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	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
2	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
3	Assessment of a numeric variational method for the solution of confined multielectron atoms. Journal of Molecular Modeling, 2021, 27, 212.	1.8	2
4	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
5	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
6	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
7	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
8	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
9	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
10	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
11	Pheâ€“Phe Di-Peptide Nanostructure Self-Assembling Modulated by Luminescent Additives. ACS Omega, 2019, 4, 606-619.	3.5	8
12	Empirical corrections in the G3X and G3X(CCSD) theories combined with a compact effective pseudopotential. Theoretical Chemistry Accounts, 2018, 137, 1.	1.4	12
13	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
14	Fully Anharmonic Vibrational Resonance Raman Spectrum of Diatomic Systems. Journal of Chemical Theory and Computation, 2018, 14, 843-855.	5.3	1
15	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
16	Algoritmos para o mÃ©todo Monte Carlo quÃ¢ntico: o ajuste variacional. , 2018, , 64-97.		0
17	Photoluminescence of Solvent-Selected Fluorescent Moieties in MEH-PPV Solutions and Films. Journal of the Brazilian Chemical Society, 2017, , .	0.6	0
18	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

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19	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
20	W1CEP theory for computational thermochemistry. Computational and Theoretical Chemistry, 2015, 1067, 84-92.	2.5	13
21	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
22	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
23	A SIMPLIFIED ROUTE TO OBTAIN THE HARTREE AND HARTREE-FOCK EQUATIONS. Quimica Nova, 2015, , .	0.3	0
24	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
25	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
26	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
27	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
28	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
29	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
30	Resolvendo a equaÃ§Ã£o de SchrÃ¶dinger utilizando procedimentos numÃ©ricos fundamentais. Quimica Nova, 2012, 35, 2076-2082.	0.3	4
31	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
32	Comparative study of BxNyCz nanojunctions fragments. Materials Research, 2011, 14, 281-286.	1.3	1
33	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
34	Double ionization energies of HCl, HBr, Cl2 and Br2 molecules: An MRCI study. Chemical Physics Letters, 2011, 506, 22-25.	2.6	13
35	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
36	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

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37	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
38	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
39	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
40	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
41	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
42	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
43	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
44	Theoretical investigation of the reducing capacity of sodium borohydride and sodium acetoxyborohydride derivatives. Computational and Theoretical Chemistry, 2007, 802, 11-16.	1.5	2
45	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
46	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
47	Polynomial expansion of basis sets: Alternatives to fully optimized exponents. Computational and Theoretical Chemistry, 2006, 760, 39-44.	1.5	1
48	Conformational isomerism and electronic interactions in some Î±-aminoketones. Computational and Theoretical Chemistry, 2006, 766, 177-183.	1.5	2
49	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
50	Analysis of the segmented contraction of basis functions using density matrix theory. Journal of Computational Chemistry, 2006, 27, 1822-1829.	3.3	4
51	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
52	Preface proceedings of the XII Brazilian Symposium of Theoretical Chemistry. International Journal of Quantum Chemistry, 2005, 103, 471-471.	2.0	0
53	An electron transfer mechanism of O4 formation. Chemical Physics Letters, 2003, 370, 789-794.	2.6	2
54	Theoretical investigation of the conformational behaviour of 3-monosubstituted 2-methylpropenes. Computational and Theoretical Chemistry, 2003, 637, 43-54.	1.5	11

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55	Electronic and structural properties of SnxTi1âˆ’xO2 solid solutions: a periodic DFT study. Catalysis Today, 2003, 85, 145-152.	4.4	71
56	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
57	Comments on the quantum Monte Carlo method and the density matrix theory. Journal of Chemical Physics, 2003, 118, 4781-4783.	3.0	4
58	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
59	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
60	Exact Gaussian expansions of Slater-type atomic orbitals. Journal of Computational Chemistry, 2002, 23, 1007-1012.	3.3	8
61	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
62	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
63	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
64	On the improvement of compact basis sets by approximated integral transforms. Computational and Theoretical Chemistry, 2001, 539, 17-27.	1.5	3
65	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
66	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
67	Regioselectivity of the nitration of phenol by acetyl nitrate adsorbed on silica gel. Tetrahedron, 1999, 55, 6733-6738.	1.9	61
68	Theoretical studies of Nile Red by ab initio and semiempirical methods. Chemical Physics Letters, 1999, 302, 505-510.	2.6	26
69	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
70	Polycarbonitrile: A semiempirical, ab initio and density functional study of molecular stability. Synthetic Metals, 1997, 85, 1127-1128.	3.9	9
71	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
72	Basis set modeling for molecular calculations using effective core potential. Journal of Computational Chemistry, 1997, 18, 1918-1929.	3.3	9

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73	A universal basis set to be used along with pseudopotentials. Chemical Physics Letters, 1997, 279, 396-402.	2.6	18
74	O ajuste de funÃ§Ãµes matemÃ¡ticas a dados experimentais. Quimica Nova, 1997, 20, 219-225.	0.3	11
75	Title is missing!. Journal of Computational Chemistry, 1997, 18, 1918.	3.3	0
76	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
77	A theoretical study of isomeric C6H4Brâ˙ ions. Chemical Physics Letters, 1995, 235, 436-443.	2.6	19
78	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
79	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
80	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
81	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
82	The application of an optimization technique to the development of universal basis sets. Canadian Journal of Chemistry, 1992, 70, 580-588.	1.1	33
83	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
84	Reliable Hellmann-Feynman forces for nuclei-centeredGTO basis of standard size. International Journal of Quantum Chemistry, 1992, 44, 311-318.	2.0	9
85	On the improvement of geometric basis sets. Computational and Theoretical Chemistry, 1992, 277, 263-277.	1.5	12
86	A modification of Koopmans' theorem by imposition of the virial theorem in molecules. Theoretica Chimica Acta, 1987, 72, 197-205.	0.8	1
87	The virial theorem as an entail for Koopmans' theorem in atomic calculations. Theoretica Chimica Acta, 1985, 67, 307-313.	0.8	2
88	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
89	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
90	Micro-determination of long-chain fatty acids in plasma and tissues by photometric titration. Analyst, The, 1980, 105, 1127.	3.5	0

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91	MecÃ¢nica QuÃ¢ntica. Revista Chemkeys, 0, 3, e021001.	0.0	3
92	Redes neurais para regressÃ£o uni- e multivariada. Revista Chemkeys, 0, 3, e021003.	0.0	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