Guilherme Colherinhas

List of Publications by Year
in descending order

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55 papers	746 citations	535685 17 h-index	685536 24 g-index
55 all docs	55 docs citations	55 times ranked	443 citing authors

#	Article	IF	Citations
1	Fullerene C60 spectroscopy in [BMIM][PF6] ionic liquid: Molecular dynamics study using polarization effects. Journal of Molecular Structure, 2022, 1250, 131887.	1.8	5
2	Molecular dynamics study of hydrogen bond in peptide membrane at 150â€“300ÂK. Journal of Molecular Liquids, 2022, 349, 118165.	2.3	4
3	Statistical and energetic analysis of hydrogen bonds in short and long peptide nanotapes/nanofibers using molecular dynamics simulations. Journal of Molecular Liquids, 2022, 359, 119308.	2.3	4
4	A molecular dynamics study of graphyne-based electrode and biocompatible ionic liquid for supercapacitor applications. Journal of Molecular Liquids, 2022, 360, 119494.	2.3	9
5	Update of CHARMM36's atomic charges for aromatic amino acids in water solution simulations and spectroscopy analysis via sequential molecular dynamics and DFT calculations. Journal of Molecular Liquids, 2021, 321, 114739.	2.3	12
6	Molecular dynamic simulations, <scp>GIAOâ€NMR</scp> and <scp>TDâ€DFT</scp> spectroscopy analyze for zwitterionic isoleucine (ILE)_N, 1â€‰â‰‰â€‰Nâ€‰â‰‰â€‰6, in water solution. Journal of Computational Chemistry, 2021, 42, 344-357.	1.5	1
7	Updating atomic charge parameters of aliphatic amino acids: a quest to improve the performance of molecular modeling via sequential molecular dynamics and DFT-GIAO-NMR calculations. Physical Chemistry Chemical Physics, 2021, 23, 8413-8425.	1.3	12
8	Atomistic molecular dynamics study on the influence of high temperatures on the structure of peptide nanomembranes candidates for organic supercapacitor electrode. Journal of Molecular Liquids, 2021, 334, 116126.	2.3	15
9	TD-DFT absorption spectrum of (poly)threonine in water: A study combining molecular dynamics and quantum mechanics calculations. Chemical Physics Letters, 2021, 779, 138876.	1.2	4
10	Hydroxylic, sulfur-containing and amidic amino acids in water solution: Atomic charges parameters for computational modeling using molecular dynamics simulation and DFT calculations. Journal of Molecular Liquids, 2021, 339, 116815.	2.3	6
11	Laminar peptide structure: Energetic and structural evaluation using molecular dynamics. Journal of Molecular Liquids, 2021, 341, 117261.	2.3	4
12	GIAO-NMR spectroscopy of the xanthineâ€™s structures in water solution using S-MC/QM methodology: an evaluation of the DFT-functionalsâ€™ efficiency. Journal of Molecular Liquids, 2021, , 117955.	2.3	1
13	The influence of polar and non-polar interactions on the self-assembly of peptide nanomembranes and their applications: An atomistic study using classical molecular dynamics. Journal of Molecular Liquids, 2020, 318, 114263.	2.3	15
14	Can CHARMM36 atomic charges described correctly the interaction between amino acid and water molecules by molecular dynamics simulations?. Journal of Molecular Liquids, 2020, 317, 113919.	2.3	18
15	A6H polypeptide membranes: Molecular dynamics simulation, GIAO-DFT-NMR and TD-DFT spectroscopy analysis. Journal of Molecular Liquids, 2020, 316, 113850.	2.3	19
16	Assessing the DOPC-cholesterol interactions and their influence on fullerene C60 partitioning in lipid bilayers. Journal of Molecular Liquids, 2020, 315, 113698.	2.3	15
17	Design and analysis of polypeptide nanofiber using full atomistic Molecular Dynamic. Journal of Molecular Liquids, 2020, 302, 112610.	2.3	14
18	Investigating the asymmetry in the EDL response of C₆₀/graphene supercapacitors. Physical Chemistry Chemical Physics, 2019, 21, 15362-15371.	1.3	17

