Joao Paulo C A Prates Ramalho

List of Publications by Year
in descending order

90	1,836	279798	302126
papers	citations	23 h-index	39 g-index

92	92	92	2617
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	The fate of three common plastic nanoparticles in water: A molecular dynamics study. Journal of Molecular Structure, 2022, 1249, 131520.	3.6	6
2	Development of new 2-piperidinium-4-styrylcoumarin derivatives with large Stokes shifts as potential fluorescent labels for biomolecules. RSC Advances, 2022, 12, 8477-8484.	3.6	1
3	New Red-Shifted 4-Styrylcoumarin Derivatives as Potential Fluorescent Labels for Biomolecules. Molecules, 2022, 27, 1461.	3.8	4
4	Interactions between Rhodamine Dyes and Model Membrane Systemsâ€"Insights from Molecular Dynamics Simulations. Molecules, 2022, 27, 1420.	3.8	10
5	Modeling Gd³⁺ Complexes for Molecular Dynamics Simulations: Toward a Rational Optimization of MRI Contrast Agents. Inorganic Chemistry, 2022, 61, 11837-11858.	4.0	3
6	Chiral enhancement via surface-confined supramolecular self-assembly at the electrified liquid/solid interface. Electrochimica Acta, 2021, 387, 138464.	5.2	3
7	Acetonitrile Adducts of Tranexamic Acid as Sensitive Ions for Quantification at Residue Levels in Human Plasma by UHPLC-MS/MS. Pharmaceuticals, 2021, 14, 1205.	3.8	1
8	Ambipolar pentacyclic diamides with interesting electrochemical and optoelectronic properties. Chemical Communications, 2020, 56, 14893-14896.	4.1	0
9	Organocatalysts for the Synthesis of Poly(ethylene terephthalateâ€coâ€isosorbide terephthalate): A Combined Experimental and DFT Study. Macromolecular Materials and Engineering, 2019, 304, 1900298.	3.6	11
10	Development of a Simple Method for Labeling and Identification of Protein Binders in Art. Heritage, 2019, 2, 2444-2456.	1.9	3
11	A chiral electrochemical system based on l-cysteine modified gold nanoparticles for propranolol enantiodiscrimination: Electroanalysis and computational modelling. Electrochimica Acta, 2019, 326, 134961.	5.2	21
12	Interaction of Bile Salts With Lipid Bilayers: An Atomistic Molecular Dynamics Study. Frontiers in Physiology, 2019, 10, 393.	2.8	11
13	A simple method for labelling and detection of proteinaceous binders in art using fluorescent coumarin derivativesâ€†. European Physical Journal Plus, 2019, 134, 1.	2.6	4
14	Methyl-cyclopentadienyl Ruthenium Compounds with 2,2â€²-Bipyridine Derivatives Display Strong Anticancer Activity and Multidrug Resistance Potential. Inorganic Chemistry, 2018, 57, 4629-4639.	4.0	36
15	A magnetic controllable tool for the selective enrichment of dimethoate from olive oil samples: A responsive molecular imprinting-based approach. Food Chemistry, 2018, 254, 309-316.	8.2	21
16	Gaining insight into the photophysical properties of a coumarin STP ester with potential for bioconjugation. New Journal of Chemistry, 2018, 42, 16635-16645.	2.8	3
17	A photoswitchable â€œhost-guestâ€•approach for the selective enrichment of dimethoate from olive oil. Analytica Chimica Acta, 2018, 1035, 60-69.	5.4	6
18	Adsorption of CO on the rutile TiO₂(110) surface: a dispersion-corrected density functional theory study. Physical Chemistry Chemical Physics, 2017, 19, 2487-2494.	2.8	11

