JosÃ© A.N.F. Gomes

List of Publications by Year
in descending order

82 papers	2,745 citations	201385 27 h-index	182168 51 g-index
91 all docs	91 docs citations	91 times ranked	2925 citing authors

#	Article	IF	Citations
1	CiÃªncia para todos. Revista De CiÃªncia Elementar, 2016, 4, .	0.0	0
2	PrÃ©mios Nobel 2016. Revista De CiÃªncia Elementar, 2016, 4, .	0.0	0
3	PISA, TIMSS e Rankings. Revista De CiÃªncia Elementar, 2016, 4, .	0.0	0
4	The subtle effect of vdW interactions upon the C60 fullerene structure. Computational and Theoretical Chemistry, 2013, 1026, 12-16.	1.1	5
5	New Parameterization Scheme of DFT-D for Graphitic Materials. Journal of Physical Chemistry A, 2013, 117, 2844-2853.	1.1	13
6	CiÃªncia elementar. Revista De CiÃªncia Elementar, 2013, 1, .	0.0	0
7	New insights into the functionalization of multi-walled carbon nanotubes with aniline derivatives. Carbon, 2012, 50, 3280-3294.	5.4	99
8	Some Comments on Topological Approaches to the Ï€-Electron Currents in Conjugated Systems. Journal of Chemical Theory and Computation, 2011, 7, 3661-3674.	2.3	24
9	A computational analysis of the insertion of carbon nanotubes into cellular membranes. Biomaterials, 2011, 32, 7079-7085.	5.7	53
10	An impact indicator for researchers. Scientometrics, 2011, 89, 607-629.	1.6	13
11	The journal relative impact: an indicator for journal assessment. Scientometrics, 2011, 89, 631-651.	1.6	9
12	Citations to scientific articles: Its distribution and dependence on the article features. Journal of Informetrics, 2010, 4, 1-13.	1.4	137
13	A research impact indicator for institutions. Journal of Informetrics, 2010, 4, 581-590.	1.4	18
14	Structure of the interface between water and self-assembled monolayers of neutral, anionic and cationic alkane thiols. Computational and Theoretical Chemistry, 2010, 946, 83-87.	1.5	10
15	Comparative analysis of the performance of commonly available density functionals in the determination of geometrical parameters for zinc complexes. Journal of Computational Chemistry, 2009, 30, 2752-2763.	1.5	51
16	Molecular dynamics simulations of mouse ferrochelatase variants: what distorts and orientates the porphyrin?. Journal of Biological Inorganic Chemistry, 2009, 14, 1119-1128.	1.1	4
17	A comparison of Scopus and Web of Science for a typical university. Scientometrics, 2009, 81, 587-600.	1.6	340
18	Effect of thetert-butiloxycarbonyl protecting group on the adsorption of protected amino-cyclopentene on the Si(100) surface. Physical Review B, 2007, 75, .	1.1	2