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19	On the calculation of magnetic properties of nucleic acids in liquid water with the sequential QM/MM method. Journal of Molecular Liquids, 2019, 294, 111611.	2.3	13
20	Understanding the stability of polypeptide membranes in ionic liquids: a theoretical molecular dynamics study. New Journal of Chemistry, 2019, 43, 10151-10161.	1.4	16
21	Solvent effects on the spectroscopic properties of Damascone derivatives: A sequential Monte Carlo/Quantum Mechanics study. Chemical Physics Letters, 2019, 730, 531-537.	1.2	12
22	Robust Entanglement Generation in Lithium Ions Mediated by Graphene Quantum Dots Interaction. Journal of Physical Chemistry A, 2019, 123, 1790-1795.	1.1	3
23	Elucidating NH2-I3V3A3G3K3-COOH and NH2-K3G3A3V3I3-COOH polypeptide membranes: A classical molecular dynamics study. Journal of Molecular Liquids, 2019, 279, 740-749.	2.3	20
24	Spectroscopic properties and soluteâ€“solvent structural analyses for A_NR polypeptides in water solution: a sequential Monte Carlo/quantum mechanics (S-MC/QM) theoretical study. New Journal of Chemistry, 2018, 42, 19692-19700.	1.4	6
25	Stability and Structural Analysis of A₆R Polypeptide Nanosheets: A Theoretical Study Using the Classical Molecular Dynamics Simulation. Journal of Physical Chemistry C, 2018, 122, 24445-24453.	1.5	18
26	Storing Energy in Biodegradable Electrochemical Supercapacitors. ACS Omega, 2018, 3, 13869-13875.	1.6	46
27	GIAO-DFT-NMR characterization of fullerene-cucurbituril complex: the effects of the C60@CB[9] host-guest mutual interactions. Journal of Molecular Modeling, 2018, 24, 181.	0.8	5
28	The influence of flexibility on the spectroscopic properties for organic molecules in solution: A theoretical study applied to A3R polypeptide. Journal of Molecular Liquids, 2018, 263, 334-341.	2.3	13
29	Solvent effects on the electrical and magnetic spectroscopic properties of azo-enaminone derivatives in methanol and in water. New Journal of Chemistry, 2018, 42, 12032-12044.	1.4	6
30	MatemÃ¡tica bÃ¡sica aplicada ao ensino de fÃsica: relaÃ§Ã£o entre competÃªncias e habilidades tÃ©cnicas necessÃ¡rias para a resoluÃ§Ã£o de problemas de fÃsica segundo o Inep. Ensino E Tecnologia Em Revista, 2018, 2, 3.	0.0	0
31	All-boron fullerene exhibits a strong affinity to inorganic anions. Chemical Physics Letters, 2017, 671, 107-112.	1.2	6
32	TD-DFT and GIAO-NMR spectroscopy studies for maltose and (Î±- and Î²)-glucose in water solution using S-MC/QM polarization methodology. Journal of Molecular Liquids, 2017, 237, 295-303.	2.3	11
33	Hydration properties of the polyalanines by atomistic molecular dynamics. Journal of Molecular Liquids, 2017, 244, 285-290.	2.3	6
34	Assessing the interaction between surfactant-like peptides and lipid membranes. RSC Advances, 2017, 7, 35973-35981.	1.7	22
35	Elucidating the stability of bolaamphiphilic polypeptide nanosheets using atomistic molecular dynamics. Physical Chemistry Chemical Physics, 2017, 19, 31921-31928.	1.3	26
36	GIAOâ¿¿DFT isotropic magnetic shielding constants and spinâ¿¿spin coupling of tartaric acid in water solution. Chemical Physics Letters, 2016, 644, 205-211.	1.2	14

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37	Potential energy surface of excited semiconductors: Graphene quantum dot and BODIPY. Chemical Physics, 2016, 474, 1-6.	0.9	9
38	Versatile interactions of boron fullerene B₈₀with gas molecules. RSC Advances, 2016, 6, 78684-78691.	1.7	4
39	Can inorganic salts tune electronic properties of graphene quantum dots?. Physical Chemistry Chemical Physics, 2015, 17, 17413-17420.	1.3	29
40	The Band Gap of Graphene Is Efficiently Tuned by Monovalent Ions. Journal of Physical Chemistry Letters, 2015, 6, 302-307.	2.1	50
41	Spectroscopic properties of vitamin E models in solution. Chemical Physics Letters, 2015, 628, 49-53.	1.2	20
42	Solvent effects on the first hyperpolarizability of retinal derivatives. Chemical Physics Letters, 2014, 598, 43-47.	1.2	16
43	Molecular Dynamics Study of Surfactant-Like Peptide Based Nanostructures. Journal of Physical Chemistry B, 2014, 118, 12215-12222.	1.2	49
44	Molecular Description of Surfactant-like Peptide Based Membranes. Journal of Physical Chemistry C, 2014, 118, 9598-9603.	1.5	29
45	Predicting the properties of a new class of hostâ€“guest complexes: C₆₀ fullerene and CB[9] cucurbituril. Physical Chemistry Chemical Physics, 2014, 16, 22823-22829.	1.3	20
46	Isotropic magnetic shielding constants of retinal derivatives in aprotic and protic solvents. Journal of Chemical Physics, 2013, 139, 094502.	1.2	20
47	13C chemical shifts of polyacetylene chains with charged conformational defects: A GIAOâ€“DFT study. Chemical Physics Letters, 2011, 503, 191-196.	1.2	10
48	Isomerization effects on chemical shifts and spinâ€spin coupling constants of polyacetylene chains: A GIAOâ€DFT study. International Journal of Quantum Chemistry, 2011, 111, 1616-1625.	1.0	17
49	Theoretical analysis of the hydration of C60 in normal and supercritical conditions. Carbon, 2011, 49, 187-192.	5.4	29
50	INTERACTION OF A TWO-LEVEL ATOM WITH A SQUEEZED DISPLACED NUMBER STATE. International Journal of Modern Physics B, 2007, 21, 2723-2733.	1.0	0
51	SCATTERING OF ATOMS BY LIGHT: MEASURING THE QUANTUM STATE OF THE FIELD IN A CAVITY. International Journal of Modern Physics B, 2006, 20, 325-339.	1.0	1
52	NONLINEAR EVEN AND ODD DISPLACED NUMBER STATE. Modern Physics Letters B, 2006, 20, 1135-1146.	1.0	4
53	Nonlinear displaced number states. Physics Letters, Section A: General, Atomic and Solid State Physics, 2005, 339, 275-282.	0.9	5
54	Alternative proposal for the generation of the displaced number state. Physica A: Statistical Mechanics and Its Applications, 2005, 351, 251-259.	1.2	13

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55	EVEN AND ODD DISPLACED NUMBER STATE. Modern Physics Letters B, 2005, 19, 1347-1360.	1.0	2