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19	Conformational Preference and Spectroscopical Characteristics of the Active Pharmaceutical Ingredient Levetiracetam. Journal of Pharmaceutical Sciences, 2017, 106, 3564-3573.	3.3	2
20	Mechanisms of removal of three widespread pharmaceuticals by two clay materials. Journal of Hazardous Materials, 2017, 323, 575-583.	12.4	66
21	Adenine as an organocatalyst for the ring-opening polymerization of lactide: scope, mechanism and access to adenine-functionalized polylactide. Reaction Chemistry and Engineering, 2016, 1, 508-520.	3.7	19
22	Diphenylhexatriene membrane probes DPH and TMA-DPH: A comparative molecular dynamics simulation study. Biochimica Et Biophysica Acta - Biomembranes, 2016, 1858, 2647-2661.	2.6	87
23	Fluorescence of nitrobenzoxadiazole (NBD)-labeled lipids in model membranes is connected not to lipid mobility but to probe location. Physical Chemistry Chemical Physics, 2016, 18, 7042-7054.	2.8	55
24	Fluorinated surfactants in solution: Diffusion coefficients of fluorinated alcohols in water. Fluid Phase Equilibria, 2016, 407, 322-333.	2.5	9
25	Behaviour of NBD-head group labelled phosphatidylethanolamines in POPC bilayers: a molecular dynamics study. Physical Chemistry Chemical Physics, 2015, 17, 20066-20079.	2.8	28
26	Design and development of molecularly imprinted polymers for the selective extraction of deltamethrin in olive oil: An integrated computational-assisted approach. Journal of Chromatography A, 2015, 1409, 1-10.	3.7	32
27	Palladium catalysed sequential imine arylation/Suzukiâ€“Miyaura coupling: synthesis of Î±-(biarylyl)benzylamines. Tetrahedron, 2015, 71, 3314-3324.	1.9	6
28	Prediction of diffusion coefficients of chlorophenols in water by computer simulation. Fluid Phase Equilibria, 2015, 396, 9-19.	2.5	20
29	Conformational landscape and low lying excited states of imatinib. Journal of Molecular Modeling, 2015, 21, 84.	1.8	5
30	Influence of the sterol aliphatic side chain on membrane properties: a molecular dynamics study. Physical Chemistry Chemical Physics, 2015, 17, 22736-22748.	2.8	13
31	A catalytic route to dibenzodiazepines involving Buchwaldâ€“Hartwig coupling: reaction scope and mechanistic consideration. RSC Advances, 2015, 5, 99990-99999.	3.6	12
32	A DFT study on the adsorption of benzodiazepines to vermiculite surfaces. Journal of Molecular Modeling, 2014, 20, 2336.	1.8	14
33	Mono(Î·5-cyclopentadienyl)metal(II) Complexes with Thienyl Acetylide Chromophores: Synthesis, Electrochemical Studies, and First Hyperpolarizabilities. Organometallics, 2014, 33, 4655-4671.	2.3	18
34	Diffusion Coefficients of Fluorinated Surfactants in Water: Experimental Results and Prediction by Computer Simulation. Journal of Chemical & Engineering Data, 2014, 59, 3151-3159.	1.9	31
35	Adsorption of sulfamethoxazole molecule on silver colloids: A joint SERS and DFT study. Journal of Molecular Structure, 2014, 1073, 71-76.	3.6	19
36	Adsorption of two phenoxyacid compounds on a clay surface: a theoretical study. Adsorption, 2013, 19, 937-944.	3.0	16

