physical Chemistry A, 2004, 108, 7253-7260.	1.1	13

#	Article	IF	Citations
73	AZA NITROGENS EFFECT ON THE ELECTRONIC PROPERTIES OF COBALT PORPHYRINE AND DERIVATIVES. Journal of the Chilean Chemical Society, 2004, 49, .	0.5	1
74	Reactivity descriptors applied to the study of cobalt porphyrin and their aza derivatives. International Journal of Quantum Chemistry, 2003, 91, 389-397.	1.0	19
75	Application of Condensed Fukui Functions to Cobalt Macrocycle Complexes. Journal of Physical Chemistry A, 2003, 107, 11483-11488.	1.1	13
76	Theoretical and experimental study of the electronic structure and spectra of Ni(II) tetraazadinaphtho[14]annulene complexes. Journal of Coordination Chemistry, 2003, 56, 1257-1267.	0.8	8
77	Theoretical study of the electron transfer reaction of hydrazine with cobalt(II) phthalocyanine and substituted cobalt(II) phthalocyanines. Journal of Coordination Chemistry, 2003, 56, 1269-1275.	0.8	16
78	Substituent Effect in the Chemical Reactivity and Selectivity of Substituted Cobalt Phthalocyanines. Journal of Physical Chemistry A, 2002, 106, 3202-3206.	1.1	32
79	Theoretical Study of Global and Local Charge Transfer Descriptors Applied to the Interaction of Cobalt Phthalocyanine with 2-Mercaptoethanol and Cobalt Phthalocyanine with Pyridine in the Gas Phase. Journal of Physical Chemistry A, 2002, 106, 11938-11944.	1.1	16
80	Theoretical study of the interaction energy profile of cobalt phthalocyanine and 2-mercaptoethanol. Effect of the graphite on the global reactivity. Computational and Theoretical Chemistry, 2002, 580, 193-200.	1.5	19
81	Donorâ€“acceptor intermolecular hardness on charge transfer reactions of substituted cobalt phthalocyanines. Journal of Electroanalytical Chemistry, 2001, 497, 55-60.	1.9	64
82	Reactivity of electrodes modified with substituted metallophthalocyanines. Correlations with redox potentials, Hammett parameters and donor?acceptor intermolecular hardness. Electrochimica Acta, 2001, 46, 3227-3235.	2.6	88
83	Reactivity of immobilized cobalt phthalocyanines for the electroreduction of molecular oxygen in terms of molecular hardness. Journal of Electroanalytical Chemistry, 2000, 489, 96-100.	1.9	72
84	Metal-centered redox chemistry of substituted cobalt phthalocyanines adsorbed on graphite and correlations with MO calculations and Hammett parameters. Electrocatalytic reduction of a disulfide. Polyhedron, 2000, 19, 2255-2260.	1.0	60
85	Paradoxical effect of the redox potential of adsorbed metallophthalocyanines on their activity for the oxidation of 2-mercaptoethanol. Inner versus outer sphere electrocatalysis. Electrochemistry Communications, 1999, 1, 389-393.	2.3	58
86	A theoretical procedure to determine interaction energies in complex systems: application to the oxygenâ€“iron tetraazaporphyrin interaction. Computational and Theoretical Chemistry, 1999, 493, 219-224.	1.5	6
87	Molecular Orbital Study of Crystalline p-Benzoquinone. Journal of Physical Chemistry A, 1999, 103, 7042-7046.	1.1	29
88	Acetic Acid Molecular Aggregates:â€‰ Energy and Softness of Hydrogen Bonding. Journal of Physical Chemistry A, 1999, 103, 8056-8061.	1.1	7
89	Linear versus volcano correlations between electrocatalytic activity and redox and electronic properties of metallophthalocyanines. Electrochimica Acta, 1998, 44, 1349-1357.	2.6	147
90	Dynamical and spectroscopic study of internal rotation in formic, thiolformic, thionformic and dithioformic acids using a reduced potential model. Computational and Theoretical Chemistry, 1998, 426, 155-163.	1.5	4

#	Article	IF	Citations
91	The Internal Rotation of Hydrogen Thioperoxide:â€‰ Energy, Chemical Potential, and Hardness Profiles. Journal of Physical Chemistry A, 1998, 102, 7864-7871.	1.1	27
92	Relations between Potential Energy, Electronic Chemical Potential, and Hardness Profiles. Journal of Physical Chemistry A, 1997, 101, 4621-4627.	1.1	45
93	Fragment chemistry of the hydrogen thioperoxide molecule; energy, chemical potential and hardness. Computational and Theoretical Chemistry, 1997, 390, 79-89.	1.5	29
94	Hardness Profile and Activation Hardness for Rotational Isomerization Processes. 1. Application to Nitrous Acid and Hydrogen Persulfide. The Journal of Physical Chemistry, 1995, 99, 5325-5330.	2.9	49
95	Hardness Profile and Activation Hardness for Rotational Isomerization Processes. 2. The Maximum Hardness Principle. The Journal of Physical Chemistry, 1995, 99, 12730-12738.	2.9	61
96	Characterization of Rotational Isomerization Processes in Monorotor Molecules. Topics in Molecular Organization and Engineering, 1995, , 97-120.	0.1	10
97	A model potential for the internal rotation of nitrosyl hyperfluorite. A comparative analysis of different theoretical methods. Chemical Physics Letters, 1994, 222, 8-14.	1.2	7
98	Theoretical analysis of the internal rotation, molecular structures and electronic properties of the XSSX series of molecules (X = H, F, Cl). Computational and Theoretical Chemistry, 1993, 282, 113-122.	1.5	18
99	Theory of one-dimension rotational isomerization: A study of thecis-trans isomerization of HS-NS compared to that of HO-NO. Molecular Engineering, 1992, 2, 17-27.	0.2	5
100	On the rotational isomerism of one rotor molecules. A comparative study of the HSSH and HXNX (X =) Tj ETQq0 0 0 rgBT /Overlock 10 T	1.5	18
101	Infrared Assignment and Formation Mechanism of Trans-Anti Thymine Dimer. Spectroscopy Letters, 1988, 21, 107-125.	0.5	3