Lucas de Azevedo Santos

List of Publications by Year
in descending order

27	412	758635 12	752256 20
papers	citations	h-index	g-index

31	31	31	446
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Substituted Corannulenes and Sumanenes as Fullerene Receptors. A Dispersion-Corrected Density Functional Theory Study. Journal of Physical Chemistry A, 2014, 118, 9521-9528.	1.1	49
2	Reductive amination of levulinic acid to different pyrrolidones on Ir/SiO 2 -SO 3 H: Elucidation of reaction mechanism. Catalysis Today, 2017, 296, 118-126.	2.2	40
3	The pnictogen bond: a quantitative molecular orbital picture. Physical Chemistry Chemical Physics, 2021, 23, 13842-13852.	1.3	39
4	Ring-annelated corannulenes as fullerene receptors. A DFT-D study. RSC Advances, 2014, 4, 29826-29833.	1.7	33
5	A Quantitative Molecular Orbital Perspective of the Chalcogen Bond. ChemistryOpen, 2021, 10, 391-401.	0.9	32
6	Nature and Strength of Lewis Acid/Base Interaction in Boron and Nitrogen Trihalides. Chemistry - an Asian Journal, 2020, 15, 4043-4054.	1.7	28
7	Halogen Bonds in Ligandâ€“Protein Systems: Molecular Orbital Theory for Drug Design. Journal of Chemical Information and Modeling, 2020, 60, 1317-1328.	2.5	27
8	Chalcogen bonds: Hierarchical ab initio benchmark and density functional theory performance study. Journal of Computational Chemistry, 2021, 42, 688-698.	1.5	21
9	Molecularly imprinted polymers for selective adsorption of quinoline: theoretical and experimental studies. RSC Advances, 2018, 8, 28775-28786.	1.7	19
10	Toward the Classical Description of Halogen Bonds: A Quantum Based Generalized Empirical Potential for Fluorine, Chlorine, and Bromine. Journal of Physical Chemistry A, 2017, 121, 2442-2451.	1.1	17
11	The Gauche Effect in XCH₂CH₂X Revisited. ChemPhysChem, 2021, 22, 641-648.	1.0	17
12	Hydrophobic Noncovalent Interactions of Inosine-Phenylalanine: A Theoretical Model for Investigating the Molecular Recognition of Nucleobases. Journal of Physical Chemistry A, 2014, 118, 5808-5817.	1.1	14
13	Could Quantum Mechanical Properties Be Reflected on Classical Molecular Dynamics? The Case of Halogenated Organic Compounds of Biological Interest. Frontiers in Chemistry, 2019, 7, 848.	1.8	13
14	Ïƒâ€Electrons Responsible for Cooperativity and Ring Equalization in Hydrogenâ€Bonded Supramolecular Polymers. ChemPlusChem, 2022, 87, .	1.3	8
15	Thermodynamic framework of hydrophobic/electrostatic interactions. Journal of Biomolecular Structure and Dynamics, 2013, 31, 995-1000.	2.0	7
16	Insights into the pharmaceuticals and mechanisms of neurological orphan diseases: Current Status and future expectations. Progress in Neurobiology, 2018, 169, 135-157.	2.8	6
17	Experimental and theoretical studies of solvent polarity influence on the preparation of molecularly imprinted polymers for the removal of estradiol from water. New Journal of Chemistry, 2019, 43, 1775-1784.	1.4	6
18	Synthesis and special characterization through X-ray analysis of 1,8-dioxooctahydroxanthenes. Arabian Journal of Chemistry, 2020, 13, 974-987.	2.3	6

#	Article	IF	Citations
19	Structural analysis of two tetraketones and theoretical investigation of the reactions involved in their preparation. Journal of Molecular Structure, 2018, 1156, 700-711.	1.8	5
20	Etherification of Hydroxymethylfurfural with Preyssler Heteropolyacids Immobilized on Magnetic Composites. ChemistrySelect, 2018, 3, 5526-5533.	0.7	5
21	The Role of Intramolecular Interactions on the Bioactive Conformation of Epinephrine. Molecular Informatics, 2019, 38, e1800167.	1.4	5
22	Dipolar repulsion in Î±-halocarbonyl compounds revisited. Physical Chemistry Chemical Physics, 2021, 23, 20883-20891.	1.3	4
23	Probing the redox-conversion of Co(<scp>ii</scp>)-disulfide to Co(<scp>iii</scp>)-thiolate complexes: the effect of ligand-field strength. Dalton Transactions, 2022, 51, 8046-8055.	1.6	4
24	Cleaner and stronger: how 8-quinolinolate facilitates formation of Co(<scp>iii</scp>)â€“thiolate from Co(<scp>ii</scp>)â€“disulfide complexes. Dalton Transactions, 2022, 51, 11675-11684.	1.6	4
25	A Quantitative Molecular Orbital Perspective of the Chalcogen Bond. ChemistryOpen, 2021, 10, 390-390.	0.9	1
26	A DFT-D study of stacking interactions between substituted buckybowls with fullerenes. , 0, , .		1
27	Ïƒâ€Electrons Responsible for Cooperativity and Ring Equalization in Hydrogenâ€Bonded Supramolecular Polymers. ChemPlusChem, 2022, 87, e202100541.	1.3	0