JosÃ© A Dobado

List of Publications by Year
in descending order

72 papers	3,131 citations	236925 25 h-index	161849 54 g-index
90 all docs	90 docs citations	90 times ranked	4129 citing authors

#	Article	IF	Citations
1	Lignin as Renewable Raw Material. ChemSusChem, 2010, 3, 1227-1235.	6.8	785
2	Chemical Bonding in Hypervalent Molecules Revised. Application of theAtoms in MoleculesTheoryto Y3X and Y3XZ (Y = H or CH3; X = N, P or As; Z = O or S) Compounds. Journal of the American Chemical Society, 1998, 120, 8461-8471.	13.7	162
3	Green and Bio-Based Solvents. Topics in Current Chemistry, 2018, 376, 18.	5.8	143
4	Weakening Câ”O Bonds: Ti(III), a New Reagent for Alcohol Deoxygenation and Carbonyl Coupling Olefination. Journal of the American Chemical Society, 2010, 132, 254-259.	13.7	127
5	CoNTub:â€‰ An Algorithm for Connecting Two Arbitrary Carbon Nanotubes. Journal of Chemical Information and Computer Sciences, 2004, 44, 1639-1646.	2.8	110
6	Chemical Bonding in Hypervalent Molecules Revised. 3.â€Application of the Atoms in Molecules Theory to Y3Xâ”CH2(X = N, P, or As; Y = H or F) and H2Xâ”CH2(X = O, S, or Se) Ylides. Journal of the American Chemical Society, 2000, 122, 1144-1149.	13.7	107
7	The three-center-four-electron (3c-4e) bond nature revisited. An atoms-in-molecules theory (AIM) and ELF study. Theoretical Chemistry Accounts, 2001, 105, 328-337.	1.4	95
8	Chemical Bonding in Hypervalent Molecules Revised. 2.â€Application of the Atoms in Molecules Theory to Y2XZ and Y2XZ2(Y = H, F, CH3; X = O, S, Se; Z = O, S) Compounds. Journal of the American Chemical Society, 1999, 121, 3156-3164.	13.7	74
9	CarbonÂ·Â·Â·Carbon Weak Interactions. Journal of Physical Chemistry A, 2009, 113, 8387-8393.	2.5	73
10	Basis set superposition error-counterpoise corrected potential energy surfaces. Application to hydrogen peroxideâ‹¯X (X=Fâ”,â€ŠClâ”, Brâ”,â€ŠLi+,â€ŠNa+) complexes. Journal of Chemical Physics, 1999, 110, 11806-11813.	3.0	71
11	On the Existence of Î±-Agostic Bonds:â€‰ Bonding Analyses of Titanium Alkyl Complexes. Organometallics, 2006, 25, 5638-5647.	2.3	63
12	On the Nature of Metalâ”Carbon Bonding:Â AIM and ELF Analyses of MCHn(n= 1â”3) Compounds Containing Early Transition Metals. Journal of Physical Chemistry A, 2005, 109, 7500-7508.	2.5	60
13	Theoretical Study on the Ureaâ”Hydrogen Peroxide 1:1 Complexes. Journal of Physical Chemistry A, 1998, 102, 778-784.	2.5	58
14	Porous nanotube network: a novel 3-D nanostructured material with enhanced hydrogen storage capacity. Chemical Communications, 2011, 47, 2303-2305.	4.1	55
15	Ab initio molecular orbital study of the hydrogen peroxide-water complex (HOOH.cntdot..cntdot..cntdot.H2O). The Journal of Physical Chemistry, 1994, 98, 1819-1825.	2.9	47
16	Recognizing a triple bond between main group atoms. Theoretical Chemistry Accounts, 2001, 105, 365-373.	1.4	43
17	Dinuclear silver(i) complexes for the design of metalâ€“ligand networks based on triazolopyrimidines. Dalton Transactions, 2011, 40, 11845.	3.3	42
18	Adenineâ”Hydrogen Peroxide System:Â DFT and MP2 Investigation. Journal of Physical Chemistry A, 1999, 103, 4755-4761.	2.5	39