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37	Behavior of Fluorescent Cholesterol Analogues Dehydroergosterol and Cholestatrienol in Lipid Bilayers: A Molecular Dynamics Study. Journal of Physical Chemistry B, 2013, 117, 5806-5819.	2.6	32
38	Accounting for van der Waals interactions between adsorbates and surfaces in density functional theory based calculations: selected examples. RSC Advances, 2013, 3, 13085.	3.6	138
39	A Family of Styrylcoumarins: Synthesis, Spectroscopic, Photophysical and Photochemical Properties. ChemPlusChem, 2013, 78, 789-792.	2.8	4
40	Benzo[c]thiophene Chromophores Linked to Cationic Fe and Ru Derivatives for NLO Materials: Synthesis Characterization and Quadratic Hyperpolarizabilities. European Journal of Inorganic Chemistry, 2013, 2013, 3506-3517.	2.0	9
41	NBD-Labeled Cholesterol Analogues in Phospholipid Bilayers: Insights from Molecular Dynamics. Journal of Physical Chemistry B, 2013, 117, 13731-13742.	2.6	31
42	Effect of Amphipathic HIV Fusion Inhibitor Peptides on POPC and POPC/Cholesterol Membrane Properties: A Molecular Simulation Study. International Journal of Molecular Sciences, 2013, 14, 14724-14743.	4.1	6
43	Molecular Dynamics Simulation of HIV Fusion Inhibitor T-1249: Insights on Peptide-Lipid Interaction. Computational and Mathematical Methods in Medicine, 2012, 2012, 1-14.	1.3	9
44	Switchable Nonlinear Optical Properties of Î·⁵-Monocyclopentadienylmetal Complexes: A DFT Approach. Journal of Chemical Information and Modeling, 2012, 52, 1970-1983.	5.4	20
45	Assessing the importance of Van der Waals interactions on the adsorption of azobenzene on the rutile TiO2(110) surface. Chemical Physics Letters, 2012, 545, 60-65.	2.6	13
46	Structure and Phase Transformations of DPPC Lipid Bilayers in the Presence of Nanoparticles: Insights from Coarse-Grained Molecular Dynamics Simulations. Langmuir, 2011, 27, 3723-3730.	3.5	80
47	Excess Thermodynamic Properties of Mixtures Involving Xenon and Light Alkanes: A Study of Their Temperature Dependence by Computer Simulation. Journal of Physical Chemistry B, 2011, 115, 9745-9765.	2.6	7
48	Recent Developments in Molecular Dynamics Simulations of Fluorescent Membrane Probes. Molecules, 2011, 16, 5437-5452.	3.8	57
49	Molecular dynamics simulations of T-20 HIV fusion inhibitor interacting with model membranes. Biophysical Chemistry, 2011, 159, 275-286.	2.8	11
50	Evaluation of phosphinoamidoesterâ€derived Pd catalysts in the asymmetric allylic alkylation reaction: Theoretical studies and mechanistic insights. Chirality, 2011, 23, 383-388.	2.6	7
51	Theoretical study of the adsorption and dissociation of azobenzene on the rutile TiO2(110) surface. Chemical Physics Letters, 2011, 501, 379-384.	2.6	16
52	Chiral monooxazolines as modular copper(I)-heterocomplex building blocks: investigations on the catalytic asymmetric cyclopropanation of alkenes. Tetrahedron, 2011, 67, 4640-4648.	1.9	8
53	Direct calculation of FÃ¶rster orientation factor of membrane probes by molecular simulation. Computational and Theoretical Chemistry, 2010, 946, 107-112.	1.5	16
54	Structure and conformation of HIV fusion inhibitor peptide T-1249 in presence of model membranes: A molecular dynamics study. Computational and Theoretical Chemistry, 2010, 946, 119-124.	1.5	9

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55	DFT studies on thiophene acetylide Ru(II) complexes for nonlinear optics: Structureâ€“function relationships and solvent effects. Computational and Theoretical Chemistry, 2010, 946, 33-42.	1.5	23
56	Adsorption of Xe atoms on the TiO2(110) surface: A density functional study. Surface Science, 2010, 604, 428-434.	1.9	15
57	Molecular simulation of C60 adsorption onto a TiO2 rutile (110) surface. Applied Surface Science, 2010, 256, 5365-5369.	6.1	4
58	A Comparison of (R,R)â€Meâ€DUPHOS and (R,R)â€DUPHOSâ€iPr Ligands in the Pd⁰â€Catalysed Asymmetric Allylic Alkylation Reaction: Stereochemical and Kinetic Considerations. European Journal of Organic Chemistry, 2009, 2009, 6311-6317.	2.4	9
59	Arylid-OX and Arylid-BOX derived catalysts: applications in catalytic asymmetric cyclopropanation. Tetrahedron: Asymmetry, 2009, 20, 1272-1278.	1.8	13
60	Fluorescent membrane probesâ€™ behavior in lipid bilayers: insights from molecular dynamics simulations. Biophysical Reviews, 2009, 1, 141-148.	3.2	37
61	The benzilic ester rearrangement: synthesis of labelled compounds and theoretical studies. Journal of Physical Organic Chemistry, 2009, 22, 735-739.	1.9	7
62	Role played by the organometallic fragment on the first hyperpolarizability of ironâ€“acetylide complexes: A TD-DFT study. Computational and Theoretical Chemistry, 2009, 900, 110-117.	1.5	19
63	Tâ€20 and Tâ€1249 HIV fusion inhibitors' structure and conformation in solution: a molecular dynamics study. Journal of Peptide Science, 2008, 14, 442-447.	1.4	18
64	Effects of fluorescent probe NBD-PC on the structure, dynamics and phase transition of DPPC. A molecular dynamics and differential scanning calorimetry study. Biochimica Et Biophysica Acta - Biomembranes, 2008, 1778, 491-501.	2.6	58
65	Experimental and Simulation Study of n-Heptane Adsorption on Rutile. Adsorption Science and Technology, 2007, 25, 517-530.	3.2	4
66	Location and dynamics of acyl chain NBD-labeled phosphatidylcholine (NBD-PC) in DPPC bilayers. A molecular dynamics and time-resolved fluorescence anisotropy study. Biochimica Et Biophysica Acta - Biomembranes, 2007, 1768, 467-478.	2.6	82
67	Adsorption of Normal Pentane on the Surface of Rutile. Experimental Results and Simulations. Langmuir, 2007, 23, 7555-7561.	3.5	9
68	Excess Thermodynamics of Mixtures Involving Xenon and Light Linear Alkanes by Computer Simulation. Journal of Physical Chemistry B, 2007, 111, 6437-6443.	2.6	7
69	Simulation study of argon adsorption on (001) faces of phyllosilicates. Applied Surface Science, 2007, 253, 5628-5632.	6.1	4
70	Cu(I) catalysed cyclopropanation of olefins: Stereoselectivity studies with Arylid-Box and Isbut-Box ligands. Journal of Organometallic Chemistry, 2007, 692, 4863-4874.	1.8	28
71	Density functional theory calculations on Î·5-monocyclopentadienylnitrilecobalt complexes concerning their second-order nonlinear optical properties. Computational and Theoretical Chemistry, 2005, 729, 109-113.	1.5	41
72	Molecular simulations of nitrogen adsorption in pure silica MCM-41 materials. Computational and Theoretical Chemistry, 2005, 729, 65-69.	1.5	26

