Pedro Morgado

List of Publications by Year in descending order

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49 papers	1,057 citations	331670 21 h-index	434195 31 g-index
49 all docs	49 docs citations	49 times ranked	1016 citing authors

#	Article	IF	Citations
1	Optimized all-atom force field for alkynes within the OPLS-AA framework. Fluid Phase Equilibria, 2022, 554, 113314.	2.5	3
2	Breaking the Structure of Liquid Hydrogenated Alcohols Using Perfluorinated tert-Butanol: A Multitechnique Approach (Infrared, Raman, and X-ray Scattering) Analyzed by DFT and Molecular Dynamics Calculations. Journal of Physical Chemistry B, 2022, 126, 1992-2004.	2.6	8
3	Gaseous hetero dimers of perfluoro tert-butyl alcohol with hydrogenated alcohols by infrared spectroscopy and quantum DFT calculations. Chemical Physics, 2021, 544, 111110.	1.9	4
4	Solubility of water in mixtures of (n-alkanes + n-perfluoroalkanes) and in n-perfluoroalkylalkanes: experiments and modelling with the SAFT-Î³ Mie group-contribution approach. Molecular Physics, 2021, 119, .	1.7	1
5	The structure of liquid perfluoro Tert-Butanol using Infrared, Raman and X-Ray scattering analyzed by quantum DFT calculations and molecular Dynamics. Chemical Physics Letters, 2021, 779, 138844.	2.6	3
6	Solubility of xenon in liquid n-alkanes and cycloalkanes by computer simulation. Towards the perfect anaesthetic. Journal of Molecular Liquids, 2021, 340, 117272.	4.9	0
7	Solubility of water in n-alkanes: New experimental measurements and molecular dynamics simulations. Fluid Phase Equilibria, 2020, 503, 112322.	2.5	10
8	Preaggregation of Asphaltenes in the Presence of Natural Polymers by Molecular Dynamics Simulation. Energy & Fuels, 2020, 34, 1581-1591.	5.1	17
9	Detailed surface characterization of highly fluorinated liquid alcohols: Experimental surface tensions, molecular simulations and soft-SAFT theory. Journal of Molecular Liquids, 2020, 300, 112294.	4.9	8
10	Solubility of water in perfluoroalkylalkanes surfactants: Evidence of specific interaction between water and the surfactant molecule. Fluid Phase Equilibria, 2020, 522, 112754.	2.5	4
11	Langmuir Films of Perfluorinated Fatty Alcohols: Evidence of Spontaneous Formation of Solid Aggregates at Zero Surface Pressure and Very Low Surface Density. Nanomaterials, 2020, 10, 2257.	4.1	5
12	Modeling the Fluid-Phase Equilibria of Semifluorinated Alkanes and Mixtures of (n-Alkanes +) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 5 & Engineering Data, 2020, 65, 5909-5919.	1.9	4
13	Towards Aqueous â€“ Fluorous â€“ Hydrogenous emulsions: Phase equilibria and liquid structure of (waterÂ+ 1H,1H-PerfluorobutanolÂ+ 1-butanol) ternary mixture. Fluid Phase Equilibria, 2020, 522, 112737.	2.5	7
14	From nano-seggregation to mesophases: probing the liquid structure of perfluoroalkylalkanes with ¹²⁹Xe NMR spectroscopy. Physical Chemistry Chemical Physics, 2020, 22, 14736-14747.	2.8	16
15	Sorption/Diffusion Contributions to the Gas Permeation Properties of Bi-Soft Segment Polyurethane/Polycaprolactone Membranes for Membrane Blood Oxygenators. Membranes, 2020, 10, 8.	3.0	9
16	Modelling the thermodynamic properties and fluid-phase equilibria of n-perfluoroalkanes and their binary mixtures with the SAFT-Î³ Mie group contribution equation of state. Molecular Physics, 2020, 118, e1722270.	1.7	2
17	Liquidâ€“liquid interfaces: Waterâ€“perfluoroalkanes and waterâ€“perfluoroalkylalkanes, experimental interfacial tensions and molecular simulation. Journal of Molecular Liquids, 2020, 312, 113385.	4.9	15
18	Surface crystallization of ionic liquid crystals. Physical Chemistry Chemical Physics, 2019, 21, 17792-17800.	2.8	6

