Luis G. Dias

List of Publications by Year
in descending order

53 papers	1,287 citations	331259 21 h-index	377514 34 g-index
53 all docs	53 docs citations	53 times ranked	2431 citing authors

#	Article	IF	Citations
1	Osmotic Method for Calculating Surface Pressure of Monolayers in Molecular Dynamics Simulations. Journal of Chemical Theory and Computation, 2022, , .	2.3	2
2	Tuning aprotic solvent properties with long alkyl chain ionic liquid for lithium-based electrolytes. Journal of Materials Chemistry A, 2022, 10, 11684-11701.	5.2	9
3	Experimental mapping of a pH gradient from a positively charged micellar interface to bulk solution. Colloids and Surfaces A: Physicochemical and Engineering Aspects, 2021, 611, 125770.	2.3	9
4	Theoretical Investigation of the Na⁺ Transport Mechanism and the Performance of Ionic Liquid-Based Electrolytes in Sodium-Ion Batteries. ACS Applied Energy Materials, 2021, 4, 4444-4458.	2.5	27
5	Development of coarse-grained force field to investigate sodium-ion transport mechanisms in cyanoborate-based ionic liquid. Journal of Molecular Liquids, 2021, 338, 116648.	2.3	6
6	In vitro enantioselective inhibition of the main human CYP450 enzymes involved in drug metabolism by the chiral pesticide tebuconazole. Toxicology Letters, 2021, 351, 1-9.	0.4	5
7	Molecular Dynamics Simulations of Polymerâ€“Ionic Liquid (1-Ethyl-3-methylimidazolium) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50 Information and Modeling, 2020, 60, 485-499.	2.5	23
8	Self-Assembly of Phosphocholine Derivatives Using the ELBA Coarse-Grained Model: Micelles, Bicelles, and Reverse Micelles. Journal of Chemical Information and Modeling, 2020, 60, 522-536.	2.5	13
9	Computational insights into substituent effects on the stability and reactivity of flavylium cation analogs of anthocyanins. Arkivoc, 2020, 2020, 146-162.	0.3	2
10	Synergistic long-range effects of mutations underlie aggregation propensities of amylin analogues. Journal of Molecular Modeling, 2019, 25, 263.	0.8	5
11	An Explanation about the Use of (S)-Citronellal as a Chiral Derivatizing Agent (CDA) in 1H and 13C NMR for Sec-Butylamine, Methylbenzylamine, and Amphetamine: A Theoretical-Experimental Study. Molecules, 2019, 24, 2830.	1.7	4
12	In vitro enantioselective study of the toxicokinetic effects of chiral fungicide tebuconazole in human liver microsomes. Ecotoxicology and Environmental Safety, 2019, 181, 96-105.	2.9	26
13	Myclobutanil enantioselective risk assessment in humans through in vitro CYP450 reactions: Metabolism and inhibition studies. Food and Chemical Toxicology, 2019, 128, 202-211.	1.8	36
14	Parallel damage in mitochondria and lysosomes is an efficient way to photoinduce cell death. Autophagy, 2019, 15, 259-279.	4.3	111
15	Citronellal assumes a folded conformation in solution due to dispersion interactions: A joint NMR-DFT analysis. Journal of Molecular Structure, 2018, 1157, 401-407.	1.8	5
16	Parameterization of a coarse-grained model of cholesterol with point-dipole electrostatics. Journal of Computer-Aided Molecular Design, 2018, 32, 1259-1271.	1.3	5
17	Methylene Blue Location in (Hydroperoxized) Cardiolipin Monolayer: Implication in Membrane Photodegradation. Journal of Physical Chemistry B, 2017, 121, 8512-8522.	1.2	10
18	Counterion-mediated Ca2+ accumulation on cationic Langmuir-Blodgett films as template for CaCO3 growth. Thin Solid Films, 2017, 638, 433-440.	0.8	5

