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	Ïƒâ€Electrons Responsible for Cooperativity and Ring Equalization in Hydrogenâ€Bonded Supramolecular Polymers. ChemPlusChem, 2022, 87, .	1.3	8
2	Ïƒâ€Electrons Responsible for Cooperativity and Ring Equalization in Hydrogenâ€Bonded Supramolecular Polymers. ChemPlusChem, 2022, 87, e202100541.	1.3	0
3	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
4	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
5	Dipolar repulsion in Î±-halocarbonyl compounds revisited. Physical Chemistry Chemical Physics, 2021, 23, 20883-20891.	1.3	4
6	The pnictogen bond: a quantitative molecular orbital picture. Physical Chemistry Chemical Physics, 2021, 23, 13842-13852.	1.3	39
7	A Quantitative Molecular Orbital Perspective of the Chalcogen Bond. ChemistryOpen, 2021, 10, 391-401.	0.9	32
8	The Gauche Effect in XCH₂CH₂X Revisited. ChemPhysChem, 2021, 22, 641-648.	1.0	17
9	Chalcogen bonds: Hierarchical ab initio benchmark and density functional theory performance study. Journal of Computational Chemistry, 2021, 42, 688-698.	1.5	21
10	A Quantitative Molecular Orbital Perspective of the Chalcogen Bond. ChemistryOpen, 2021, 10, 390-390.	0.9	1
11	Synthesis and special characterization through X-ray analysis of 1,8-dioxooctahydroxanthenes. Arabian Journal of Chemistry, 2020, 13, 974-987.	2.3	6
12	Nature and Strength of Lewis Acid/Base Interaction in Boron and Nitrogen Trihalides. Chemistry - an Asian Journal, 2020, 15, 4043-4054.	1.7	28
13	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
14	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
15	The Role of Intramolecular Interactions on the Bioactive Conformation of Epinephrine. Molecular Informatics, 2019, 38, e1800167.	1.4	5
16	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
17	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
18	Etherification of Hydroxymethylfurfural with Preyssler Heteropolyacids Immobilized on Magnetic Composites. ChemistrySelect, 2018, 3, 5526-5533.	0.7	5

#	Article	IF	Citations
19	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
20	Molecularly imprinted polymers for selective adsorption of quinoline: theoretical and experimental studies. RSC Advances, 2018, 8, 28775-28786.	1.7	19
21	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
22	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
23	Ring-annelated corannulenes as fullerene receptors. A DFT-D study. RSC Advances, 2014, 4, 29826-29833.	1.7	33
24	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
25	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
26	Thermodynamic framework of hydrophobic/electrostatic interactions. Journal of Biomolecular Structure and Dynamics, 2013, 31, 995-1000.	2.0	7
27	A DFT-D study of stacking interactions between substituted buckybowls with fullerenes. , 0, , .		1