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	Singleâ€Stranded DNA as Supramolecular Template for Oneâ€Dimensional Palladium(II) Arrays. Angewandte Chemie - International Edition, 2021, 60, 10089-10094.	13.8	17
2	Singleâ€Stranded DNA as Supramolecular Template for Oneâ€Dimensional Palladium(II) Arrays. Angewandte Chemie, 2021, 133, 10177-10182.	2.0	0
3	Thread based microfluidic platform for urinary creatinine analysis. Sensors and Actuators B: Chemical, 2020, 305, 127407.	7.8	17
4	Comparative Structural Study of Metal-Mediated Base Pairs Formed outside and inside DNA Molecules. Inorganic Chemistry, 2020, 59, 9325-9338.	4.0	3
5	Multiscale Modeling of Lignocellulosic Biomass. , 2020, , 1627-1648.		1
6	Green and Bio-Based Solvents. Topics in Current Chemistry, 2018, 376, 18.	5.8	143
7	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
8	Multiscale Modeling of Lignocellulosic Biomass. , 2018, , 1-22.		1
9	The role of weak interactions in lignin polymerization. Journal of Molecular Modeling, 2017, 23, 80.	1.8	18
10	A computational study of bulk porous two-dimensional polymers related to graphyne. Physical Chemistry Chemical Physics, 2016, 18, 21305-21314.	2.8	1
11	Designing novel nanoporous architectures of carbon nanotubes for hydrogen storage. International Journal of Hydrogen Energy, 2014, 39, 9825-9829.	7.1	30
12	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
13	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
14	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
15	Structural Consequences of the N7 and C8 Translocation on the Metal Binding Behavior of Adenine. Inorganic Chemistry, 2013, 52, 1916-1925.	4.0	7
16	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
17	Dinuclear silver(i) complexes for the design of metalâ€“ligand networks based on triazolopyrimidines. Dalton Transactions, 2011, 40, 11845.	3.3	42
18	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

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19	Edge effects, electronic arrangement, and aromaticity patterns on finite-length carbon nanotubes. Physical Chemistry Chemical Physics, 2011, 13, 12844.	2.8	18
20	Porous nanotube network: a novel 3-D nanostructured material with enhanced hydrogen storage capacity. Chemical Communications, 2011, 47, 2303-2305.	4.1	55
21	Protecting-Group-Free Synthesis of Chokols. Journal of Organic Chemistry, 2011, 76, 2494-2501.	3.2	27
22	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
23	Causes of energy destabilization in carbon nanotubes with topological defects. Theoretical Chemistry Accounts, 2011, 128, 445-456.	1.4	6
24	NMR assignment in regioisomeric hydroquinones. Magnetic Resonance in Chemistry, 2011, 49, 358-365.	1.9	13
25	Lignin as Renewable Raw Material. ChemSusChem, 2010, 3, 1227-1235.	6.8	785
26	Reversible Attachment of Platinum Alloy Nanoparticles to Nonfunctionalized Carbon Nanotubes. ACS Nano, 2010, 4, 2438-2444.	14.6	31
27	Weakening Câˆ’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
28	CarbonÂ·Â·Â·Carbon Weak Interactions. Journal of Physical Chemistry A, 2009, 113, 8387-8393.	2.5	73
29	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
30	Evidence of an Unexpectedly Long Câˆ’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
31	Clarâˆ’KekulÃ© Structuring in Armchair Carbon Nanotubes. Organic Letters, 2008, 10, 1991-1994.	4.6	26
32	Electrochemically and photochemically active Palladium(ii) heterotopic metallacalix[3]arenes. Chemical Communications, 2008, , 3735.	4.1	19
33	On the Existence of Î±-Agostic Bonds:â€‰ Bonding Analyses of Titanium Alkyl Complexes. Organometallics, 2006, 25, 5638-5647.	2.3	63
34	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
35	On the Nature of Metalâˆ’Carbon Bonding:Â AIM and ELF Analyses of MCHn(n= 1âˆ’3) Compounds Containing Early Transition Metals. Journal of Physical Chemistry A, 2005, 109, 7500-7508.	2.5	60
36	Structure and theoretical NMR chemical shifts of modified cyclodextrinsâ€. Computational and Theoretical Chemistry, 2004, 672, 127-132.	1.5	15

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37	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
38	CoNTub:â€‰ An Algorithm for Connecting Two Arbitrary Carbon Nanotubes. Journal of Chemical Information and Computer Sciences, 2004, 44, 1639-1646.	2.8	110
39	Bonding of Atomic Phosphorus to Polycyclic Hydrocarbons and Curved Graphitic Surfaces. Journal of the American Chemical Society, 2003, 125, 2301-2306.	13.7	10
40	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
41	Structure and bonding of weak hydrogen peroxide complexes. Computational and Theoretical Chemistry, 2002, 580, 117-126.	1.5	25
42	Structurally Different Dinuclear Copper(II) Complexes with the Same Triazolopyrimidine Bridging Ligand. European Journal of Inorganic Chemistry, 2002, 2002, 811-818.	2.0	15
43	Structural and electronic effects of the interaction of metal cations with benzene. Computational and Theoretical Chemistry, 2002, 589-590, 337-347.	1.5	20
44	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
45	Recognizing a triple bond between main group atoms. Theoretical Chemistry Accounts, 2001, 105, 365-373.	1.4	43
46	Stabilization in neutral bicyclic sulfoxide compounds. Journal of Computational Chemistry, 2000, 21, 322-327.	3.3	9
47	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
48	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
49	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
50	Multiple Bonding in Four-Coordinated Titanium(IV) Compounds. Inorganic Chemistry, 2000, 39, 2831-2836.	4.0	30
51	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
52	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
53	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
54	N-O and P-O Bond Nature in Hypervalent Compounds: is Bader Analysis Basis-Set and Geometry Independent?. , 2000, , 337-353.		1

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55	Stabilization in neutral bicyclic sulfoxide compounds. Journal of Computational Chemistry, 2000, 21, 322.	3.3	0
56	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
57	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
58	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
59	On the bonding isomerism in three-co-ordinated copper(I) thiocyanates. Journal of the Chemical Society Dalton Transactions, 1999, , 489-496.	1.1	10
60	Adenineâ‹¯Hydrogen Peroxide System:Â DFT and MP2 Investigation. Journal of Physical Chemistry A, 1999, 103, 4755-4761.	2.5	39
61	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
62	Ab initio molecular study of hydrogen peroxide.. Computational and Theoretical Chemistry, 1998, 433, 181-192.	1.5	14
63	para-Fluoro benzyl substituted bis(indenyl) metallocenes as catalyst precursors in ethene polymerization. Journal of Organometallic Chemistry, 1998, 553, 173-178.	1.8	18
64	Theoretical Study on the Ureaâ‹¯Hydrogen Peroxide 1:1 Complexes. Journal of Physical Chemistry A, 1998, 102, 778-784.	2.5	58
65	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
66	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
67	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
68	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
69	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
70	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
71	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
72	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