#	Article	IF	Citations
19	Epoxides, Cyclic Sulfites, and Sulfate from Natural Pentacyclic Triterpenoids:Â Theoretical Calculations and Chemical Transformations. Journal of Organic Chemistry, 2003, 68, 4833-4844.	3.2	38
20	Silver(I)â€Mediated Base Pairs in DNA Sequences Containing 7â€Deazaguanine/Cytosine: towards DNA with Entirely Metallated Watsonâ€“Crick Base Pairs. Chemistry - A European Journal, 2018, 24, 4583-4589.	3.3	35
21	Reversible Attachment of Platinum Alloy Nanoparticles to Nonfunctionalized Carbon Nanotubes. ACS Nano, 2010, 4, 2438-2444.	14.6	31
22	Ab initio molecular orbital calculation of the hydrogen peroxide dimer: study of basis set superposition error. The Journal of Physical Chemistry, 1993, 97, 7499-7504.	2.9	30
23	Multiple Bonding in Four-Coordinated Titanium(IV) Compounds. Inorganic Chemistry, 2000, 39, 2831-2836.	4.0	30
24	Designing novel nanoporous architectures of carbon nanotubes for hydrogen storage. International Journal of Hydrogen Energy, 2014, 39, 9825-9829.	7.1	30
25	CoNTub v2.0 - Algorithms for Constructing C3-Symmetric Models of Three-Nanotube Junctions. Journal of Chemical Information and Modeling, 2011, 51, 1492-1505.	5.4	27
26	Protecting-Group-Free Synthesis of Chokols. Journal of Organic Chemistry, 2011, 76, 2494-2501.	3.2	27
27	Clarâ€™KekulÃ© Structuring in Armchair Carbon Nanotubes. Organic Letters, 2008, 10, 1991-1994.	4.6	26
28	Structure and bonding of weak hydrogen peroxide complexes. Computational and Theoretical Chemistry, 2002, 580, 117-126.	1.5	25
29	A comparative molecular mechanics, semiempirical and ab initio study of saturated five-membered rings. Computational and Theoretical Chemistry, 1994, 303, 205-212.	1.5	23
30	MRCI Calculations of the Ground and Excited State Potential Energy Surfaces of the 2,4-Pentadien-1-iminium Cation. The Journal of Physical Chemistry, 1996, 100, 18282-18288.	2.9	23
31	Regioselective Enzymatic Acylations of Polyhydroxylated Eudesmanes:Â Semisynthesis, Theoretical Calculations, and Biotransformation of Cyclic Sulfites. Journal of Organic Chemistry, 2000, 65, 8214-8223.	3.2	22
32	Structure and bonding of H2O2Â·Â·Â·X complexes with (X = NO+, CN-, HCN, HNC, CO). Physical Chemistry Chemical Physics, 2000, 2, 4089-4094.	2.8	21
33	Study by fluorescence of calix[4]arenes bearing heterocycles with anions: highly selective detection of iodide. Journal of Inclusion Phenomena and Macrocyclic Chemistry, 2014, 80, 369-375.	1.6	21
34	Ab Initio Calculations of the Hydrogen Peroxide-Hydrogen Halide Complexes (HOOH.cntdot..cntdot..cntdot.XH, X = F, Cl). The Journal of Physical Chemistry, 1994, 98, 7819-7822.	2.9	20
35	Structural and electronic effects of the interaction of metal cations with benzene. Computational and Theoretical Chemistry, 2002, 589-590, 337-347.	1.5	20
36	Electrochemically and photochemically active Palladium(ii) heterotopic metallacalix[3]arenes. Chemical Communications, 2008, , 3735.	4.1	19

#	Article	IF	Citations
37	From 7-azaindole to adenine: molecular recognition aspects on mixed-ligand Cu(ii) complexes with deaza-adenine ligands. Dalton Transactions, 2013, 42, 6119.	3.3	19
38	para-Fluoro benzyl substituted bis(indenyl) metallocenes as catalyst precursors in ethene polymerization. Journal of Organometallic Chemistry, 1998, 553, 173-178.	1.8	18
39	Chemical Bonding to N, P, and As in Ylides and Their Boron Analogues. Journal of Physical Chemistry A, 2004, 108, 9188-9195.	2.5	18
40	Edge effects, electronic arrangement, and aromaticity patterns on finite-length carbon nanotubes. Physical Chemistry Chemical Physics, 2011, 13, 12844.	2.8	18
41	The role of weak interactions in lignin polymerization. Journal of Molecular Modeling, 2017, 23, 80.	1.8	18
42	Insights on the binding ability of a new adenine analog: 7-amine-1,2,4-triazolo[1,5-a]pyrimidine. Synthesis and magnetic study of the first copper(<scp>ii</scp>) complexes. Dalton Transactions, 2012, 41, 1755-1764.	3.3	17
43	Thread based microfluidic platform for urinary creatinine analysis. Sensors and Actuators B: Chemical, 2020, 305, 127407.	7.8	17
44	Singleâ€Stranded DNA as Supramolecular Template for Oneâ€Dimensional Palladium(II) Arrays. Angewandte Chemie - International Edition, 2021, 60, 10089-10094.	13.8	17
45	Structurally Different Dinuclear Copper(II) Complexes with the Same Triazolopyrimidine Bridging Ligand. European Journal of Inorganic Chemistry, 2002, 2002, 811-818.	2.0	15
46	Structure and theoretical NMR chemical shifts of modified cyclodextrinsâ€. Computational and Theoretical Chemistry, 2004, 672, 127-132.	1.5	15
47	Evidence of an Unexpectedly Long Câ^'C Bond (>2.7 Ã...) in 1,3-Metalladiyne Complexes [Cp₂MCCR]₂(M = Ti, Zr):â€‰ QTAIM and ELF Analyses. Journal of Physical Chemistry A, 2008, 112, 3414-3423.	2.5	15
48	Ab initio molecular study of hydrogen peroxide.. Computational and Theoretical Chemistry, 1998, 433, 181-192.	1.5	14
49	Metalâ€“metal closed-shell interaction in M 2 X 2 (M=Ag, Cu; X=Cl, Br, I) and related compounds [Ag 2 Br 2](PH 3) 3 and [Cu 2 Cl 2](PH 3) 2 : an RHF, MP2 and DFT study. Computational and Theoretical Chemistry, 1999, 493, 249-257.	1.5	14
50	On the Aromaticity and Meisenheimer Rearrangement of Strained Heterocyclic Amine, Phosphine, and Arsine Oxides. Journal of Organic Chemistry, 2000, 65, 8574-8581.	3.2	14
51	The structure and molecular mechanics calculations of the cyclic (1 â†' 2)-Î²-d-glucan secreted by Rhizobium tropici CIAT 899. Journal of Molecular Structure, 1993, 301, 211-226.	3.6	13
52	NMR assignment in regioisomeric hydroquinones. Magnetic Resonance in Chemistry, 2011, 49, 358-365.	1.9	13
53	N, P, and As Ylides and Aza- and Arsa-Wittig Reactions from Topological Analyses of Electron Density. Journal of Physical Chemistry A, 2011, 115, 8316-8326.	2.5	12
54	Insight into the informational-structure behavior of the Diels-Alder reaction of cyclopentadiene and maleic anhydride. Journal of Molecular Modeling, 2014, 20, 2361.	1.8	12

