Thiago Messias Cardozo

List of Publications by Year
in descending order

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26	401	687220 13	752573 20
papers	citations	h-index	g-index

26	26	26	478
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	The anomeric effect: the dominance of exchange effects in closed-shell systems. Organic and Biomolecular Chemistry, 2013, 11, 299-308.	1.5	49
2	Energy partitioning for generalized product functions: The interference contribution to the energy of generalized valence bond and spin coupled wave functions. Journal of Chemical Physics, 2009, 130, 104102.	1.2	44
3	Nature of the Chemical Bond and Origin of the Inverted Dipole Moment in Boron Fluoride: A Generalized Valence Bond Approach. Journal of Physical Chemistry A, 2015, 119, 5335-5343.	1.1	35
4	Chemical Bonding in the N₂ Molecule and the Role of the Quantum Mechanical Interference Effect. Journal of Physical Chemistry A, 2009, 113, 12541-12548.	1.1	23
5	Dynamics of benzene excimer formation from the parallel-displaced dimer. Physical Chemistry Chemical Physics, 2019, 21, 13916-13924.	1.3	23
6	Interference Effect and the Nature of the Ï€-Bonding in 1,3-Butadiene^{â€}. Journal of Physical Chemistry A, 2010, 114, 8798-8805.	1.1	22
7	Interference Energy in Câ€“H and Câ€“C Bonds of Saturated Hydrocarbons: Dependence on the Type of Chain and Relationship to Bond Dissociation Energy. Journal of Physical Chemistry A, 2013, 117, 4025-4034.	1.1	22
8	The non-covalent nature of the molecular structure of the benzene molecule. Physical Chemistry Chemical Physics, 2014, 16, 11024-11030.	1.3	22
9	Absorption and Fluorescence Spectra of Poly(p-phenylenevinylene) (PPV) Oligomers: An ab Initio Simulation. Journal of Physical Chemistry A, 2015, 119, 1787-1795.	1.1	22
10	The role of quantum-mechanical interference and quasi-classical effects in conjugated hydrocarbons. Physical Chemistry Chemical Physics, 2012, 14, 5479.	1.3	20
11	The Nature of the Singlet and Triplet States of Cyclobutadiene as Revealed by Quantum Interference. ChemPhysChem, 2016, 17, 288-295.	1.0	19
12	On the metastability of doubly charged homonuclear diatomics. Physical Chemistry Chemical Physics, 2017, 19, 19352-19359.	1.3	17
13	Solvent effects on the decarboxylation of trichloroacetic acid: insights from ab initio molecular dynamics simulations. Physical Chemistry Chemical Physics, 2018, 20, 21988-21998.	1.3	15
14	New class of molecules predicted to exhibit non-linear optical properties. Journal of Materials Science, 2005, 40, 3549-3551.	1.7	12
15	Excitonic and charge transfer interactions in tetracene stacked and T-shaped dimers. Journal of Chemical Physics, 2021, 154, 044306.	1.2	11
16	Impact of low-cost methods in the description of excimer and exciplex formation: pyreneâ€“pyrene and pyreneâ€“naphthalene case studies. Theoretical Chemistry Accounts, 2020, 139, 1.	0.5	9
17	Characterization of (NH₃)_n₌₁₋₆NH⁺ Clusters Produced by ²⁵²Cf Fragments Impact onto a NH₃ Condensed Target. Journal of Physical Chemistry A, 2007, 111, 8302-8307.	1.1	8
18	Dinuclear copper(<scp>ii</scp>) complexes containing oxamate and blocking ligands: crystal structure, magnetic properties, and DFT calculations. New Journal of Chemistry, 2020, 44, 2597-2608.	1.4	6

#	Article	IF	Citations
19	Taming the Antiferromagnetic Beast: Computational Design of Ultrashort Mnâ^'Mn Bonds Stabilized by Nâ€Heterocyclic Carbenes. Chemistry - A European Journal, 2021, 27, 12126-12136.	1.7	6
20	Using an interval branch-and-bound algorithm in the Hartree-Fock method. International Journal of Quantum Chemistry, 2005, 103, 500-504.	1.0	4
21	DABCO-promoted photocatalytic Câ€"H functionalization of aldehydes. Beilstein Journal of Organic Chemistry, 2021, 17, 2959-2967.	1.3	4
22	A general new method for calculating the molecular nonpolar surface for analysis of LC-MS data. International Journal of Mass Spectrometry, 2021, 461, 116495.	0.7	3
23	An experimental and theoretical description of the (NH3)â~'1{NH3â€"Hâ€"H2O}+ cluster ions produced by fast ion bombardment. Chemical Physics Letters, 2009, 474, 185-189.	1.2	2
24	Nonradiative relaxation mechanisms of the elusive silole molecule. Physical Chemistry Chemical Physics, 2021, 23, 26561-26574.	1.3	2
25	Experimental and theoretical studies of a greener catalytic system for saturated hydrocarbon chlorination composed by trichloroisocyanuric acid and a copper(II) compound. Applied Catalysis A: General, 2018, 562, 150-158.	2.2	1
26	On the calculated first hyperpolarizability of substituted tri-cyclohexadien-2-yl-amines: Novel targets for experimental research. Computational and Theoretical Chemistry, 2007, 811, 337-343.	1.5	0