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73	Surface topography problem and argon adsorption on crystalline faces: Monte-Carlo and lattice-gas model simulations. Applied Surface Science, 2005, 252, 529-537.	6.1	2
74	Adsorption of Ar atoms on the relaxed defect-freeTiO2(110)surface. Physical Review B, 2005, 71, .	3.2	17
75	Isbut-Box: A new chiral C2 symmetric bis-oxazoline for catalytic enantioselective synthesis. Journal of Molecular Catalysis A, 2005, 236, 38-45.	4.8	20
76	Cesiumauride Ammonia (1/1), CsAuâ‹…NH3: A Crystalline Analogue to Alkali Metals Dissolved in Ammonia?. Angewandte Chemie - International Edition, 2002, 41, 120-124.	13.8	53
77	Adsorption integral equation via complex approximation with constraints: kernel of general form. Journal of Computational Chemistry, 2001, 22, 1058-1066.	3.3	1
78	On the Structure of a Local Isotherm and Solution to the Adsorption Integral Equation. Langmuir, 2000, 16, 1918-1923.	3.5	7
79	Phase diagram of C60 from ab initio intermolecular potential. Journal of Chemical Physics, 2000, 113, 738-743.	3.0	29
80	First-Principles Determination of the Dispersion Interaction between Fullerenes and Their Intermolecular Potential. Physical Review Letters, 1997, 79, 3873-3876.	7.8	106
81	Influence of surface ionization on the adsorption of aqueous zinc species by activated carbons. Carbon, 1997, 35, 403-410.	10.3	60
82	High dimensional geometry in statistical mechanics. A new microcanonical sampling method. Pure and Applied Chemistry, 1996, 68, 1509-1514.	1.9	3
83	Hypervolumes in microcanonical Monte Carlo. Computer Physics Communications, 1995, 90, 73-80.	7.5	7
84	Path integral Monte Carlo simulations: Study of the efficiency of energy estimators. Journal of Chemical Physics, 1995, 103, 5720-5724.	3.0	9
85	Numerical simulation of surface ionisation and specific adsorption on a two-site model of a carbon surface. Journal of the Chemical Society, Faraday Transactions, 1995, 91, 2179.	1.7	22
86	Light metal ions in water: Quantal and classical simulations for 7Li+. Journal of Molecular Liquids, 1994, 60, 237-249.	4.9	0
87	Improved propagators for the path integral study of quantum systems. Journal of Chemical Physics, 1993, 98, 3300-3305.	3.0	2
88	A Monte Carlo and transfer-matrix grid path-integral study of the vibrational structure of Br2 in solid argon. Chemical Physics Letters, 1991, 184, 53-60.	2.6	10
89	Theoretical Study on the Influence of Iron Mordant in the Optical Properties of Natural Dyes. Materials Science Forum, 0, 587-588, 608-612.	0.3	0
90	Recent Developments in the Study of the Behavior of Fluorescent Membrane Probes in Lipid Bilayers: Molecular Dynamics Approach. , 0, , .		0