Gloria I Cardenas-Jiron

List of Publications by Year
in descending order

101 papers	2,048 citations	257450 24 h-index	289244 40 g-index
101 all docs	101 docs citations	101 times ranked	1895 citing authors

#	Article	IF	Citations
1	Linear versus volcano correlations between electrocatalytic activity and redox and electronic properties of metallophthalocyanines. Electrochimica Acta, 1998, 44, 1349-1357.	5.2	147
2	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.	2.5	89
3	Reactivity of electrodes modified with substituted metallophthalocyanines. Correlations with redox potentials, Hammett parameters and donor?acceptor intermolecular hardness. Electrochimica Acta, 2001, 46, 3227-3235.	5.2	88
4	Reactivity of immobilized cobalt phthalocyanines for the electroreduction of molecular oxygen in terms of molecular hardness. Journal of Electroanalytical Chemistry, 2000, 489, 96-100.	3.8	72
5	Theoretical and Spectroscopic Study of Nickel(II) Porphyrin Derivatives. Journal of Physical Chemistry A, 2007, 111, 2706-2714.	2.5	65
6	Donorâ€“acceptor intermolecular hardness on charge transfer reactions of substituted cobalt phthalocyanines. Journal of Electroanalytical Chemistry, 2001, 497, 55-60.	3.8	64
7	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
8	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.	2.2	60
9	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.	4.7	58
10	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
11	Experimental and Theoretical Study of the Activity of Substituted Metallophthalocyanines for Nitrite Electro-oxidation. Journal of the Electrochemical Society, 2004, 151, E32.	2.9	47
12	Relations between Potential Energy, Electronic Chemical Potential, and Hardness Profiles. Journal of Physical Chemistry A, 1997, 101, 4621-4627.	2.5	45
13	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.	2.5	45
14	Electropreparation and characterization of polyNiTSPc films. An EQCM study. Journal of Electroanalytical Chemistry, 2005, 580, 94-104.	3.8	43
15	Electrical Characteristics of Cobalt Phthalocyanine Complexes Adsorbed on Graphene. Journal of Physical Chemistry C, 2011, 115, 16052-16062.	3.1	38
16	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
17	Substituent Effect in the Chemical Reactivity and Selectivity of Substituted Cobalt Phthalocyanines. Journal of Physical Chemistry A, 2002, 106, 3202-3206.	2.5	32
18	B12N12 cluster as a collector of noble gases: A quantum chemical study. Physica E: Low-Dimensional Systems and Nanostructures, 2020, 115, 113697.	2.7	32

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19	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.	3.8	30
20	Fragment chemistry of the hydrogen thioperoxide molecule; energy, chemical potential and hardness. Computational and Theoretical Chemistry, 1997, 390, 79-89.	1.5	29
21	Molecular Orbital Study of Crystalline p-Benzoquinone. Journal of Physical Chemistry A, 1999, 103, 7042-7046.	2.5	29
22	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.	2.5	29
23	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.	2.8	28
24	The Internal Rotation of Hydrogen Thioperoxide:â€‰ Energy, Chemical Potential, and Hardness Profiles. Journal of Physical Chemistry A, 1998, 102, 7864-7871.	2.5	27
25	Excited States of Light-Harvesting Systems Based on Fullerene/Graphene Oxide and Porphyrin/Smaragdyrin. Journal of Physical Chemistry C, 2017, 121, 4859-4872.	3.1	23
26	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.	2.7	23
27	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.	2.5	22
28	Inhibitory effect of aromatic geranyl derivatives isolated from Heliotropium filifolium on infectious pancreatic necrosis virus replication. Veterinary Microbiology, 2010, 141, 53-58.	1.9	22
29	Electron Transport Properties through Graphene Oxideâ€“Cobalt Phthalocyanine Complexes. Journal of Physical Chemistry C, 2013, 117, 23664-23675.	3.1	22
30	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.	4.7	20
31	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
32	Reactivity descriptors applied to the study of cobalt porphyrin and their aza derivatives. International Journal of Quantum Chemistry, 2003, 91, 389-397.	2.0	19
33	The boron nitride (B116N124) fullerene: Stability and electronic properties from DFT simulations. Chemical Physics Letters, 2020, 741, 137097.	2.6	19
34	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
35	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
36	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.	2.5	18

