Julian Cruz-Borbolla

List of Publications by Year
in descending order

66	1,085	567247 15	434170 31
papers	citations	h-index	g-index

67	67	67	1171
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Development of a predictive model for corrosion inhibition of carbon steel by imidazole and benzimidazole derivatives. Corrosion Science, 2016, 108, 23-35.	6.6	177
2	A New Specific Mechanism for the Acid Catalysis of the Addition Step in the Baeyerâ˜Villiger Rearrangement. Organic Letters, 2006, 8, 1763-1765.	4.6	92
3	Reactivity properties of derivatives of 2-imidazoline: an ab initio DFT study. International Journal of Quantum Chemistry, 2001, 85, 546-556.	2.0	91
4	Interaction of Imidazoline Compounds with Fen(n= 1â˜'4 Atoms) as a Model for Corrosion Inhibition:â€‰ DFT and Electrochemical Studies. Journal of Physical Chemistry C, 2007, 111, 9853-9866.	3.1	87
5	Density Functional Theory and Electrochemical Studies: Structureâ€“Efficiency Relationship on Corrosion Inhibition. Journal of Chemical Information and Modeling, 2015, 55, 2391-2402.	5.4	53
6	Benzimidazole ligands in the corrosion inhibition for carbon steel in acid medium: DFT study of its interaction on Fe30 surface. Journal of Molecular Structure, 2016, 1119, 314-324.	3.6	53
7	The influence of iodide in corrosion inhibition by organic compounds on carbon steel: Theoretical and experimental studies. Applied Surface Science, 2020, 514, 145928.	6.1	47
8	Theoretical Study of the Hg2+ Recognition by 1,3-Diphenyl-Thiourea. Journal of Physical Chemistry A, 2003, 107, 9000-9007.	2.5	31
9	Pyriteâ˜Arsenopyrite Galvanic Interaction and Electrochemical Reactivity. Journal of Physical Chemistry C, 2008, 112, 10453-10461.	3.1	31
10	DFT studies of Î±-diimines adsorption over Fen surface (n=1, 4, 9 and 14) as a model for metal surface coating. Chemical Physics Letters, 2010, 485, 142-151.	2.6	30
11	Surface tension of hydrocarbon chains at the liquidâ€“vapour interface. Molecular Physics, 2008, 106, 1055-1059.	1.7	25
12	Substituent Effects in the Migration Step of the Baeyerâ˜Villiger Rearrangement. A Theoretical Study. Journal of Physical Chemistry A, 2005, 109, 3383-3390.	2.5	23
13	DFT analysis: Fe4 cluster and Fe(110) surface interaction studies with pyrrole, furan, thiophene, and selenophene molecules. Structural Chemistry, 2014, 25, 115-126.	2.0	20
14	Subtle Câ€“HÂ·Â·Â·Hal (Hal = Cl, Br) Bonding as Predominant Synthon in the Assembly of Supramolecular Architectures Based on Luminescent Tin(IV) Complexes. Crystallography, Hirshfeld Surfaces, DFT Calculations, and Fluorescence. Crystal Growth and Design, 2014, 14, 3742-3757.	3.0	19
15	Mathematical Models Generated for the Prediction of Corrosion Inhibition Using Different Theoretical Chemistry Simulations. Materials, 2020, 13, 5656.	2.9	18
16	DFT studies on the phenol and thiophenol interaction on an undecagold cluster surface. Chemical Physics Letters, 2008, 455, 64-71.	2.6	16
17	Electrochemical and theoretical studies of the interactions of a pyridyl-based corrosion inhibitor with iron clusters (Fe15, Fe30, Fe45, and Fe60). Journal of Molecular Modeling, 2017, 23, 342.	1.8	16
18	Formal synthesis of (â˜')-flustramine B and its absolute configuration assignment by vibrational circular dichroism exciton chirality. Tetrahedron: Asymmetry, 2015, 26, 710-720.	1.8	13

