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List of Publications by Year in descending order

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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	Aromaticity and Ring Currents. <i>Chemical Reviews</i> , 2001, 101, 1349-1384.	23.0	554
2	A comparison of Scopus and Web of Science for a typical university. <i>Scientometrics</i> , 2009, 81, 587-600.	1.6	340
3	Citations to scientific articles: Its distribution and dependence on the article features. <i>Journal of Informetrics</i> , 2010, 4, 1-13.	1.4	137
4	New insights into the functionalization of multi-walled carbon nanotubes with aniline derivatives. <i>Carbon</i> , 2012, 50, 3280-3294.	5.4	99
5	Molecular Dynamics Simulation of the Water/2-Heptanone Liquid-Liquid Interface. <i>Journal of Physical Chemistry B</i> , 1999, 103, 6290-6299.	1.2	74
6	A DFT study of the methanol oxidation catalyzed by a copper surface. <i>Surface Science</i> , 2001, 471, 59-70.	0.8	74
7	Interaction of halide ions with copper: the DFT approach. <i>Chemical Physics Letters</i> , 1996, 257, 609-615.	1.2	62
8	Topological elements of the magnetically induced orbital current densities. <i>Journal of Chemical Physics</i> , 1983, 78, 4585-4591.	1.2	59
9	Adsorption of the formate species on copper surfaces: a DFT study. <i>Surface Science</i> , 1999, 432, 279-290.	0.8	55
10	Topology of the electronic current density in molecules. <i>Physical Review A</i> , 1983, 28, 559-566.	1.0	53
11	A computational analysis of the insertion of carbon nanotubes into cellular membranes. <i>Biomaterials</i> , 2011, 32, 7079-7085.	5.7	53
12	Comparative analysis of the performance of commonly available density functionals in the determination of geometrical parameters for zinc complexes. <i>Journal of Computational Chemistry</i> , 2009, 30, 2752-2763.	1.5	51
13	Molecular Dynamics Study of the Transfer of Iodide across Two Liquid/Liquid Interfaces. <i>Journal of Physical Chemistry B</i> , 1999, 103, 8930-8939.	1.2	50
14	The adsorption of ethylene on the (100) surfaces of platinum, palladium and nickel: a DFT study. <i>Computational and Theoretical Chemistry</i> , 2001, 542, 263-271.	1.5	44
15	Ring magnetic susceptibilities in conjugated hydrocarbons. <i>Molecular Physics</i> , 1975, 30, 713-732.	0.8	43
16	On the use of the ring current concept. <i>Molecular Physics</i> , 1980, 40, 765-769.	0.8	41
17	First-principles study of the adsorption of formaldehyde on the clean and atomic oxygen covered Cu(111) surface. <i>Journal of Chemical Physics</i> , 2004, 120, 7843-7854.	4.8	46
18	Quantum and simulation studies of X ²⁺ (H ₂ O) _n systems. <i>Electrochimica Acta</i> , 1999, 45, 659-673.	2.6	39

#	ARTICLE	IF	CITATIONS
19	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
20	Theoretical study of arginine-carboxylate interactions. Computational and Theoretical Chemistry, 1999, 463, 81-90.	1.5	37
21	Calculated magnetic properties of some isomers of pyracylene. Journal of Organic Chemistry, 1981, 46, 719-727.	1.7	34
22	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
23	Ab initio copper-water interaction potential for the simulation of aqueous solutions. Journal of Computational Chemistry, 1993, 14, 629-638.	1.5	31
24	Computational study of calix[4]arene derivatives and complexation with Zn ²⁺ . Chemical Physics, 2005, 310, 109-122.	0.9	31
25	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
26	Molecular Dynamics Study of the Calcium Ion Transfer across the Water/Nitrobenzene Interface. ChemPhysChem, 2002, 3, 946-951.	1.0	29
27	Theory for a general system of increments for the properties of polycyclic hydrocarbons. Theoretica Chimica Acta, 1981, 59, 333-356.	0.9	27
28	Delocalized magnetic currents in benzene. Journal of Chemical Physics, 1983, 78, 3133-3139.	1.2	26
29	The optical activity of methane. Chemical Physics Letters, 1976, 39, 519-520.	1.2	25
30	Physics, 1983, 79, 3320-3327.	1.2	24
31	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
32	Some Comments on Topological Approaches to the π -Electron Currents in Conjugated Systems. Journal of Chemical Theory and Computation, 2011, 7, 3661-3674.	2.3	24
33	The role of many-body interactions in the stability of hydrated Cu ²⁺ clusters. Chemical Physics, 1990, 141, 379-392.	0.9	23
34	The number of spanning trees in buckminsterfullerene. Journal of Computational Chemistry, 1991, 12, 1118-1124.	1.5	19
35	Molecular Simulation of the Interface between Two Immiscible Electrolyte Solutions. Journal of Physical Chemistry B, 2001, 105, 981-993.	1.2	19
36	Charge and current densities for approximate molecular wavefunctions. Molecular Physics, 1976, 32, 1063-1074.	0.8	18

