Rogerio Custodio

List of Publications by Year
in descending order

94	1,085	430874 18	501196 28
papers	citations	h-index	g-index

98	98	98	1057
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Periodic study on the structural and electronic properties of bulk, oxidized and reduced SnO 2 (1 1 0) surfaces and the interaction with O 2. Surface Science, 2002, 511, 408-420.	1.9	100
2	Electronic and structural properties of SnxTi1â˜'xO2 solid solutions: a periodic DFT study. Catalysis Today, 2003, 85, 145-152.	4.4	71
3	Regioselectivity of the nitration of phenol by acetyl nitrate adsorbed on silica gel. Tetrahedron, 1999, 55, 6733-6738.	1.9	61
4	Simultaneous electroanalytical determination of hydroquinone and catechol in the presence of resorcinol at an SiO₂/C electrode spin-coated with a thin film of Nb₂O₅. Analyst, The, 2013, 138, 315-324.	3.5	55
5	Application of an optimization technique to the discretized version of the Griffin-Hill-Wheeler-Hartree-Fock equations. International Journal of Quantum Chemistry, 1992, 42, 411-423.	2.0	41
6	On the Accuracy of the Direct Method to Calculate pK_a from Electronic Structure Calculations. Journal of Physical Chemistry A, 2021, 125, 65-73.	2.5	39
7	The application of an optimization technique to the development of universal basis sets. Canadian Journal of Chemistry, 1992, 70, 580-588.	1.1	33
8	Molecular Structure of the Molybdenum Oxo-Diperoxo Compound MoO(O2)2(OPy)(H2O):Â A Computational and X-ray Study. Inorganic Chemistry, 2001, 40, 6022-6025.	4.0	28
9	Theoretical studies of Nile Red by ab initio and semiempirical methods. Chemical Physics Letters, 1999, 302, 505-510.	2.6	26
10	Electroactive Properties of 1-propyl-3-methylimidazolium Ionic Liquid Covalently Bonded on Mesoporous Silica Surface: Development of an Electrochemical Sensor Probed for NADH, Dopamine and Uric Acid Detection. Electrochimica Acta, 2014, 123, 435-440.	5.2	26
11	Sulfide and Sulfoxide Oxidations by Mono- and Diperoxo Complexes of Molybdenum. A Density Functional Study. Journal of Organic Chemistry, 2003, 68, 5870-5874.	3.2	24
12	Implementation of pseudopotential in the G3 theory for molecules containing first-, second-, and non-transition third-row atoms. Journal of Chemical Physics, 2011, 135, 034106.	3.0	24
13	Electrical field effects on dipole moment, structure and energetic of (H2O)n (2â©½nâ©½15) cluster. Computational and Theoretical Chemistry, 2009, 915, 170-177.	1.5	21
14	G4CEP: A G4 theory modification by including pseudopotential for molecules containing first-, second- and third-row representative elements. Journal of Chemical Physics, 2016, 144, 204118.	3.0	21
15	Infrared Vibrational Intensities, Polar Tensors, and Core Electron Energies of the Group IV Hydrides and the Fluorosilanes. Journal of Physical Chemistry A, 1998, 102, 4615-4622.	2.5	20
16	Why Do Peroxomolybdenum Complexes Chemoselectively Oxidize the Sulfur Centers of Unsaturated Sulfides and Sulfoxides? A DFT Analysis. European Journal of Organic Chemistry, 2005, 2005, 2406-2415.	2.4	20
17	A theoretical study of isomeric C6H4Brâ˜' ions. Chemical Physics Letters, 1995, 235, 436-443.	2.6	19
18	A universal basis set to be used along with pseudopotentials. Chemical Physics Letters, 1997, 279, 396-402.	2.6	18

