

Tarciso Andrade-Filho

List of Publications by Year in descending order

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34
papers

346
citations

932766

10
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839053

18
g-index

35
all docs

35
docs citations

35
times ranked

340
citing authors

#	ARTICLE	IF	CITATIONS
1	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
2	Water-driven stabilization of diphenylalanine nanotube structures. <i>Theoretical Chemistry Accounts</i> , 2016, 135, 1.	0.5	40
3	The effects of water molecules on the electronic and structural properties of peptide nanotubes. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 7555.	1.3	38
4	Multifunctional biosensors based on peptide-polyelectrolyte conjugates. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 3223-3233.	1.3	30
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	Polarized Raman and Infrared Spectroscopy and ab Initio Calculation of Palmitic and Stearic Acids in the Bm and C Forms. <i>Journal of Physical Chemistry A</i> , 2017, 121, 4830-4842.	1.1	19
7	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
8	The UV-vis absorption spectrum of the flavonol quercetin in methanolic solution: A theoretical investigation. <i>European Physical Journal E</i> , 2009, 29, 253-259.	0.7	17
9	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
10	Theoretical investigation of the electronic absorption spectrum of Piceatannol in methanolic solution. <i>Theoretical Chemistry Accounts</i> , 2008, 121, 147-153.	0.5	11
11	Experimental and theoretical spectroscopic characterization, NLO response, and reactivity of the pharmacological agent spilanthal and analogues. <i>Journal of Molecular Structure</i> , 2021, 1227, 129423.	1.8	9
12	Encapsulation ability of silicon carbide and boron nitride nanotubes for spilanthal molecule. <i>Journal of Nanostructure in Chemistry</i> , 2021, 11, 203-213.	5.3	9
13	Theoretical study of thieno[3,4-b]pyrazine derivatives with enhanced NLO response. <i>Chemical Physics Letters</i> , 2021, 781, 138976.	1.2	8
14	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
15	Theoretical study of the adsorption of diphenylalanine on pristine graphene. <i>Theoretical Chemistry Accounts</i> , 2020, 139, 1.	0.5	7
16	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
17	Insights and modelling on the nonlinear optical response, reactivity, and structure of chalcones and dihydrochalcones. <i>Journal of Molecular Structure</i> , 2021, 1246, 131182.	1.8	6
18	Thermodynamics study of biokerosene from coconut and palm kernel oils and JP-8 aircraft fuels in the gas phase by the DFT method. <i>Journal of Molecular Modeling</i> , 2020, 26, 79.	0.8	5

#	ARTICLE	IF	CITATIONS
19	Structural behavior of phenylalanine-tryptophan peptide nanotubes at anhydrous conditions: a theoretical investigation. <i>Theoretical Chemistry Accounts</i> , 2019, 138, 1.	0.5	4
20	Prediction of electronic and vibrational properties of poly (hexamethylene biguanide) hydrochloride: A combined theoretical and experimental investigation. <i>Journal of Molecular Structure</i> , 2021, 1246, 131176.	1.8	4
21	Simulation of Iron Corrosion Inhibition by Biological Molecules Thymol and Carvacrol.. <i>Materials Letters</i> , 2022, 308, 131249.	1.3	4
22	A DFT analysis of electronic, reactivity, and NLO responses of a reactive orange dye: the role of Hartree-Fock exchange corrections. <i>Journal of Molecular Modeling</i> , 2022, 28, 85.	0.8	4
23	Structural and electronic properties of amorphous bismuth calcium borate from first-principle calculations. <i>Structural Chemistry</i> , 2021, 32, 1589-1595.	1.0	3
24	Molecular Docking of Azithromycin, Ritonavir, Lopinavir, Oseltamivir, Ivermectin and Heparin Interacting with Coronavirus Disease 2019 Main and Severe Acute Respiratory Syndrome Coronavirus-2 3C-Like Proteases. <i>Journal of Nanoscience and Nanotechnology</i> , 2021, 21, 2075-2089.	0.9	3
25	Theoretical investigation of adsorption of kojic acid on carbon nanotubes. <i>Materials Letters</i> , 2021, 294, 129769.	1.3	3
26	Hydration-dependent band gap tunability of self-assembled phenylalanyl tryptophan nanotubes. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2021, 134, 114910.	1.3	3
27	Understanding the Stokes shift and nonlinear optical behavior of 1-nitro-2-phenylethane: A sequential Monte Carlo/Quantum Mechanics discussion. <i>Chemical Physics Letters</i> , 2022, 804, 139867.	1.2	3
28	Elucidating the crystal structure of the antimalarial drug (±)-mefloquine hydrochloride: a tetragonal hydrated species. <i>Journal of Applied Crystallography</i> , 2014, 47, 1380-1386.	1.9	2
29	Solvent polarity effects on thermochemical and NMR parameters of spilanthol pharmacological agent: an experimental and DFT investigation. <i>Structural Chemistry</i> , 2020, 31, 2281-2292.	1.0	2
30	Insights on the crossing of the two lowest n-π* and π-π* absorption lines of thieno[3,4-b]pyrazine in an aqueous environment. <i>Chemical Physics Letters</i> , 2021, 768, 138366.	1.2	2
31	Effect of the Electric Field on DNA Bases as Pigments for Nanodevices: A First-Principles Study. <i>Journal of Nanoscience and Nanotechnology</i> , 2020, 20, 2603-2610.	0.9	1
32	Designing a novel organometallic chalcone with an enormous second-harmonic generation response. <i>Materials Today Communications</i> , 2022, , 103762.	0.9	1
33	Hormones Nanofiltration in Carbon Nanotubes and Boron Nitride Nanotubes Using Uniform External Electric Field Through Molecular Dynamics. <i>Journal of Nanoscience and Nanotechnology</i> , 2021, 21, 5499-5509.	0.9	0
34	Experimental and Theoretical Optical Properties of β -Carotene in Oleic Acid Solution. <i>Journal of Bionanoscience</i> , 2010, 4, 104-108.	0.4	0