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19	Spectroscopic studies and molecular modelling of the aflatoxin M1-bovine Î±-lactalbumin complex formation. Journal of Photochemistry and Photobiology B: Biology, 2020, 209, 111957.	3.8	13
20	Synthesis, structural study and biological activity of new derivatives of chrysin containing a 2-mercaptopyridyl or 5-(trifluoromethyl)-2-mercaptopyridyl fragments. Journal of Molecular Structure, 2016, 1110, 196-207.	3.6	12
21	Study on the intramolecular transannular chalcogenâ€“tin interactions in dithiastannecine compounds. Polyhedron, 2012, 33, 367-377.	2.2	11
22	Synthesis of Ir(<scp>iii</scp>) complexes with Tp^{Me2} and acac ligands and their reactivity with electrophiles. Dalton Transactions, 2015, 44, 13881-13889.	3.3	11
23	Absolute configuration assignment of 3-oxindolylacetyl-4-phenyloxazolidinone derivatives. Tetrahedron: Asymmetry, 2011, 22, 2085-2098.	1.8	10
24	Fe n Clusters (nÂ=Â2â€“7) Interaction with Furan Ring: DFT Studies over Iron Surface Suitability for Furan Adsorption. Journal of Cluster Science, 2011, 22, 459-471.	3.3	10
25	Experimental and theoretical studies of Câ€“Hâ‹¯M interactions in palladium and platinum complexes derived from 1,2-bis-(2-hydroxymethylphenylthio)ethane. Polyhedron, 2015, 87, 181-193.	2.2	10
26	Mechanosynthesis of Photochromic Oligophenyleneimines: Optical, Electrochemical and Theoretical Studies. Molecules, 2019, 24, 849.	3.8	9
27	Understanding of benzimidazole based ionic liquid as an efficient corrosion inhibitor for carbon steel: Experimental and theoretical studies. Journal of Molecular Liquids, 2022, 358, 119204.	4.9	9
28	Ruthenium(II) complexes containing benzimidazolic tripodal ligands. Inorganica Chimica Acta, 2015, 431, 258-265.	2.4	8
29	A new computational model for the prediction of toxicity of phosphonate derivatives using QSPR. Molecular Diversity, 2018, 22, 269-280.	3.9	8
30	Orlistat interaction with sibutramine and carnitine. A physicochemical and theoretical study. Journal of Molecular Structure, 2014, 1062, 1-12.	3.6	7
31	Synthetic, spectroscopic and structural behavior of unsaturated functionalized N -heterocyclic carbene complexes of group 11. Polyhedron, 2017, 137, 97-111.	2.2	7
32	Reaction mechanism for hydrogen production using the Pd4 cluster and formic acid by DFT. Chemical Physics Letters, 2020, 755, 137794.	2.6	7
33	Effects of Bentonite on p-Methoxybenzyl Acetate: A Theoretical Model for Oligomerization via an Electrophilic-Substitution Mechanism. Molecules, 2011, 16, 1761-1775.	3.8	6
34	Absolute configuration assignment of 3-indolylacetate esters. Tetrahedron: Asymmetry, 2012, 23, 1279-1293.	1.8	6
35	Activation of aldehydes by exocyclic iridium(i)-Î·4:Ï€2-diene complexes derived from 1,3-oxazolidin-2-ones. Dalton Transactions, 2016, 45, 16878-16888.	3.3	6
36	2-Cyano-2-indolylpropanoic acid as a chiral derivatizing agent for the absolute configuration assignment of secondary alcohols and primary amines by 1 H NMR and VCD. Tetrahedron: Asymmetry, 2017, 28, 762-782.	1.8	6