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19	A DFT study of the chemisorption of methoxy on clean and low oxygen precovered Ru(0001) surfaces. Surface Science, 2007, 601, 2473-2485.	0.8	14
20	Microscopic detail provided for the adsorption of protected amino-cyclopentene on Si(100). Chemical Physics Letters, 2007, 448, 111-114.	1.2	0
21	Theoretical study on the structure and conformational features of distally dibromo-dipropoxythiacalix[4]arene derivatives and their Zn2+ complexes. Theoretical Chemistry Accounts, 2007, 117, 431-440.	0.5	6
22	Comparative study on the transition metal complexes of a novel thiacalix[4]arene derivative. Chemical Physics, 2006, 320, 193-206.	0.9	7
23	QM/QM study of the coverage effects on the adsorption of amino-cyclopentene at the Si(100) surface. Journal of Computational Chemistry, 2006, 27, 1892-1897.	1.5	4
24	Comparative study of novel sulfonylcalix[4]arene derivative compounds. Computational and Theoretical Chemistry, 2005, 729, 83-90.	1.5	6
25	Computational study of calix[4]arene derivatives and complexation with Zn2+. Chemical Physics, 2005, 310, 109-122.	0.9	31
26	Comparative Density Functional Theory Study on Thiacalix[4]arene Binding Modes for Zn2+ and Cu2+. Journal of Physical Chemistry A, 2005, 109, 10742-10752.	1.1	12
27	A new strategy to model the Si(100) surface. Comptes Rendus Chimie, 2005, 8, 1461-1468.	0.2	9
28	Adsorption of protected and unprotected amino-cyclopentene at the Si(100) surface modeled with a hybrid quantum mechanical cluster technique. Physical Review B, 2005, 72, .	1.1	6
29	Fermi resonance coupling in the Câ€“H stretching region of methoxide adsorbed on clean Ru(001): a combined RAIRS and theoretical study. Surface Science, 2004, 566-568, 965-970.	0.8	13
30	Structure and conformational equilibrium of new thiacalix[4]arene derivatives. Chemical Physics Letters, 2004, 385, 368-373.	1.2	17
31	Structure and Properties of Hexadecyltrimethylammonium Chloride Monolayers in Contact with Oil Films with Different Thicknesses. Journal of Physical Chemistry B, 2004, 108, 17153-17159.	1.2	2
32	Cluster model DFT study of acetylene adsorption on the Cu (100) surface. Computational and Theoretical Chemistry, 2003, 629, 251-261.	1.5	12
33	Molecular Dynamics Study of a Hexadecyltrimethylammonium Chloride Monolayer at the Interface between Two Immiscible Liquids. Langmuir, 2003, 19, 958-966.	1.6	6
34	Molecular Dynamics Study of the Calcium Ion Transfer across the Water/Nitrobenzene Interface. ChemPhysChem, 2002, 3, 946-951.	1.0	29
35	The adsorption of ethylene on the (110) surfaces of copper, silver and platinum: a DFT study. Computational and Theoretical Chemistry, 2002, 582, 159-169.	1.5	24
36	Aromaticity and Ring Currents. Chemical Reviews, 2001, 101, 1349-1384.	23.0	554

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37	A DFT study of the methanol oxidation catalyzed by a copper surface. Surface Science, 2001, 471, 59-70.	0.8	74
38	A Theoretical Study of the Gas-Phase Pyrolysis of 2-Azidoacetic Acid. Journal of Physical Chemistry A, 2001, 105, 3140-3147.	1.1	18
39	Molecular Simulation of the Interface between Two Immiscible Electrolyte Solutions. Journal of Physical Chemistry B, 2001, 105, 981-993.	1.2	19
40	First-principles study of the adsorption of formaldehyde on the clean and atomic oxygen covered Cu(1) Tj ETQq0 0 0 rgBT /Overlock 10	4.8	40
41	The search for a new model structure of beta-factor XIIa. Journal of Computer-Aided Molecular Design, 2001, 15, 309-322.	1.3	5
42	The adsorption of ethylene on the (100) surfaces of platinum, palladium and nickel: a DFT study. Computational and Theoretical Chemistry, 2001, 542, 263-271.	1.5	44
43	Comparative study of geometry and bonding character for methoxy radical adsorption on noble metals. Computational and Theoretical Chemistry, 2000, 503, 189-200.	1.5	32
44	A theoretical study of dioxymethylene, proposed as intermediate in the oxidation of formaldehyde to formate over copper. Surface Science, 2000, 446, 283-293.	0.8	18
45	Influence of Ion Size and Charge in Ion Transfer Processes Across a Liquid|Liquid Interface. Journal of Physical Chemistry B, 2000, 104, 2278-2286.	1.2	38
46	Parallel Implementation of a Monte Carlo Molecular Simulation Program. Journal of Chemical Information and Computer Sciences, 2000, 40, 588-592.	2.8	6
47	Quantum and simulation studies of Xâ˜(H2O)n systems. Electrochimica Acta, 1999, 45, 659-673.	2.6	39
48	Theoretical study of arginineâ€“carboxylate interactions. Computational and Theoretical Chemistry, 1999, 463, 81-90.	1.5	37
49	A theoretical approach to the adsorption of ions on metal surfaces. Computational and Theoretical Chemistry, 1999, 463, 113-123.	1.5	16
50	Molecular dynamics simulation of the water/1,2-dichloroethane interface. Computational and Theoretical Chemistry, 1999, 463, 151-156.	1.5	13
51	Cluster model study of methoxy radical adsorption on the Cu (111) surface. Computational and Theoretical Chemistry, 1999, 463, 163-168.	1.5	18
52	Simulations of liquid water in contact with a Cu(100) surface. Computational and Theoretical Chemistry, 1999, 464, 227-238.	1.5	11
53	Influence of interionic separation in electron transfer reactions. Computational and Theoretical Chemistry, 1999, 488, 169-178.	1.5	0
54	Adsorption of the formate species on copper surfaces: a DFT study. Surface Science, 1999, 432, 279-290.	0.8	55

