

# Guilherme Colherinhas

## List of Publications by Year in descending order

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55  
papers

746  
citations

471371

17  
h-index

610775

24  
g-index

55  
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55  
docs citations

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times ranked

396  
citing authors

#	ARTICLE	IF	CITATIONS
1	Fullerene C60 spectroscopy in [BMIM][PF6] ionic liquid: Molecular dynamics study using polarization effects. <i>Journal of Molecular Structure</i> , 2022, 1250, 131887.	1.8	5
2	Molecular dynamics study of hydrogen bond in peptide membrane at 150–300 Å. <i>Journal of Molecular Liquids</i> , 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. <i>Journal of Molecular Liquids</i> , 2022, 359, 119308.	2.3	4
4	A molecular dynamics study of graphyne-based electrode and biocompatible ionic liquid for supercapacitor applications. <i>Journal of Molecular Liquids</i> , 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. <i>Journal of Molecular Liquids</i> , 2021, 321, 114739.	2.3	12
6	Molecular dynamic simulations, GIAO-NMR and TD-DFT spectroscopy analyze for zwitterionic isoleucine ( <i>ILE</i> ) <sub>N</sub> , 1 <sup>st</sup> in water solution. <i>Journal of Computational Chemistry</i> , 2021, 42, 344-357.	1.3	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. <i>Physical Chemistry Chemical Physics</i> , 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. <i>Journal of Molecular Liquids</i> , 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. <i>Chemical Physics Letters</i> , 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. <i>Journal of Molecular Liquids</i> , 2021, 339, 116815.	2.3	6
11	Laminar peptide structure: Energetic and structural evaluation using molecular dynamics. <i>Journal of Molecular Liquids</i> , 2021, 341, 117261.	2.3	4
12	GIAO-NMR spectroscopy of the xanthine <sup>TM</sup> s structures in water solution using S-MC/QM methodology: an evaluation of the DFT-functionals <sup>TM</sup> efficiency. <i>Journal of Molecular Liquids</i> , 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. <i>Journal of Molecular Liquids</i> , 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?. <i>Journal of Molecular Liquids</i> , 2020, 317, 113919.	2.3	18
15	A6H polypeptide membranes: Molecular dynamics simulation, GIAO-DFT-NMR and TD-DFT spectroscopy analysis. <i>Journal of Molecular Liquids</i> , 2020, 316, 113850.	2.3	19
16	Assessing the DOPC-cholesterol interactions and their influence on fullerene C60 partitioning in lipid bilayers. <i>Journal of Molecular Liquids</i> , 2020, 315, 113698.	2.3	15
17	Design and analysis of polypeptide nanofiber using full atomistic Molecular Dynamic. <i>Journal of Molecular Liquids</i> , 2020, 302, 112610.	2.3	14
18	Investigating the asymmetry in the EDL response of C <sub>60</sub> /graphene supercapacitors. <i>Physical Chemistry Chemical Physics</i> , 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. <i>Journal of Molecular Liquids</i> , 2019, 294, 111611.	2.3	13
20	Understanding the stability of polypeptide membranes in ionic liquids: a theoretical molecular dynamics study. <i>New Journal of Chemistry</i> , 2019, 43, 10151-10161.	1.4	16
21	Solvent effects on the spectroscopic properties of Damascone derivatives: A sequential Monte Carlo/Quantum Mechanics study. <i>Chemical Physics Letters</i> , 2019, 730, 531-537.	1.2	12
22	Robust Entanglement Generation in Lithium Ions Mediated by Graphene Quantum Dots Interaction. <i>Journal of Physical Chemistry A</i> , 2019, 123, 1790-1795.	1.1	3
23	Elucidating NH <sub>2</sub> -I3V3A3G3K3-COOH and NH <sub>2</sub> -K3G3A3V3I3-COOH polypeptide membranes: A classical molecular dynamics study. <i>Journal of Molecular Liquids</i> , 2019, 279, 740-749.	2.3	20
24	Spectroscopic properties and solute-solvent structural analyses for A <sub>N</sub> polypeptides in water solution: a sequential Monte Carlo/quantum mechanics (S-MC/QM) theoretical study. <i>New Journal of Chemistry</i> , 2018, 42, 19692-19700.	1.4	6
25	Stability and Structural Analysis of A <sub>6</sub> Polypeptide Nanosheets: A Theoretical Study Using the Classical Molecular Dynamics Simulation. <i>Journal of Physical Chemistry C</i> , 2018, 122, 24445-24453.	1.5	18
26	Storing Energy in Biodegradable Electrochemical Supercapacitors. <i>ACS Omega</i> , 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. <i>Journal of Molecular Modeling</i> , 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. <i>Journal of Molecular Liquids</i> , 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. <i>New Journal of Chemistry</i> , 2018, 42, 12032-12044.	1.4	6
30	Matemática básica aplicada ao ensino de física: relação entre competências e habilidades técnicas necessárias para a resolução de problemas de física segundo o Inep. <i>Ensino E Tecnologia Em Revista</i> , 2018, 2, 3.	0.0	0
31	All-boron fullerene exhibits a strong affinity to inorganic anions. <i>Chemical Physics Letters</i> , 2017, 671, 107-112.	1.2	6
32	TD-DFT and GIAO-NMR spectroscopy studies for maltose and (1±- and 1 <sup>2</sup> )-glucose in water solution using S-MC/QM polarization methodology. <i>Journal of Molecular Liquids</i> , 2017, 237, 295-303.	2.3	11
33	Hydration properties of the polyalanines by atomistic molecular dynamics. <i>Journal of Molecular Liquids</i> , 2017, 244, 285-290.	2.3	6
34	Assessing the interaction between surfactant-like peptides and lipid membranes. <i>RSC Advances</i> , 2017, 7, 35973-35981.	1.7	22
35	Elucidating the stability of bolaamphiphilic polypeptide nanosheets using atomistic molecular dynamics. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 31921-31928.	1.3	26
36	GIAO-DFT isotropic magnetic shielding constants and spin-spin coupling of tartaric acid in water solution. <i>Chemical Physics Letters</i> , 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 B <sub>80</sub> with 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 host-guest complexes: C <sub>60</sub> 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	<sup>13</sup> C chemical shifts of polyacetylene chains with charged conformational defects: A GIAO-DFT study. Chemical Physics Letters, 2011, 503, 191-196.	1.2	10
48	Isomerization effects on chemical shifts and spin-spin coupling constants of polyacetylene chains: A GIAO-DFT study. International Journal of Quantum Chemistry, 2011, 111, 1616-1625.	1.0	17
49	Theoretical analysis of the hydration of C <sub>60</sub> 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