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37	Simulation of water solutions of Ni ²⁺ at infinite dilution. <i>Chemical Physics</i> , 1993, 176, 97-108.	0.9	18
38	Cluster model study of methoxy radical adsorption on the Cu (111) surface. <i>Computational and Theoretical Chemistry</i> , 1999, 463, 163-168.	1.5	18
39	A theoretical study of dioxymethylene, proposed as intermediate in the oxidation of formaldehyde to formate over copper. <i>Surface Science</i> , 2000, 446, 283-293.	0.8	18
40	A Theoretical Study of the Gas-Phase Pyrolysis of 2-Azidoacetic Acid. <i>Journal of Physical Chemistry A</i> , 2001, 105, 3140-3147.	1.1	18
41	A research impact indicator for institutions. <i>Journal of Informetrics</i> , 2010, 4, 581-590.	1.4	18
42	Structure and conformational equilibrium of new thiacalix[4]arene derivatives. <i>Chemical Physics Letters</i> , 2004, 385, 368-373.	1.2	17
43	Density-functional methods for the study of the ground-state vibrations of the guanidinium ion. <i>International Journal of Quantum Chemistry</i> , 1997, 61, 725-739.	1.0	16
44	A theoretical approach to the adsorption of ions on metal surfaces. <i>Computational and Theoretical Chemistry</i> , 1999, 463, 113-123.	1.5	16
45	A DFT study of the chemisorption of methoxy on clean and low oxygen precovered Ru(0001) surfaces. <i>Surface Science</i> , 2007, 601, 2473-2485.	0.8	14
46	Classical dynamics of a coupled double well oscillator in condensed media. II. <i>Journal of Chemical Physics</i> , 1984, 80, 1826-1830.	1.2	13
47	Molecular dynamics simulation of the water/1,2-dichloroethane interface. <i>Computational and Theoretical Chemistry</i> , 1999, 463, 151-156.	1.5	13
48	Fermi resonance coupling in the C-H stretching region of methoxide adsorbed on clean Ru(001): a combined RAIRS and theoretical study. <i>Surface Science</i> , 2004, 566-568, 965-970.	0.8	13
49	An impact indicator for researchers. <i>Scientometrics</i> , 2011, 89, 607-629.	1.6	13
50	New Parameterization Scheme of DFT-D for Graphitic Materials. <i>Journal of Physical Chemistry A</i> , 2013, 117, 2844-2853.	1.1	13
51	Cluster model DFT study of acetylene adsorption on the Cu (100) surface. <i>Computational and Theoretical Chemistry</i> , 2003, 629, 251-261.	1.5	12
52	Comparative Density Functional Theory Study on Thiacalix[4]arene Binding Modes for Zn ²⁺ and Cu ²⁺ . <i>Journal of Physical Chemistry A</i> , 2005, 109, 10742-10752.	1.1	12
53	Simulations of liquid water in contact with a Cu(100) surface. <i>Computational and Theoretical Chemistry</i> , 1999, 464, 227-238.	1.5	11
54	Structure of the interface between water and self-assembled monolayers of neutral, anionic and cationic alkane thiols. <i>Computational and Theoretical Chemistry</i> , 2010, 946, 83-87.	1.5	10