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55	Methoxy radical reaction to formaldehyde on clean and hydroxy radical-covered copper (111) surfaces: a density functional theory study. Surface Science, 1999, 443, 165-176.	0.8	29
56	A DFT study of dioxymethylene adsorption on the copper (111) surface. Electrochimica Acta, 1999, 45, 653-658.	2.6	9
57	Molecular Dynamics Simulation of the Water/2-Heptanone Liquid-Liquid Interface. Journal of Physical Chemistry B, 1999, 103, 6290-6299.	1.2	74
58	Molecular Dynamics Study of the Transfer of Iodide across Two Liquid/Liquid Interfaces. Journal of Physical Chemistry B, 1999, 103, 8930-8939.	1.2	50
59	Molecular Dynamics Simulation of Liquid 2-Heptanone, Pure and Saturated with Water. Journal of Physical Chemistry B, 1999, 103, 1176-1184.	1.2	9
60	Density-functional methods for the study of the ground-state vibrations of the guanidinium ion. International Journal of Quantum Chemistry, 1997, 61, 725-739.	1.0	16
61	Interaction of halide ions with copper: the DFT approach. Chemical Physics Letters, 1996, 257, 609-615.	1.2	62
62	Simulation of the electron transfer process Cu2+ + Cu+ â‡Œ Cu+ + Cu2+ in aqueous solution. Computational and Theoretical Chemistry, 1996, 371, 185-190.	1.5	1
63	Light metal ions in water: Quantal and classical simulations for 7Li+. Journal of Molecular Liquids, 1994, 60, 237-249.	2.3	0
64	Ab initiocopper-water interaction potential for the simulation of aqueous solutions. Journal of Computational Chemistry, 1993, 14, 629-638.	1.5	31
65	Simulation of water solutions of Ni2+ at infinite dilution. Chemical Physics, 1993, 176, 97-108.	0.9	18
66	Analysis of the interaction energy in the Cu+-H2O and Cl?-H2O systems, with CP corrections to the BSSE of the separate terms, and MC simulations of the aqueous systems with and without CP corrections. Theoretica Chimica Acta, 1992, 82, 165-187.	0.9	9
67	The number of spanning trees in buckminsterfullerene. Journal of Computational Chemistry, 1991, 12, 1118-1124.	1.5	19
68	The role of many-body interactions in the stability of hydrated Cu2+ clusters. Chemical Physics, 1990, 141, 379-392.	0.9	23
69	The Cu+â€“H2O interaction potential and its application to the study of [Cu(H2O)n]+clusters at different temperatures. Journal of the Chemical Society, Faraday Transactions 2, 1988, 84, 693-704.	1.1	9
70	Classical dynamics of a coupled double well oscillator in condensed media. II. Journal of Chemical Physics, 1984, 80, 1826-1830.	1.2	13
71	Short-time description of chemical reaction by Stochastic methods. International Journal of Quantum Chemistry, 1983, 23, 473-476.	1.0	3
72	Topology of the electronic current density in molecules. Physical Review A, 1983, 28, 559-566.	1.0	53

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73	Physics, 1983, 79, 3320-3327.	1.2	24
74	Topological elements of the magnetically induced orbital current densities. Journal of Chemical Physics, 1983, 78, 4585-4591.	1.2	59
75	Delocalized magnetic currents in benzene. Journal of Chemical Physics, 1983, 78, 3133-3139.	1.2	26
76	Topological theory of the electronic currents in benzene. Molecular Physics, 1982, 47, 1227-1230.	0.8	7
77	Calculated magnetic properties of some isomers of pyracylene. Journal of Organic Chemistry, 1981, 46, 719-727.	1.7	34
78	Theory for a general system of increments for the properties of polycyclic hydrocarbons. Theoretica Chimica Acta, 1981, 59, 333-356.	0.9	27
79	On the use of the ring current concept. Molecular Physics, 1980, 40, 765-769.	0.8	41
80	Charge and current densities for approximate molecular wavefunctions. Molecular Physics, 1976, 32, 1063-1074.	0.8	18
81	The optical activity of methane. Chemical Physics Letters, 1976, 39, 519-520.	1.2	25
82	Ring magnetic susceptibilities in conjugated hydrocarbons. Molecular Physics, 1975, 30, 713-732.	0.8	43