GeÃ³rgia M A Junqueira

List of Publications by Year
in descending order

31 papers	383 citations	759233 12 h-index	839539 18 g-index
31 all docs	31 docs citations	31 times ranked	459 citing authors

#	Article	IF	Citations
1	Vibrational spectroscopy and aromaticity investigation of squarate salts: A theoretical and experimental approach. Journal of Molecular Structure, 2006, 794, 63-70.	3.6	44
2	New Insights on Chemical Oxidation of Single-Wall Carbon Nanotubes: A Theoretical Study. Journal of Physical Chemistry C, 2009, 113, 10079-10084.	3.1	31
3	Theoretical analysis of the oxocarbons: structure and spectroscopic properties of croconate ion and its coordination compound with lithium. Physical Chemistry Chemical Physics, 2001, 3, 3499-3505.	2.8	26
4	Theoretical analysis of the oxocarbons: The solvent and counter-ion effects on the structure and spectroscopic properties of the squarate ion. Physical Chemistry Chemical Physics, 2003, 5, 437-445.	2.8	26
5	Vibrational spectroscopy for milk fat quantification: line shape analysis of the Raman and infrared spectra. Journal of Raman Spectroscopy, 2016, 47, 692-698.	2.5	19
6	Structural and vibrational study of graphene oxide via coronene based models: theoretical and experimental results. Materials Research Express, 2016, 3, 055020.	1.6	18
7	Theoretical analysis of the oxocarbons: The role played by the solvent and counter-ions in the electronic spectrum of the deltate ion. Physical Chemistry Chemical Physics, 2002, 4, 2517-2523.	2.8	17
8	Extrapolating to the One-Electron Basis Set Limit in Polarizability Calculations. Journal of Physical Chemistry A, 2008, 112, 10413-10419.	2.5	15
9	Ab initio calculation of electric properties for the BH, CO, CS and N2 molecules. Computational and Theoretical Chemistry, 2009, 913, 200-206.	1.5	15
10	Theoretical study of structure and non-linear optical properties of Zn(II) porphyrin adsorbed on carbon nanotubes. Computational and Theoretical Chemistry, 2010, 959, 92-100.	1.5	15
11	Enhancement of nonlinear optical properties of graphene oxide-based structures: pushâ€“pull models. RSC Advances, 2016, 6, 94437-94450.	3.6	15
12	Theoretical study of oxocarbons: structure and vibrational spectrum of the D6h and C2 forms of the rhodizonate ion. Computational and Theoretical Chemistry, 2004, 684, 141-147.	1.5	13
13	Theoretical study of structure and properties of a molecular reactor based on the urea-linked Î²-cyclodextrin dimer. Computational and Theoretical Chemistry, 2007, 809, 95-102.	1.5	13
14	Solvent effects on reactivity properties of dicarba-closo-dodecarboranes isomers. Chemical Physics Letters, 2012, 538, 54-59.	2.6	12
15	The role of sulfate in the chemical synthesis of graphene oxide. Materials Chemistry and Physics, 2018, 215, 203-210.	4.0	12
16	Detection of antibiotic residues in Cow's milk: A theoretical and experimental vibrational study. Journal of Molecular Structure, 2020, 1215, 128221.	3.6	12
17	Theoretical analysis of the oxocarbons: the electronic spectrum of the rhodizonate ion. Computational and Theoretical Chemistry, 2005, 719, 31-39.	1.5	11
18	Theoretical study of the solvent effect on the aromaticity of benzene: a NICS analysis. Journal of Molecular Modeling, 2014, 20, 2152.	1.8	9

#	Article	IF	Citations
19	Exploring the effect of substitutional doping on the electronic properties of graphene oxide. Journal of Materials Science, 2018, 53, 7516-7526.	3.7	9
20	Theoretical study of nonlinear optical properties of oxocarbon derivatives. International Journal of Quantum Chemistry, 2010, 110, 489-497.	2.0	7
21	Remarkable aromaticity of cobalt bis(dicarbollide) derivatives: a NICS study. Theoretical Chemistry Accounts, 2018, 137, 1.	1.4	7
22	Reply to the â€˜Comment on â€œTheoretical analysis of the oxocarbons: structure and spectroscopic properties of croconate ion and its coordination compound with lithiumâ€â€™, by M. C. C. Ribeiro and A. O. Cavalcante, Phys. Chem. Chem. Phys., 2002, 4, 2917. Physical Chemistry Chemical Physics, 2002, 4, 2919-2920.	2.8	6
23	Estudo teÃ³rico de propriedades Ã³pticas nÃ£o-lineares de nanotubos de carbono de parede Ãºnica quimicamente modificados. Quimica Nova, 2009, 32, 315-321.	0.3	6
24	Molecular properties of coordination compounds of the croconate ion with first-row sivalent transition metals: a quantum mechanical study. Journal of the Brazilian Chemical Society, 2007, 18, 1379-1387.	0.6	5
25	Substituent effects on molecular properties of dicarba-closo-dodecarborane derivatives. Journal of Molecular Modeling, 2014, 20, 2275.	1.8	5
26	Gaussian basis sets for ab initio calculation of NLO properties of polyatomic molecules. Journal of Computational Methods in Sciences and Engineering, 2010, 10, 239-256.	0.2	4
27	Theoretical study of nonlinear optical properties of cobalt bis (dicarbollide) derivatives: the effect of substituents. Theoretical Chemistry Accounts, 2015, 134, 1.	1.4	4
28	AplicaÃ§Ã£o de mecÃ¢nica molecular em quÃmica inorgÃ¢nica. Quimica Nova, 1999, 22, 396-404.	0.3	4
29	Graphene oxide in water: a systematic computational experimental study. Graphene Technology, 2020, 5, 1-8.	1.9	3
30	9th Congress on Electronic Structure: Principles and Applications (ESPA 2014). , 2016, , .		0
31	Theoretical Studies of Milk: Solvent Effects on the Molecular Properties of Retinoid Compounds. Quarks, 2020, 2, 19-26.	0.3	0