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55	The Cu+H ₂ O interaction potential and its application to the study of [Cu(H ₂ O) _n] ⁺ clusters at different temperatures. <i>Journal of the Chemical Society, Faraday Transactions 2</i> , 1988, 84, 693-704.	1.1	9
56	Analysis of the interaction energy in the Cu ⁺ -H ₂ O and Cl ⁻ -H ₂ O systems, with CP corrections to the BSSE of the separate terms, and MC simulations of the aqueous systems with and without CP corrections. <i>Theoretica Chimica Acta</i> , 1992, 82, 165-187.	0.9	9
57	A DFT study of dioxymethylene adsorption on the copper (111) surface. <i>Electrochimica Acta</i> , 1999, 45, 653-658.	2.6	9
58	Molecular Dynamics Simulation of Liquid 2-Heptanone, Pure and Saturated with Water. <i>Journal of Physical Chemistry B</i> , 1999, 103, 1176-1184.	1.2	9
59	A new strategy to model the Si(100) surface. <i>Comptes Rendus Chimie</i> , 2005, 8, 1461-1468.	0.2	9
60	The journal relative impact: an indicator for journal assessment. <i>Scientometrics</i> , 2011, 89, 631-651.	1.6	9
61	Topological theory of the electronic currents in benzene. <i>Molecular Physics</i> , 1982, 47, 1227-1230.	0.8	7
62	Comparative study on the transition metal complexes of a novel thiacalix[4]arene derivative. <i>Chemical Physics</i> , 2006, 320, 193-206.	0.9	7
63	Parallel Implementation of a Monte Carlo Molecular Simulation Program. <i>Journal of Chemical Information and Computer Sciences</i> , 2000, 40, 588-592.	2.8	6
64	Molecular Dynamics Study of a Hexadecyltrimethylammonium Chloride Monolayer at the Interface between Two Immiscible Liquids. <i>Langmuir</i> , 2003, 19, 958-966.	1.6	6
65	Comparative study of novel sulfonylcalix[4]arene derivative compounds. <i>Computational and Theoretical Chemistry</i> , 2005, 729, 83-90.	1.5	6
66	Adsorption of protected and unprotected amino-cyclopentene at the Si(100) surface modeled with a hybrid quantum mechanical cluster technique. <i>Physical Review B</i> , 2005, 72, .	1.1	6
67	Theoretical study on the structure and conformational features of distally dibromo-dipropoxythiacalix[4]arene derivatives and their Zn ²⁺ complexes. <i>Theoretical Chemistry Accounts</i> , 2007, 117, 431-440.	0.5	6
68	The search for a new model structure of beta-factor XIIIa. <i>Journal of Computer-Aided Molecular Design</i> , 2001, 15, 309-322.	1.3	5
69	The subtle effect of vdW interactions upon the C60 fullerene structure. <i>Computational and Theoretical Chemistry</i> , 2013, 1026, 12-16.	1.1	5
70	QM/QM study of the coverage effects on the adsorption of amino-cyclopentene at the Si(100) surface. <i>Journal of Computational Chemistry</i> , 2006, 27, 1892-1897.	1.5	4
71	Molecular dynamics simulations of mouse ferrochelatase variants: what distorts and orientates the porphyrin?. <i>Journal of Biological Inorganic Chemistry</i> , 2009, 14, 1119-1128.	1.1	4
72	Short-time description of chemical reaction by Stochastic methods. <i>International Journal of Quantum Chemistry</i> , 1983, 23, 473-476.	1.0	3

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73	Structure and Properties of Hexadecyltrimethylammonium Chloride Monolayers in Contact with Oil Films with Different Thicknesses. <i>Journal of Physical Chemistry B</i> , 2004, 108, 17153-17159.	1.2	2
74	Effect of the tert-butoxycarbonyl protecting group on the adsorption of protected amino-cyclopentene on the Si(100) surface. <i>Physical Review B</i> , 2007, 75, .	1.1	2
75	Simulation of the electron transfer process $Cu^{2+} + Cu^+ \rightleftharpoons Cu^+ + Cu^{2+}$ in aqueous solution. <i>Computational and Theoretical Chemistry</i> , 1996, 371, 185-190.	1.5	1
76	Light metal ions in water: Quantal and classical simulations for $7Li^+$. <i>Journal of Molecular Liquids</i> , 1994, 60, 237-249.	2.3	0
77	Influence of interionic separation in electron transfer reactions. <i>Computational and Theoretical Chemistry</i> , 1999, 488, 169-178.	1.5	0
78	Microscopic detail provided for the adsorption of protected amino-cyclopentene on Si(100). <i>Chemical Physics Letters</i> , 2007, 448, 111-114.	1.2	0
79	Ciência elementar. <i>Revista De Ciência Elementar</i> , 2013, 1, .	0.0	0
80	Ciência para todos. <i>Revista De Ciência Elementar</i> , 2016, 4, .	0.0	0
81	Prêmios Nobel 2016. <i>Revista De Ciência Elementar</i> , 2016, 4, .	0.0	0
82	PISA, TIMSS e Rankings. <i>Revista De Ciência Elementar</i> , 2016, 4, .	0.0	0