

VinÃ-cius Manzoni

List of Publications by Year in descending order

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Version: 2024-02-01

26
papers

353
citations

759055

12
h-index

839398

18
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26
all docs

26
docs citations

26
times ranked

237
citing authors

#	ARTICLE	IF	CITATIONS
1	Unveiling the relationship between structural and polarization effects on the first hyperpolarizability of a merocyanine dye. <i>Journal of Chemical Physics</i> , 2022, 156, 014305.	1.2	7
2	Quantum binding energy features of the drug olmesartan bound to angiotensin type-1 receptors in the therapeutics of stroke. <i>New Journal of Chemistry</i> , 2021, 45, 19487-19496.	1.4	2
3	Insights on the crossing of the two lowest n- π^* and $\pi-\pi^*$ absorption lines of thieno[3,4-b]pyrazine in an aqueous environment. <i>Chemical Physics Letters</i> , 2021, 768, 138366.	1.2	2
4	Solvent effects on Stokes shifts, and NLO response of thieno[3,4-b]pyrazine: A comprehensive QM/MM investigation. <i>Journal of Molecular Liquids</i> , 2021, 335, 115996.	2.3	18
5	Adsorption study of 4-nitrophenol onto kaolinite (001) surface: A van der Waals density functional study. <i>Materials Chemistry and Physics</i> , 2021, 271, 124887.	2.0	7
6	Solvent enhancement and isomeric effects on the NLO properties of a photoinduced cis-trans azomethine chromophore: A sequential MC/QM study. <i>Journal of Molecular Liquids</i> , 2021, 340, 116887.	2.3	12
7	Theoretical study of thieno[3,4-b]pyrazine derivatives with enhanced NLO response. <i>Chemical Physics Letters</i> , 2021, 781, 138976.	1.2	8
8	Exploring the Binding Mechanism of GABA _B Receptor Agonists and Antagonists through in Silico Simulations. <i>Journal of Chemical Information and Modeling</i> , 2020, 60, 1005-1018.	2.5	16
9	Theoretical study of a recently synthesized azo dyes useful for OLEDs. <i>Materials Letters</i> , 2020, 280, 128535.	1.3	26
10	A theoretical study of the magnetic shielding of ¹⁵ N of formamide in liquid water. <i>Journal of Molecular Liquids</i> , 2020, 320, 114415.	2.3	11
11	Thermal and solvatochromic effects on the emission properties of a thienyl-based dansyl derivative. <i>RSC Advances</i> , 2020, 10, 28484-28491.	1.7	9
12	Observation and Analysis of Incoherent Second-Harmonic Generation in Gold Nanoclusters with Six Atoms. <i>Journal of Physical Chemistry C</i> , 2020, 124, 15440-15447.	1.5	7
13	Giant values obtained for first hyperpolarizabilities of methyl orange: a DFT investigation. <i>Theoretical Chemistry Accounts</i> , 2019, 138, 1.	0.5	23
14	Strong enhancement of NLO response of methyl orange dyes through solvent effects: A sequential Monte Carlo/DFT investigation. <i>Optical Materials</i> , 2019, 94, 152-159.	1.7	41
15	Solvent effects on low-lying absorptions and vibrational spectra of thieno[3,4-b]pyrazines: the role of unconventional C-H \cdots N bonds. <i>Chemical Papers</i> , 2019, 73, 1519-1527.	1.0	7
16	Outlining migrainous through dihydroergotamine-serotonin receptor interactions using quantum biochemistry. <i>New Journal of Chemistry</i> , 2018, 42, 2401-2412.	1.4	21
17	The electrostatic embedding contribution to DFT calculations of ligand-amino acid residues interaction. <i>Journal of Molecular Modeling</i> , 2018, 24, 211.	0.8	1
18	The role of electrostatic interactions and solvent polarity on the ¹⁵ N NMR shielding of azines. <i>Chemical Physics Letters</i> , 2017, 686, 189-194.	1.2	12

#	ARTICLE	IF	CITATIONS
19	An insightful approach for understanding solvatochromic reversal. Chemical Physics Letters, 2016, 655-656, 30-34.	1.2	15
20	The quantum biophysics of the isoniazid adduct NADH binding to its InhA reductase target. New Journal of Chemistry, 2014, 38, 2946.	1.4	18
21	Comparison of polarizable continuum model and quantum mechanics/molecular mechanics solute electronic polarization: Study of the optical and magnetic properties of diazines in water. Journal of Chemical Physics, 2011, 135, 144103.	1.2	26
22	Density functional theory study of the electronic properties of naphthofuranquinone compounds with antitrypanocidal activity. International Journal of Quantum Chemistry, 2011, 111, 1270-1279.	1.0	3
23	Study of the optical and magnetic properties of pyrimidine in water combining PCM and QM/MM methodologies. Physical Chemistry Chemical Physics, 2010, 12, 14023.	1.3	47
24	Correlation and complexity analysis of well logs via Lyapunov, Hurst, Lempel-Ziv and neural network algorithms. Physica A: Statistical Mechanics and Its Applications, 2009, 388, 747-754.	1.2	12
25	Recognition ability of the fully connected Hopfield neural network under a persistent stimulus field. Physica A: Statistical Mechanics and Its Applications, 2009, 388, 1279-1288.	1.2	1
26	Parallel and orthogonal stimulus in ultradiluted neural networks. Physical Review E, 2006, 74, 046117.	0.8	1