

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
g-index

26
all docs

26
docs citations

26
times ranked

237
citing authors

#	ARTICLE	IF	CITATIONS
1	Study of the optical and magnetic properties of pyrimidine in water combining PCM and QM/MM methodologies. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 14023.	1.3	47
2	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
3	Comparison of polarizable continuum model and quantum mechanics/molecular mechanics solute electronic polarization: Study of the optical and magnetic properties of diazines in water. <i>Journal of Chemical Physics</i> , 2011, 135, 144103.	1.2	26
4	Theoretical study of a recently synthesized azo dyes useful for OLEDs. <i>Materials Letters</i> , 2020, 280, 128535.	1.3	26
5	Giant values obtained for first hyperpolarizabilities of methyl orange: a DFT investigation. <i>Theoretical Chemistry Accounts</i> , 2019, 138, 1.	0.5	23
6	Outlining migrainous through dihydroergotamine's serotonin receptor interactions using quantum biochemistry. <i>New Journal of Chemistry</i> , 2018, 42, 2401-2412.	1.4	21
7	The quantum biophysics of the isoniazid adduct NADH binding to its InhA reductase target. <i>New Journal of Chemistry</i> , 2014, 38, 2946.	1.4	18
8	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
9	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
10	An insightful approach for understanding solvatochromic reversal. <i>Chemical Physics Letters</i> , 2016, 655-656, 30-34.	1.2	15
11	Correlation and complexity analysis of well logs via Lyapunov, Hurst, Lempel's Ziv and neural network algorithms. <i>Physica A: Statistical Mechanics and Its Applications</i> , 2009, 388, 747-754.	1.2	12
12	The role of electrostatic interactions and solvent polarity on the 15N NMR shielding of azines. <i>Chemical Physics Letters</i> , 2017, 686, 189-194.	1.2	12
13	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
14	A theoretical study of the magnetic shielding of 15N of formamide in liquid water. <i>Journal of Molecular Liquids</i> , 2020, 320, 114415.	2.3	11
15	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
16	Theoretical study of thieno[3,4-b]pyrazine derivatives with enhanced NLO response. <i>Chemical Physics Letters</i> , 2021, 781, 138976.	1.2	8
17	Solvent effects on low-lying absorptions and vibrational spectra of thieno[3,4-b]pyrazines: the role of unconventional C-H...N bonds. <i>Chemical Papers</i> , 2019, 73, 1519-1527.	1.0	7
18	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

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19	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
20	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
21	Density functional theory study of the electronic properties of naphthofuranquinone compounds with antitrypanocidal activity. <i>International Journal of Quantum Chemistry</i> , 2011, 111, 1270-1279.	1.0	3
22	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
23	Insights on the crossing of the two lowest $n\pi^*$ 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
24	Parallel and orthogonal stimulus in ultradiluted neural networks. <i>Physical Review E</i> , 2006, 74, 046117.	0.8	1
25	Recognition ability of the fully connected Hopfield neural network under a persistent stimulus field. <i>Physica A: Statistical Mechanics and Its Applications</i> , 2009, 388, 1279-1288.	1.2	1
26	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