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19	Spontaneous self-assembly and structure of perfluoroalkylalkane surfactant hemimicelles by molecular dynamics simulations. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 14868-14873.	7.1	34
20	Structure of Langmuir Monolayers of Perfluorinated Fatty Acids: Evidence of a New 2D Smectic C Phase. Molecules, 2019, 24, 3590.	3.8	7
21	From nano-emulsions to phase separation: evidence of nano-segregation in (alkane + perfluoroalkane) mixtures using ¹²⁹Xe NMR Spectroscopy. Physical Chemistry Chemical Physics, 2019, 21, 3742-3751.	2.8	21
22	Understanding the interactions of imidazolium-based ionic liquids with cell membrane models. Physical Chemistry Chemical Physics, 2018, 20, 29764-29777.	2.8	27
23	Alkane Coiling in Perfluoroalkane Solutions: A New Primitive Solvophobic Effect. Langmuir, 2017, 33, 11429-11435.	3.5	28
24	Perfluoropolyethers: Development of an All-Atom Force Field for Molecular Simulations and Validation with New Experimental Vapor Pressures and Liquid Densities. Journal of Physical Chemistry B, 2017, 121, 6588-6600.	2.6	16
25	Crystalline-like structures and multilayering in Langmuir films of ionic liquids at the airâ€“water interface. Chemical Communications, 2016, 52, 5585-5588.	4.1	10
26	Liquid Mixtures Involving Hydrogenated and Fluorinated Alcohols: Thermodynamics, Spectroscopy, and Simulation. Journal of Physical Chemistry B, 2016, 120, 10091-10105.	2.6	27
27	SAFT-Î³ force field for the simulation of molecular fluids: 8. Hetero-segmented coarse-grained models of perfluoroalkylalkanes assessed with new vapourâ€“liquid interfacial tension data. Molecular Physics, 2016, 114, 2597-2614.	1.7	41
28	Vapor pressure and liquid density of fluorinated alcohols: Experimental, simulation and GC-SAFT-VR predictions. Fluid Phase Equilibria, 2016, 425, 297-304.	2.5	17
29	Fluorinated surfactants in solution: Diffusion coefficients of fluorinated alcohols in water. Fluid Phase Equilibria, 2016, 407, 322-333.	2.5	9
30	Vapor Pressure of Perfluoroalkylalkanes: The Role of the Dipole. Journal of Physical Chemistry B, 2015, 119, 1623-1632.	2.6	30
31	High-temperature vapourâ€“liquid equilibrium for ethanolâ€“1-propanol mixtures and modeling with SAFT-VR. Fluid Phase Equilibria, 2015, 398, 5-9.	2.5	4
32	Prediction of diffusion coefficients of chlorophenols in water by computer simulation. Fluid Phase Equilibria, 2015, 396, 9-19.	2.5	20
33	Cation Alkyl Side Chain Length and Symmetry Effects on the Surface Tension of Ionic Liquids. Langmuir, 2014, 30, 6408-6418.	3.5	75
34	Charge Templates in Aromatic Plus Ionic Liquid Systems Revisited: NMR Experiments and Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2014, 118, 5772-5780.	2.6	21
35	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
36	Probing the Structure of Liquids with ¹²⁹Xe NMR Spectroscopy: n-Alkanes, Cycloalkanes, and Branched Alkanes. Journal of Physical Chemistry B, 2013, 117, 9014-9024.	2.6	21

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37	Using ¹²⁹Xe NMR to Probe the Structure of Ionic Liquids. Journal of Physical Chemistry Letters, 2013, 4, 2758-2762.	4.6	26
38	Liquid Mixtures Involving Hydrogenated and Fluorinated Chains: (p, Ï¸ T, x) Surface of (Ethanol + 2,2,2-Trifluoroethanol), Experimental and Simulation. Journal of Physical Chemistry B, 2013, 117, 9709-9717.	2.6	31
39	Viscosity of liquid systems involving hydrogenated and fluorinated substances: Liquid mixtures of (hexane+perfluorohexane). Fluid Phase Equilibria, 2013, 358, 161-165.	2.5	22
40	High-temperature vapourâ€“liquid equilibrium for the (water+alcohol) systems and modelling with SAFT-VR: 2. Water-1-propanol. Journal of Chemical Thermodynamics, 2013, 60, 15-18.	2.0	11
41	High-temperature vapourâ€“liquid equilibrium for the waterâ€“alcohol systems and modeling with SAFT-VR: 1. Waterâ€“ethanol. Fluid Phase Equilibria, 2013, 341, 48-53.	2.5	16
42	Systems Involving Hydrogenated and Fluorinated Chains: Volumetric Properties of Perfluoroalkanes and Perfluoroalkylalkane Surfactants. Journal of Physical Chemistry B, 2011, 115, 15013-15023.	2.6	34
43	Viscosity of Liquid Perfluoroalkanes and Perfluoroalkylalkane Surfactants. Journal of Physical Chemistry B, 2011, 115, 9130-9139.	2.6	42
44	Perfluoroalkanes and perfluoroalkylalkane surfactants in solution: Partial molar volumes in n-octane and hetero-SAFT-VR modelling. Fluid Phase Equilibria, 2011, 306, 76-81.	2.5	28
45	Solution Behavior of Perfluoroalkanes and Perfluoroalkylalkane Surfactants in n-Octane. Journal of Physical Chemistry C, 2007, 111, 15962-15968.	3.1	34
46	Liquid Phase Behavior of Perfluoroalkylalkane Surfactants. Journal of Physical Chemistry B, 2007, 111, 2856-2863.	2.6	52
47	Fluid-Phase Behavior of {1-Hexyl-3-methylimidazolium Bis(trifluoromethylsulfonyl) Imide, [C6mim][NTf2], + C2â^'C8n-Alcohol} Mixtures:â€‰ Liquidâ^'Liquid Equilibrium and Excess Volumesâ€¡. Journal of Chemical & Engineering Data, 2006, 51, 2215-2221.	1.9	104
48	Predicting the Phase Behavior of Nitrogen +n-Alkanes for Enhanced Oil Recovery from the SAFT-VR Approach:Â Examining the Effect of the Quadrupole Moment. Journal of Physical Chemistry B, 2006, 110, 24083-24092.	2.6	43
49	Modelling the phase behaviour and excess properties of alkane + perfluoroalkane binary mixtures with the SAFTâ€“VR approach. Fluid Phase Equilibria, 2005, 228-229, 389-393.	2.5	53