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19	Assessment of G3(MP2)//B3 theory including a pseudopotential for molecules containing first-, second-, and third-row representative elements. Journal of Chemical Physics, 2013, 139, 184108.	3.0	17
20	A study of the rotational barriers for some organic compounds using the G3 and G3CEP theories. Journal of Molecular Modeling, 2014, 20, 2199.	1.8	17
21	Can the linear combination of atomic orbital coefficients (the weight function) be used to improve the wavefunction?. Computational and Theoretical Chemistry, 1993, 281, 75-87.	1.5	16
22	Double ionization energies of HCl, HBr, Cl2 and Br2 molecules: An MRCI study. Chemical Physics Letters, 2011, 506, 22-25.	2.6	13
23	W1CEP theory for computational thermochemistry. Computational and Theoretical Chemistry, 2015, 1067, 84-92.	2.5	13
24	On the improvement of geometric basis sets. Computational and Theoretical Chemistry, 1992, 277, 263-277.	1.5	12
25	A theoretical and spectroscopic study of conformational structures of piroxicam. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2010, 75, 901-907.	3.9	12
26	Empirical corrections in the G3X and G3X(CCSD) theories combined with a compact effective pseudopotential. Theoretical Chemistry Accounts, 2018, 137, 1.	1.4	12
27	Theoretical investigation of the conformational behaviour of 3-monosubstituted 2-methylpropenes. Computational and Theoretical Chemistry, 2003, 637, 43-54.	1.5	11
28	Investigation of the Nile Red spectra by semi-empirical calculations and spectrophotometric measurements. International Journal of Quantum Chemistry, 2006, 106, 2624-2632.	2.0	11
29	Uma abordagem simplificada do mÃ©todo Monte Carlo QuÃ¢ntico: da soluÃ§Ã£o de integrais ao problema da distribuiÃ§Ã£o eletrÃ´nica. Quimica Nova, 2008, 31, 433-444.	0.3	11
30	O ajuste de funÃ§Ãµes matemÃ¡ticas a dados experimentais. Quimica Nova, 1997, 20, 219-225.	0.3	11
31	Influence of polarization functions on atomic properties of bridge N and H atoms of HCN â€¦ HCN. Computational and Theoretical Chemistry, 1995, 335, 11-23.	1.5	10
32	Pyrrolizidine alkaloids necine bases:Ab initio, semiempirical, and molecular mechanics approaches to molecular properties. Journal of Computational Chemistry, 1996, 17, 156-166.	3.3	10
33	The use of the generator coordinate method for designing basis set. Application to oxo-diperoxo molybdenum complexes. Computational and Theoretical Chemistry, 2002, 589-590, 251-264.	1.5	10
34	Accurate calculation of C1s core electron binding energies of some carbon hydrates and substituted benzenes. Computational and Theoretical Chemistry, 2010, 959, 106-112.	1.5	10
35	Design of a New Molecularly Imprinted Polymer Selective for Hydrochlorothiazide Based on Theoretical Predictions Using Gibbs Free Energy. Journal of the Brazilian Chemical Society, 2016, , .	0.6	10
36	Assessment of pK_a Determination for Monocarboxylic Acids with an Accurate Theoretical Composite Method: G4CEP. Journal of Physical Chemistry A, 2019, 123, 8314-8320.	2.5	10

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37	Reliable Hellmann-Feynman forces for nuclei-centeredGTO basis of standard size. International Journal of Quantum Chemistry, 1992, 44, 311-318.	2.0	9
38	Polycarbonitrile: A semiempirical, ab initio and density functional study of molecular stability. Synthetic Metals, 1997, 85, 1127-1128.	3.9	9
39	Basis set modeling for molecular calculations using effective core potential. Journal of Computational Chemistry, 1997, 18, 1918-1929.	3.3	9
40	Valence basis sets for tellurium: Weight functions as a basis set development tool and initial molecular applications. Computational and Theoretical Chemistry, 1994, 315, 163-172.	1.5	8
41	The correlation of proton affinities with atomic charges and electronegativities for the group 14 to 17 hydrides. Journal of Computational Chemistry, 2000, 21, 1119-1131.	3.3	8
42	Exact Gaussian expansions of Slater-type atomic orbitals. Journal of Computational Chemistry, 2002, 23, 1007-1012.	3.3	8
43	Evaluations of the BET, I-Point, and Î±-Plot Procedures for the Routine Determination of External Specific Surface Areas of Highly Dispersed and Porous Silicas. Langmuir, 2011, 27, 187-195.	3.5	8
44	G3(MP2)-CEP theory and applications for compounds containing atoms from representative first, second and third row elements of the periodic table. Journal of Molecular Modeling, 2015, 21, 204.	1.8	8
45	Partial combination of composite strategy and the B3LYP functional for the calculation of enthalpies of formation. Journal of Molecular Modeling, 2019, 25, 62.	1.8	8
46	Pheâ€“Phe Di-Peptide Nanostructure Self-Assembling Modulated by Luminescent Additives. ACS Omega, 2019, 4, 606-619.	3.5	8
47	Koopmans' approximation applied in atoms and diatomic molecules using the diffusion quantum Monte Carlo method. International Journal of Quantum Chemistry, 2008, 108, 2459-2466.	2.0	7
48	Exploring the G3 method in the study of rotational barrier of some simple molecules. International Journal of Quantum Chemistry, 2010, 110, 2006-2014.	2.0	7
49	An interpretation of the phenol nitration mechanism in the gas phase using G3(MP2)//B3-CEP theory. Journal of Molecular Modeling, 2014, 20, 2524.	1.8	7
50	An energetic analysis of the Diels-Alder endo:exo selectivity reaction by using composite methods. Computational and Theoretical Chemistry, 2018, 1123, 161-168.	2.5	7
51	G3(MP2)//B3-SBK: A revision of a composite theory for calculations of thermochemical properties including some non-transition elements beyond the fourth period. Computational and Theoretical Chemistry, 2019, 1149, 1-7.	2.5	7
52	Assessment of a composite method based on selected density functional theory methods and complete basis set extrapolation formulas. International Journal of Quantum Chemistry, 2019, 119, e25892.	2.0	6
53	The reduction mechanism at the mercury electrode in neutral and alkaline aqueous media of an hydroxytriphenylmethane dye: Eriochrome Azurol B. Journal of Electroanalytical Chemistry and Interfacial Electrochemistry, 1982, 139, 143-156.	0.1	5
54	Systematic Sequences of Geometric Relativistic Basis Sets. I:s- and p-Block Elements up to Xe. Theoretical Chemistry Accounts, 2006, 115, 398-409.	1.4	5

