Tarciso Andrade-Filho

List of Publications by Year
in descending order

34	346	933264 10	839398 18
papers	citations	h-index	g-index

35	35	35	340
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Simulation of Iron Corrosion Inhibition by Biological Molecules Thymol and Carvacrol.. Materials Letters, 2022, 308, 131249.	1.3	4
2	A DFT analysis of electronic, reactivity, and NLO responses of a reactive orange dye: the role of Hartree-Fock exchange corrections. Journal of Molecular Modeling, 2022, 28, 85.	0.8	4
3	Designing a novel organometallic chalcone with an enormous second-harmonic generation response. Materials Today Communications, 2022, , 103762.	0.9	1
4	Understanding the Stokes shift and nonlinear optical behavior of 1-nitro-2-phenylethane: A sequential Monte Carlo/Quantum Mechanics discussion. Chemical Physics Letters, 2022, 804, 139867.	1.2	3
5	Experimental and theoretical spectroscopic characterization, NLO response, and reactivity of the pharmacological agent spilanthol and analogues. Journal of Molecular Structure, 2021, 1227, 129423.	1.8	9
6	Encapsulation ability of silicon carbide and boron nitride nanotubes for spilanthol molecule. Journal of Nanostructure in Chemistry, 2021, 11, 203-213.	5.3	9
7	Structural and electronic properties of amorphous bismuth calcium borate from first-principle calculations. Structural Chemistry, 2021, 32, 1589-1595.	1.0	3
8	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. Journal of Nanoscience and Nanotechnology, 2021, 21, 2075-2089.	0.9	3
9	Insights on the crossing of the two lowest n-Ï€â^— and Ï€-Ï€â^— absorption lines of thieno[3,4-b]pyrazine in an aqueous environment. Chemical Physics Letters, 2021, 768, 138366.	1.2	2
10	Theoretical investigation of adsorption of kojic acid on carbon nanotubes. Materials Letters, 2021, 294, 129769.	1.3	3
11	Solvent effects on Stokes shifts, and NLO response of thieno[3,4-b]pyrazine: A comprehensive QM/MM investigation. Journal of Molecular Liquids, 2021, 335, 115996.	2.3	18
12	Adsorption study of 4-nitrophenol onto kaolinite (001) surface: A van der Waals density functional study. Materials Chemistry and Physics, 2021, 271, 124887.	2.0	7
13	Solvent enhancement and isomeric effects on the NLO properties of a photoinduced cis-trans azomethine chromophore: A sequential MC/QM study. Journal of Molecular Liquids, 2021, 340, 116887.	2.3	12
14	Hydration-dependent band gap tunability of self-assembled phenylalanyl tryptophan nanotubes. Physica E: Low-Dimensional Systems and Nanostructures, 2021, 134, 114910.	1.3	3
15	Theoretical study of thieno[3,4-b]pyrazine derivatives with enhanced NLO response. Chemical Physics Letters, 2021, 781, 138976.	1.2	8
16	Hormones Nanofiltration in Carbon Nanotubes and Boron Nitride Nanotubes Using Uniform External Electric Field Through Molecular Dynamics. Journal of Nanoscience and Nanotechnology, 2021, 21, 5499-5509.	0.9	0
17	Insights and modelling on the nonlinear optical response, reactivity, and structure of chalcones and dihydrochalcones. Journal of Molecular Structure, 2021, 1246, 131182.	1.8	6
18	Prediction of electronic and vibrational properties of poly (hexamethylene biguanide) hydrochloride: A combined theoretical and experimental investigation. Journal of Molecular Structure, 2021, 1246, 131176.	1.8	4

#	Article	IF	Citations
19	Effect of the Electric Field on DNA Bases as Pigments for Nanodevices: A First-Principles Study. Journal of Nanoscience and Nanotechnology, 2020, 20, 2603-2610.	0.9	1
20	Observation and Analysis of Incoherent Second-Harmonic Generation in Gold Nanoclusters with Six Atoms. Journal of Physical Chemistry C, 2020, 124, 15440-15447.	1.5	7
21	Thermodynamics study of biokerosene from coconut and palm kernel oils and JP-8 aircraft fuels in the gas phase by the DFT method. Journal of Molecular Modeling, 2020, 26, 79.	0.8	5
22	Solvent polarity effects on thermochemical and NMR parameters of spilanthol pharmacological agent: an experimental and DFT investigation. Structural Chemistry, 2020, 31, 2281-2292.	1.0	2
23	Theoretical study of the adsorption of diphenylalanine on pristine graphene. Theoretical Chemistry Accounts, 2020, 139, 1.	0.5	7
24	Giant values obtained for first hyperpolarizabilities of methyl orange: a DFT investigation. Theoretical Chemistry Accounts, 2019, 138, 1.	0.5	23
25	Strong enhancement of NLO response of methyl orange dyes through solvent effects: A sequential Monte Carlo/DFT investigation. Optical Materials, 2019, 94, 152-159.	1.7	41
26	Structural behavior of phenylalanineâ€“tryptophan peptide nanotubes at anhydrous conditions: a theoretical investigation. Theoretical Chemistry Accounts, 2019, 138, 1.	0.5	4
27	Polarized Raman and Infrared Spectroscopy and ab Initio Calculation of Palmitic and Stearic Acids in the Bm and C Forms. Journal of Physical Chemistry A, 2017, 121, 4830-4842.	1.1	19
28	Water-driven stabilization of diphenylalanine nanotube structures. Theoretical Chemistry Accounts, 2016, 135, 1.	0.5	40
29	Multifunctional biosensors based on peptideâ€“polyelectrolyte conjugates. Physical Chemistry Chemical Physics, 2016, 18, 3223-3233.	1.3	30
30	Elucidating the crystal structure of the antimalarial drug (Â±)-mefloquine hydrochloride: a tetragonal hydrated species. Journal of Applied Crystallography, 2014, 47, 1380-1386.	1.9	2
31	The effects of water molecules on the electronic and structural properties of peptide nanotubes. Physical Chemistry Chemical Physics, 2013, 15, 7555.	1.3	38
32	Experimental and Theoretical Optical Properties of Î²-Carotene in Oleic Acid Solution. Journal of Bionanoscience, 2010, 4, 104-108.	0.4	0
33	The UV-vis absorption spectrum of the flavonol quercetin in methanolic solution: A theoretical investigation. European Physical Journal E, 2009, 29, 253-259.	0.7	17
34	Theoretical investigation of the electronic absorption spectrum of Piceatannol in methanolic solution. Theoretical Chemistry Accounts, 2008, 121, 147-153.	0.5	11