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37	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.	2.4	17
38	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.	2.8	17
39	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.	2.5	16
40	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.	2.2	16
41	Synthetic N-substituted metal aza-macrocyclic complexes: properties and applications. Journal of Coordination Chemistry, 2005, 58, 89-109.	2.2	16
42	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.	2.5	16
43	Flow-Induced Î²-Hairpin Folding of the Glycoprotein Ibα Î²-Switch. Biophysical Journal, 2010, 99, 1182-1191.	0.5	16
44	A new sterically hindered asymmetric zinc phthalocyanine as an efficient sensitizer for dye-sensitized solar cells. New Journal of Chemistry, 2022, 46, 714-725.	2.8	16
45	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.	1.4	15
46	Theoretical Study on the Electronic Excitations of a Porphyrin-Polypyridyl Ruthenium(II) Photosensitizer. Journal of Physical Chemistry A, 2011, 115, 11988-11997.	2.5	15
47	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.	3.1	15
48	Molecular magnetic properties of heteroporphyrins: a theoretical analysis. Physical Chemistry Chemical Physics, 2007, 9, 5644.	2.8	14
49	Application of Condensed Fukui Functions to Cobalt Macrocycle Complexes. Journal of Physical Chemistry A, 2003, 107, 11483-11488.	2.5	13
50	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.	2.5	13
51	Understanding the Hydrolysis Mechanism of Ethyl Acetate Catalyzed by an Aqueous Molybdocene: A Computational Chemistry Investigation. Inorganic Chemistry, 2015, 54, 1223-1231.	4.0	13
52	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.	3.3	13
53	Doping Effects in the Charge Transport of Grapheneâ€“Porphyrins. Journal of Physical Chemistry C, 2016, 120, 2013-2026.	3.1	12
54	Covalent functionalization of octagraphene with magnetic octahedral B6â˜ and non-planar C6â˜ clusters. Physica E: Low-Dimensional Systems and Nanostructures, 2017, 94, 196-203.	2.7	12

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55	Spin-filter transport and magnetic properties in a binuclear Cu(ii) expanded porphyrin based molecular junction. Dalton Transactions, 2019, 48, 8418-8426.	3.3	12
56	Solvent Effect on Density Functional Reactivity Indexes Applied to Substituted Nickel Phthalocyanines. Journal of Physical Chemistry A, 2004, 108, 6045-6051.	2.5	11
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.	2.5	11
58	Nitric Oxide Oxidation Mediated by Substituted Nickel Phthalocyanines: A Theoretical Viewpoint. Journal of Physical Chemistry C, 2012, 116, 16979-16984.	3.1	11
59	Experimental and theoretical characterization of Ru(II) complexes with polypyridine and phosphine ligands. Journal of Organometallic Chemistry, 2009, 694, 3781-3792.	1.8	10
60	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.	3.9	10
61	Tautomerization mechanism and spectral properties of porphyrinâ€“glucose complexes as models of antibacterial material. Theoretical Chemistry Accounts, 2016, 135, 1.	1.4	10
62	Theoretical assessment of TD-DFT applied to a ferrocene-based complex. Computational and Theoretical Chemistry, 2017, 1118, 65-74.	2.5	10
63	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.	2.8	10
64	Characterization of Rotational Isomerization Processes in Monorotor Molecules. Topics in Molecular Organization and Engineering, 1995, , 97-120.	0.1	10
65	Theoretical study of the binding nature of glassy carbon with nickel(II) phthalocyanine complexes. Chemical Physics, 2009, 365, 164-169.	1.9	9
66	Atypical antioxidant activity of non-phenolic amino-coumarins. RSC Advances, 2018, 8, 1927-1933.	3.6	9
67	Interpreting Aromaticity and Antiaromaticity through Bifurcation Analysis of the Induced Magnetic Field. ChemistryOpen, 2019, 8, 321-326.	1.9	9
68	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.	3.1	9
69	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.	3.9	9
70	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.	2.2	8
71	Theoretical evidence of the Ni(III) participation in the chlorophenol oxidation on tetrasulphonated nickel phthalocyanine. International Journal of Quantum Chemistry, 2008, 108, 2586-2594.	2.0	8
72	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.	1.8	8