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55	A Novel Computational Approach for Development of Highly Selective Fenitrothion Imprinted Polymer: Theoretical Predictions and Experimental Validations. Journal of the Brazilian Chemical Society, 2014, , .	0.6	5
56	A method for the determination of the Hartree-Fock limit: application to closed-shell atoms. Computational and Theoretical Chemistry, 1997, 394, 95-100.	1.5	4
57	A CONVENIENT PREPARATION OF 1,2,3,4,5,6,7,8-OCTAHYDRO-NAPHTHALENE SKELETON. SYNTHESIS OF (Â±)-ISOCARIDIENE. Synthetic Communications, 2002, 32, 1393-1399.	2.1	4
58	Comments on the quantum Monte Carlo method and the density matrix theory. Journal of Chemical Physics, 2003, 118, 4781-4783.	3.0	4
59	Analysis of the segmented contraction of basis functions using density matrix theory. Journal of Computational Chemistry, 2006, 27, 1822-1829.	3.3	4
60	The Auger spectra and the calculation of double-ionization potentials for H2O and NH3 using the Diffusion Quantum Monte Carlo method. Chemical Physics Letters, 2009, 482, 148-152.	2.6	4
61	Resolvendo a equaÃ§Ã£o de SchrÃ¶dinger utilizando procedimentos numÃ©ricos fundamentais. Quimica Nova, 2012, 35, 2076-2082.	0.3	4
62	Theoretical study of the internal rotational barriers of fluorine, chlorine, bromine, and iodine-substituted ethanes. Computational and Theoretical Chemistry, 2019, 1166, 112589.	2.5	4
63	On the improvement of compact basis sets by approximated integral transforms. Computational and Theoretical Chemistry, 2001, 539, 17-27.	1.5	3
64	Quatro alternativas para resolver a equaÃ§Ã£o de SchrÃ¶dinger para o Ã¡tomo de hidrogÃªnio. Quimica Nova, 2002, 25, 159-170.	0.3	3
65	An Investigation of Chlorophenol Proton Affinities and Their Influence on the Biological Activity of Microorganisms. Journal of Physical Chemistry A, 2006, 110, 2021-2026.	2.5	3
66	Substituent effect in n-hexanes and n-hexatrienes based on core-electron binding energies calculated with density-functional theory. Computational and Theoretical Chemistry, 2009, 916, 119-124.	1.5	3
67	Determination of Enthalpies of Formation of Fatty Acids and Esters by Density Functional Theory Calculations with an Empirical Correction. Industrial & Engineering Chemistry Research, 2015, 54, 9545-9549.	3.7	3
68	MecÃ¢nica QuÃ¢ntica. Revista Chemkeys, 0, 3, e021001.	0.0	3
69	The virial theorem as an entail for Koopmans' theorem in atomic calculations. Theoretica Chimica Acta, 1985, 67, 307-313.	0.8	2
70	An electron transfer mechanism of O4 formation. Chemical Physics Letters, 2003, 370, 789-794.	2.6	2
71	Conformational isomerism and electronic interactions in some Î±-aminoketones. Computational and Theoretical Chemistry, 2006, 766, 177-183.	1.5	2
72	Theoretical investigation of the reducing capacity of sodium borohydride and sodium acetoxyborohydride derivatives. Computational and Theoretical Chemistry, 2007, 802, 11-16.	1.5	2

