Maximiliano Segala

List of Publications by Year
in descending order

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23 papers	365 citations	840776 11 h-index	794594 19 g-index
23 all docs	23 docs citations	23 times ranked	479 citing authors

#	Article	IF	Citations
1	Understanding the Strong Metalâ€“Support Interaction (SMSI) Effect in Cu_xNi_{1â€“x}/CeO₂ (0 < x < 1) Nanoparticles for Enhanced Catalysis. ACS Applied Nano Materials, 2019, 2, 2559-2573.	5.0	44
2	First hyperpolarizability in a new benzimidazole derivative. Chemical Physics, 2004, 305, 115-121.	1.9	37
3	Cyclic trinuclear copper(<scp>i</scp>), silver(<scp>i</scp>), and gold(<scp>i</scp>) complexes: a theoretical insight. Dalton Transactions, 2015, 44, 377-385.	3.3	36
4	First hyperpolarizability in proton-transfer benzoxazoles: computer-aided design, synthesis and study of a new model compound. Chemical Physics, 2001, 273, 1-10.	1.9	35
5	Geometry, solvent, and polar effects on the relationship between calculated core-electron binding energy shifts (Î”CEBE) and Hammett substituent (Ïƒ) constants. Computational and Theoretical Chemistry, 2006, 758, 61-69.	1.5	29
6	Density functional theory calculation of 2p core-electron binding energies of Si, P, S, Cl, and Ar in gas-phase molecules. Journal of Electron Spectroscopy and Related Phenomena, 2006, 151, 9-13.	1.7	28
7	K-shell core-electron binding energies for phosphorus- and sulfur-containing molecules calculated by density functional theory. Journal of Electron Spectroscopy and Related Phenomena, 2010, 182, 141-144.	1.7	27
8	New insights on the electronic factor of the SMSI effect in Pd/TiO2 nanoparticles. Applied Surface Science, 2022, 574, 151647.	6.1	22
9	An evaluation of exchange-correlation functionals for the calculations of the ionization energies for atoms and molecules. Journal of Electron Spectroscopy and Related Phenomena, 2009, 171, 18-23.	1.7	21
10	Heterocyclic dyes displaying excited-state intramolecular proton-transfer reactions (ESIPT): computational study of the substitution effect on the electronic absorption spectra of 2-(2â€²-hydroxyphenyl)-1,3-benzoxazole derivativesâ€Šâ€. Journal of the Chemical Society Perkin Transactions II, 1999, , 1123-1128.	0.9	18
11	Computational study of the geometry and electronic structure of triazolephthalocyanines. Journal of Materials Chemistry, 2002, 12, 1256-1261.	6.7	13
12	Equilibrium Conformations and Surface Charge Regulation of Spherical Polymer Brushes in Stretched Regimes. Macromolecules, 2022, 55, 35-48.	4.8	8
13	Is HAM/3 (hydrogenic atoms in molecules, version 3) a semiempirical version of dft (density functional) Tj ETQq1 1 0.784314 rgBT /Ov	0.6	6
14	Tuning MoS₂ reactivity toward halogenation. Journal of Materials Chemistry C, 2019, 7, 14672-14677.	5.5	6
15	Evaluation of Electron Donation as a Mechanism for the Stabilisation of Chalcogenateâ€Protected Gold Nanoclusters. ChemPhysChem, 2016, 17, 3102-3111.	2.1	5
16	How Do Secondary Phosphine Oxides Interact with Silver Nanoclusters? Insights from Computation. Journal of Physical Chemistry C, 2018, 122, 21449-21461.	3.1	5
17	Adsorption of polyelectrolytes on charged microscopically patterned surfaces. Journal of Molecular Liquids, 2019, 294, 111673.	4.9	5
18	Core Electron Binding Energy (CEBE) as Descriptors in Quantitative Structureâ€“Activity Relationship (QSAR) Analysis of Cytotoxicities of a Series of Simple Phenols. QSAR and Combinatorial Science, 2007, 26, 378-384.	1.4	4

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19	Density functional theory calculation of 2p spectra of SiH₄, PH₃, H₂S, HCl, and Ar. International Journal of Quantum Chemistry, 2008, 108, 1358-1368.	2.0	4
20	Electrolytes in regimes of strong confinement: surface charge modulations, osmotic equilibrium and electroneutrality. Soft Matter, 2020, 16, 10488-10505.	2.7	4
21	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
22	Conformational analyses and SAR studies of antispermatogenic hexahydroindenopyridines. Computational and Theoretical Chemistry, 2003, 633, 93-104.	1.5	3
23	Polarization Dependence in the Carbon K-Edge Photofragmentation of MAPDST Photoresist: An Experimental and Theoretical Study. Journal of Physical Chemistry C, 2018, 122, 28619-28628.	3.1	2