#	Article	IF	Citations
55	On the bonding isomerism in three-co-ordinated copper(I) thiocyanates. Journal of the Chemical Society Dalton Transactions, 1999, , 489-496.	1.1	10
56	Bonding of Atomic Phosphorus to Polycyclic Hydrocarbons and Curved Graphitic Surfaces. Journal of the American Chemical Society, 2003, 125, 2301-2306.	13.7	10
57	Stabilization in neutral bicyclic sulfoxide compounds. Journal of Computational Chemistry, 2000, 21, 322-327.	3.3	9
58	A theoretical investigation on the reactivity of 6-amino-3-methylpyrimidin-4(3H)-ones towards DMAD. Tandem Diels-Alder retro Diels-Alder (DA/RDA) reaction. Tetrahedron, 1996, 52, 13721-13732.	1.9	8
59	Semi-Synthesis of Triterpene A-ring Derivatives from Oleanolic and Maslinic Acids. Theoretical and experimental ¹³C chemical shifts. Journal of Chemical Research, 2000, 2000, 56-57.	1.3	7
60	Conformational Analysis of Thiosugars: Theoretical NMR Chemical Shifts and 3 J H,H Coupling Constants of 5â€Thioâ€Pyranose Monosaccharides. Journal of Carbohydrate Chemistry, 2006, 25, 557-594.	1.1	7
61	Structural Consequences of the N7 and C8 Translocation on the Metal Binding Behavior of Adenine. Inorganic Chemistry, 2013, 52, 1916-1925.	4.0	7
62	Causes of energy destabilization in carbon nanotubes with topological defects. Theoretical Chemistry Accounts, 2011, 128, 445-456.	1.4	6
63	Theoretical Bonding Description of Alkylidene Chalcogen (O, S, Se) Difluorides (H2CXF2):Â Planar versus Bent Conformations. Inorganic Chemistry, 1999, 38, 6257-6260.	4.0	5
64	Theoretical characterization of 5-oxo, 7-oxo and 5-oxo-7-amino[1,2,4]triazolo[1,5-a]pyrimidinesâ€Šâ€. Perkin Transactions II RSC, 2000, , 1675-1680.	1.1	4
65	Comparative Structural Study of Metal-Mediated Base Pairs Formed outside and inside DNA Molecules. Inorganic Chemistry, 2020, 59, 9325-9338.	4.0	3
66	CAL3JHH: a Java program to calculate the vicinal coupling constants (3 J H,H) of organic molecules. Journal of Computer-Aided Molecular Design, 2008, 22, 907-914.	2.9	2
67	A computational study of bulk porous two-dimensional polymers related to graphyne. Physical Chemistry Chemical Physics, 2016, 18, 21305-21314.	2.8	1
68	Multiscale Modeling of Lignocellulosic Biomass. , 2018, , 1-22.		1
69	N-O and P-O Bond Nature in Hypervalent Compounds: is Bader Analysis Basis-Set and Geometry Independent?. , 2000, , 337-353.		1
70	Multiscale Modeling of Lignocellulosic Biomass. , 2020, , 1627-1648.		1
71	Singleâ€Stranded DNA as Supramolecular Template for Oneâ€Dimensional Palladium(II) Arrays. Angewandte Chemie, 2021, 133, 10177-10182.	2.0	0
72	Stabilization in neutral bicyclic sulfoxide compounds. Journal of Computational Chemistry, 2000, 21, 322.	3.3	0