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37	On the interaction of anisole and thioanisole derivatives with gold clusters studied by DFT. Computational and Theoretical Chemistry, 2018, 1126, 54-64.	2.5	6
38	A theoretical and experimental approach to evaluate zein-calcium interaction in nixtamalization process. Food Chemistry, 2019, 297, 124995.	8.2	6
39	Synthesis, Raman, X-ray diffraction, and density functional studies of antimony(III) heterotetracycles displaying intramolecular transannular interactions OÂâ†'ÂSb. Structural Chemistry, 2013, 24, 1555-1564.	2.0	5
40	Synthesis and structural characterization of 10 Group metal complexes with anionic tridentate S,N,N donor Schiff bases derived from pyridylbenzothiazolines. Polyhedron, 2017, 135, 169-179.	2.2	5
41	Determination of antibiotics in feedstuff samples by microemulsion electrokinetic chromatography using fullerene as additive. Electrophoresis, 2018, 39, 2228-2235.	2.4	5
42	Theoretical Studies on Iron Surface Coating: Adsorption of Furan Derivatives Over Fen Clusters (n =) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 5	0.9	4
43	Structural differences in eight- and ten-membered heterocyclic tin compounds displaying transannular interactions Oâ‹¯Sn: An experimental and theoretical study. Polyhedron, 2012, 40, 1-10.	2.2	4
44	DFT and docking studies of rhodostreptomycins A and B and their interactions with solvated/nonsolvated Mg2+ and Ca2+ ions. Journal of Molecular Modeling, 2013, 19, 4823-4836.	1.8	4
45	Reduced density gradient as a novel approach for estimating QSAR descriptors, and its application to 1, 4-dihydropyridine derivatives with potential antihypertensive effects. Journal of Molecular Modeling, 2016, 22, 296.	1.8	4
46	Palladium(II) complexes bearing di-(2-picolyl)amine functionalized chrysin fragments. An experimental and theoretical study. Journal of Molecular Structure, 2017, 1145, 112-120.	3.6	4
47	Intramolecular interactions Snâ€"D in organotin heterocyclic compounds [{D(C6H4CH2)}SnBr2]. Inorganic Chemistry Communication, 2018, 97, 44-48.	3.9	4
48	Nonconventional Câ€"HÂ·Â·Â·Cu Interaction Between Copper Cun Clusters (nâ€‰=â€‰3â€"20) and Aromatic Compounds. Journal of Cluster Science, 2021, 32, 1155-1173.	3.3	4
49	Activation of Ptâ€"O and Ptâ€"H bonds: DFT studies on adsorption of [Gd(H2O)n]3+ (n=8â€"9) with Ptn (n=3â€"7) cluster. Computational and Theoretical Chemistry, 2014, 1047, 47-54.	2.5	3
50	Synthesis, X-ray diffraction, and density functional studies of tin(IV) compounds containing a pincer-type SNS ligand. Structural Chemistry, 2015, 26, 189-198.	2.0	3
51	Theoretical and experimental studies of phenol oxidation by ruthenium complex with N,N,N-tris(benzimidazol-2yl-methyl)amine. Journal of Molecular Modeling, 2015, 21, 224.	1.8	3
52	Theoretical study: Electronic structure and receptor interaction of four type bis-1,4-dihydropyridine molecules. Computational and Theoretical Chemistry, 2018, 1123, 102-110.	2.5	3
53	CO substitution vs C Si cleavage in the reactions of [(Î¼-H)M3(CO)9(CCSiR3)] (Mâ€¯=â€¯Ru, Râ€¯=â€¯Me, Ph; Mâ€¯=â€¯Os,) Tj ETQq1 492, 8-17.	2.4	3
54	Coordination from Heteroscorpionate Ligand Towards Pd(II) via Pdâ‹¯â‹¯Hî´â"C(sp3) Interaction: Structural and Catalytic Studies. European Journal of Inorganic Chemistry, 2021, 2021, 2661-2668.	2.0	3

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55	Synthesis and characterization of organopalladium(II) complexes of N,N,Sâ€“tridentate sulfur-containing Schiff bases derived from 2-(2-pyridyl)benzothiazolines. Polyhedron, 2022, 214, 115635.	2.2	3
56	Structural Changes in CuII Complexes of Potential Octadentate Ligands by Coordination with Carboxylate/Carboxylic Acid: DFT, TD-DFT, and Experimental Studies. Australian Journal of Chemistry, 2010, 63, 965.	0.9	2
57	Preferred Binding of Carboxylates by Chiral Urea Derivatives ContainingÎ±-Phenylethyl Group. Helvetica Chimica Acta, 2016, 99, 416-424.	1.6	2
58	Synthesis and Characterization of Amide Stationary Phases for the Determination of Sulfonamides by Sequential Injection Chromatography. Analytical Letters, 2016, 49, 676-689.	1.8	2
59	Coordination diversity in tin compounds with bis(benzoxazole)phenol as a polydentate ligand: Synthesis and crystal structure studies. Journal of Coordination Chemistry, 2018, 71, 3790-3805.	2.2	2
60	Synthesis and characterization of azathiaethers macrocyclic rings decorated with one or two 2-pyridylmethyl fragments. Journal of Molecular Structure, 2019, 1176, 54-65.	3.6	1
61	Câ€“H â‹¯Pd interactions in palladium complexes derived from tetrasulfur-difluorinated ligands. Experimental, computational and catalytic studies. Polyhedron, 2019, 173, 114115.	2.2	1
62	The chemical reactivity and QSPR of organic compounds applied to dye-sensitized solar cells using DFT. Journal of Molecular Graphics and Modelling, 2021, 104, 107852.	2.4	1
63	Reactivity of TpMe2Ir(C2H4)(DMAD) with carboxylic acids. A DFT study on geometrical isomers and structural characterization. Journal of Organometallic Chemistry, 2011, 696, 748-757.	1.8	0
64	Synthesis and Mechanosynthesis of <i>N, N</i>â€™-bis (thylthyenil)-2,3-butanediimine with Corrosion Inhibitor Properties. Advanced Materials Research, 0, 976, 64-69.	0.3	0
65	Assessment of Simultaneous Global Optimization of Geometry and Total Spin of Small Iron Clusters. Journal of Chemical Theory and Computation, 2022, 18, 4565-4573.	5.3	0
66	Actividad catalÃ‡tica de complejos de Paladio (II) con ligandos O,N,S tridentados. PÃ„DI BoletÃn CientÃfico De Ciencias BÃ¡sicas E IngenierÃas Del ICBI, 2022, 10, 66-69.	0.0	0