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19	Ion dehydration controls adsorption at the micellar interface: hydrotropic ions. Physical Chemistry Chemical Physics, 2017, 19, 30658-30666.	1.3	9
20	Development of constant-pH simulation methods in implicit solvent and applications in biomolecular systems. Biophysical Reviews, 2017, 9, 699-728.	1.5	40
21	Electrostatics analysis of the mutational and pH effects of the N-terminal domain self-association of the major ampullate spidroin. Soft Matter, 2016, 12, 5600-5612.	1.2	38
22	New perylenequinone derivatives from the endophytic fungus Alternaria tenuissima SS77. Tetrahedron Letters, 2016, 57, 3185-3189.	0.7	15
23	An overview of molecular dynamics simulations of oxidized lipid systems, with a comparison of ELBA and MARTINI force fields for coarse grained lipid simulations. Biochimica Et Biophysica Acta - Biomembranes, 2016, 1858, 2498-2511.	1.4	41
24	Synthesis and spectroscopic properties of luminescent tantalum(v)-Î²-diketonate complexes and their use as optical sensors and the preparation of nanostructured Ta2O5. Dalton Transactions, 2015, 44, 3829-3836.	1.6	11
25	Aggregation of photosensitizers: the role of dispersion and solvation on dimer formation energetics. Theoretical Chemistry Accounts, 2015, 134, 1.	0.5	16
26	Molecular Dynamics Simulations of the Initial-State Predict Product Distributions of Dediazoniation of Aryldiazonium in Binary Solvents. Journal of Organic Chemistry, 2015, 80, 8637-8642.	1.7	5
27	Interaction of cyclic and linear Labaditin peptides with anionic and zwitterionic micelles. Journal of Colloid and Interface Science, 2015, 438, 39-46.	5.0	6
28	Developing electrodes chemically modified with cucurbit[6]uril to detect 3,4-methylenedioxymethamphetamine (MDMA) by voltammetry. Electrochimica Acta, 2014, 121, 188-193.	2.6	44
29	A Mixed Culture of Endophytic Fungi Increases Production of Antifungal Polyketides. Journal of Chemical Ecology, 2013, 39, 1335-1342.	0.9	68
30	Effect of Counterions on the Shape, Hydration, and Degree of Order at the Interface of Cationic Micelles: The Triflate Case. Langmuir, 2013, 29, 4193-4203.	1.6	33
31	Ab initio studies of pristine and oxidized Cu3Au(100) and (111) surfaces. Journal of Materials Science, 2012, 47, 7594-7600.	1.7	7
32	Self-assembled films from chitosan and poly(vinyl sulfonic acid) on NafionÂ® for direct methanol fuel cell. Journal of the Brazilian Chemical Society, 2012, 23, 531-537.	0.6	6
33	Interactions between 1â€butylâ€3â€methylimidazolium tetrafluoroborate ionic liquid and Î³â€Al₂O₃ (100) surface calculated by density functional theory. International Journal of Quantum Chemistry, 2012, 112, 3234-3239.	1.0	14
34	Labaditin, a cyclic peptide with rich biotechnological potential: preliminary toxicological studies and structural changes in water and lipid membrane environment. Amino Acids, 2011, 40, 135-144.	1.2	22
35	Substituent effects on the pHâ€dependent multiequilibria of flavylium salt analogs of anthocyanins. Journal of Physical Organic Chemistry, 2011, 24, 1201-1208.	0.9	12
36	Diketopiperazines produced by endophytic fungi found in association with two Asteraceae species. Phytochemistry, 2010, 71, 1423-1429.	1.4	40

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37	Signatures of oxygen on<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>Cu</mml:mtext></mml:mrow><mml:mn>3</mml:mn></mml:msu From isolated impurity to oxide regimes. Physical Review B, 2010, 82, .	1.1	9
38	1-(2-Quinolyl)-2-naphthol: A new intra-intermolecular photoacidâ€“photobase molecule. Journal of Photochemistry and Photobiology A: Chemistry, 2008, 194, 37-48.	2.0	19
39	Resonance Raman study of polyynes encapsulated in single-wall carbon nanotubes. Physical Review B, 2007, 76, .	1.1	51
40	A computational study of substituted flavylium salts and their quinonoidal conjugate-bases: S0 -> S1 electronic transition, absolute pKa and reduction potential calculations by DFT and semiempirical methods. Journal of the Brazilian Chemical Society, 2007, 18, 1537-1546.	0.6	38
41	Chemical identification in the (100) surface using scanning tunneling microscopy and first-principles calculations. Surface Science, 2007, 601, 5540-5545.	0.8	16
42	Predicting Hydration Free Energies of Neutral Compounds by a Parametrization of the Polarizable Continuum Model. Journal of Physical Chemistry A, 2005, 109, 11322-11327.	1.1	9
43	Calculation of the Dipole Moment for Polypeptides Using the Generalized Born-Electronegativity Equalization Method:â€‰ Results in Vacuum and Continuum-Dielectric Solvent. Journal of Physical Chemistry B, 2004, 108, 4171-4177.	1.2	22
44	Parameterization of the electronegativity equalization method based on the charge model 1. Physical Chemistry Chemical Physics, 2002, 4, 5933-5936.	1.3	31
45	Effect of Urea on Biomimetic Systems:Â Neither Water 3-D Structure Rupture nor Direct Mechanism, Simply a More â€œPolar Waterâ€• Langmuir, 2002, 18, 319-324.	1.6	64
46	A simple method for the fast calculation of charge redistribution of solutes in an implicit solvent model. Chemical Physics, 2002, 282, 237-243.	0.9	4
47	Modulation of methylene blue photochemical properties based on adsorption at aqueous micelle interfaces. Physical Chemistry Chemical Physics, 2002, 4, 2320-2328.	1.3	222
48	SSPBE: um programa para soluÃ§Ã£o numÃ©rica da equaÃ§Ã£o de Poisson-Boltzmann em simetria esfÃ©rica com modelo de adsorÃ§Ã£o. Quimica Nova, 2002, 25, 1029-1033.	0.3	0
49	Hydrolysis of 1,8- and 2,3-naphthalic anhydrides and the mechanism of cyclization of 1,8-naphthalic acid in aqueous solutionsThe IUPAC name for naphthalic acid is napthalenedicarboxylic acid.Electronic supplementary information (ESI) available: tables containing the values of the rate constants. See http://www.rsc.org/suppdata/p2/b1/b104148g/. Perkin Transactions II RSC, 2001, , 2342-2350.	1.1	22
50	Analysis of the Bromide Ion Distribution in the Water Pool of Reverse Micelles of Hexadecyltrimethylammonium Bromide in Chloroform/n-Dodecane and Isooctane/n-Hexanol by Chemical Trapping. Langmuir, 2001, 17, 1060-1068.	1.6	23
51	Single-beam interface thermal lensing. Applied Optics, 1999, 38, 1213.	2.1	5
52	Critical Micelle Concentration and Average Aggregation Number Estimate of Zwitterionic Amphiphiles:â€‰ Salt Effect. Langmuir, 1997, 13, 5756-5758.	1.6	22
53	Assessment of Solute-Micelle Interactions in Electrokinetic Chromatography Using Quantitative Structure-Retention Relationships. , 0, , 345-366.		0