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73	An investigation of the electronic structure of some 3-monosubstituted-2-methylpropenes through computational chemistry and photoelectron spectroscopy. Chemical Physics, 2008, 349, 263-268.	1.9	2
74	Assessment of a numeric variational method for the solution of confined multielectron atoms. Journal of Molecular Modeling, 2021, 27, 212.	1.8	2
75	On the role of vibrational selective scaling for the calculation of enthalpies of formation using a composite method. Theoretical Chemistry Accounts, 2020, 139, 1.	1.4	2
76	An application of the virial theorem to study AH2 structures II. Use of CNDO/2 wavefunctions. Theoretica Chimica Acta, 1985, 67, 413-424.	0.8	1
77	A modification of Koopmans' theorem by imposition of the virial theorem in molecules. Theoretica Chimica Acta, 1987, 72, 197-205.	0.8	1
78	Hartreeâ€“Fock and density functional theory analysis of propylene insertion in Al(CH3)3/TiCl3/TiO2 (red.) in the presence of a Lewis base. Journal of Molecular Catalysis A, 1999, 146, 191-198.	4.8	1
79	Polynomial expansion of basis sets: Alternatives to fully optimized exponents. Computational and Theoretical Chemistry, 2006, 760, 39-44.	1.5	1
80	Comparative study of BxNyCz nanojunctions fragments. Materials Research, 2011, 14, 281-286.	1.3	1
81	Fully Anharmonic Vibrational Resonance Raman Spectrum of Diatomic Systems. Journal of Chemical Theory and Computation, 2018, 14, 843-855.	5.3	1
82	A grid-based variational method to the solution of the SchrÃ¶dinger equation: the q-exponential and the near Hartree-Fock results for the ground state atomic energies. Journal of Molecular Modeling, 2018, 24, 188.	1.8	1
83	Systematic Convergence of the Numerical Taylor Series to the Best Standard and Its Potential Implication for the Development of Composite Methods. Journal of Chemical Theory and Computation, 2021, 17, 2231-2243.	5.3	1
84	The Structures ofEandZMethyl Octa-6-ene-2,4-Diynoate by Total Synthesis and NMR. Journal of the Brazilian Chemical Society, 1995, 6, 361-364.	0.6	1
85	Reply to the â€œComment on â€˜On the Accuracy of the Direct Method to Calculate pK_a from Electronic Structure Calculationsâ€™â€•. Journal of Physical Chemistry A, 2022, 126, 650-651.	2.5	1
86	Micro-determination of long-chain fatty acids in plasma and tissues by photometric titration. Analyst, The, 1980, 105, 1127.	3.5	0
87	Preface proceedings of the XII Brazilian Symposium of Theoretical Chemistry. International Journal of Quantum Chemistry, 2005, 103, 471-471.	2.0	0
88	Photoluminescence of Solvent-Selected Fluorescent Moieties in MEH-PPV Solutions and Films. Journal of the Brazilian Chemical Society, 2017, , .	0.6	0
89	Redes neurais para regressÃ£o uni- e multivariada. Revista Chemkeys, 0, 3, e021003.	0.0	0
90	Title is missing!. Journal of Computational Chemistry, 1997, 18, 1918.	3.3	0

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91	A SIMPLIFIED ROUTE TO OBTAIN THE HARTREE AND HARTREE-FOCK EQUATIONS. Quimica Nova, 2015, , .	0.3	0
92	Algoritmos para o mÃ©todo Monte Carlo quÃ¢ntico: o ajuste variacional. , 2018, , 64-97.		0
93	Polycarbonitrile: an evaluation using electronic structure methods to analyze their respective electronic and structural stability. , 0, , .		0
94	A partÃcula na caixa. Revista Chemkeys, 0, 3, e021004.	0.0	0