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73	Local and macrocyclic (anti)aromaticity of porphyrinoids revealed by the topology of the induced magnetic field. Physical Chemistry Chemical Physics, 2020, 22, 21267-21274.	2.8	8
74	A model potential for the internal rotation of nitrosyl hyperfluorite. A comparative analysis of different theoretical methods. Chemical Physics Letters, 1994, 222, 8-14.	2.6	7
75	Acetic Acid Molecular Aggregates:â€‰ Energy and Softness of Hydrogen Bonding. Journal of Physical Chemistry A, 1999, 103, 8056-8061.	2.5	7
76	Nickel(II) complexes with tetraaza macrocycles in the electrocatalytic oxidation of sulfite. Journal of Coordination Chemistry, 2006, 59, 1467-1475.	2.2	7
77	Quantitative structure property relationships to evaluate the photosensitizing capability in porphyrins and chlorins. International Journal of Quantum Chemistry, 2011, 111, 1570-1582.	2.0	7
78	Reaction Kinetics of Phenolic Antioxidants toward Photoinduced Pyranine Free Radicals in Biological Models. Journal of Physical Chemistry B, 2017, 121, 6331-6340.	2.6	7
79	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.	2.0	7
80	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
81	A computational study on the stabilityâ€“aromaticity correlation of triply N-confused porphyrins: CMMSE-09. Journal of Mathematical Chemistry, 2010, 48, 137-144.	1.5	6
82	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.	2.5	6
83	Assessment of the photosensitization properties of cationic porphyrins in interaction with DNA nucleotide pairs. Journal of Molecular Modeling, 2013, 19, 2913-2924.	1.8	6
84	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.	3.9	6
85	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
86	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
87	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.	2.8	4
88	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.	2.5	4
89	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.	2.8	4
90	A photo-induced spin crossover based molecular switch and spin filter operating at room temperature. Dalton Transactions, 2021, 50, 6578-6587.	3.3	4

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91	Infrared Assignment and Formation Mechanism of Trans-Anti Thymine Dimer. Spectroscopy Letters, 1988, 21, 107-125.	1.0	3
92	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.	1.2	3
93	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.	2.5	2
94	A three-layer ONIOM model for the outside binding of cationic porphyrins and nucleotide pair DNA. Journal of Molecular Modeling, 2013, 19, 811-824.	1.8	2
95	Insights on the Reactivity of Terminal Phosphanido Metal Complexes toward Activated Alkynes from Theoretical Computations. Inorganic Chemistry, 2017, 56, 6652-6661.	4.0	2
96	Zinc phthalocyanine absorbance in the near-infrared with application for transparent and colorless dye-sensitized solar cells. Comptes Rendus Chimie, 2021, 24, 157-170.	0.5	2
97	Excited Electronic States of Porphyrin-Based Assemblies Using Density Functional Theory. , 2016, , 233-289.		1
98	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.	3.1	1
99	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
100	AZA NITROGENS EFFECT ON THE ELECTRONIC PROPERTIES OF COBALT PORPHYRINE AND DERIVATIVES. Journal of the Chilean Chemical Society, 2004, 49, .	1.2	1
101	Near-Infrared Optical Properties and Charge Transport in Expanded Porphyrins. ECS Meeting Abstracts, 2021, MA2021-01, 761-761.	0.0	0