

Pedro Morgado

List of Publications by Year in descending order

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49
papers

1,057
citations

331259

21
h-index

433756

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. <i>Fluid Phase Equilibria</i> , 2022, 554, 113314.	1.4	3
2	Breaking the Structure of Liquid Hydrogenated Alcohols Using Perfluorinated <i>tert</i> -Butanol: A Multitechnique Approach (Infrared, Raman, and X-ray Scattering) Analyzed by DFT and Molecular Dynamics Calculations. <i>Journal of Physical Chemistry B</i> , 2022, 126, 1992-2004.	1.2	8
3	Gaseous hetero dimers of perfluoro <i>tert</i> -butyl alcohol with hydrogenated alcohols by infrared spectroscopy and quantum DFT calculations. <i>Chemical Physics</i> , 2021, 544, 111110.	0.9	4
4	Solubility of water in mixtures of (n-alkanes + n-perfluoroalkanes) and in n-perfluoroalkylalkanes: experiments and modelling with the SAFT- λ^3 Mie group-contribution approach. <i>Molecular Physics</i> , 2021, 119, .	0.8	1
5	The structure of liquid perfluoro <i>Tert</i> -Butanol using Infrared, Raman and X-Ray scattering analyzed by quantum DFT calculations and molecular Dynamics. <i>Chemical Physics Letters</i> , 2021, 779, 138844.	1.2	3
6	Solubility of xenon in liquid n-alkanes and cycloalkanes by computer simulation. Towards the perfect anaesthetic. <i>Journal of Molecular Liquids</i> , 2021, 340, 117272.	2.3	0
7	Solubility of water in n-alkanes: New experimental measurements and molecular dynamics simulations. <i>Fluid Phase Equilibria</i> , 2020, 503, 112322.	1.4	10
8	Preaggregation of Asphaltenes in the Presence of Natural Polymers by Molecular Dynamics Simulation. <i>Energy & Fuels</i> , 2020, 34, 1581-1591.	2.5	17
9	Detailed surface characterization of highly fluorinated liquid alcohols: Experimental surface tensions, molecular simulations and soft-SAFT theory. <i>Journal of Molecular Liquids</i> , 2020, 300, 112294.	2.3	8
10	Solubility of water in perfluoroalkylalkanes surfactants: Evidence of specific interaction between water and the surfactant molecule. <i>Fluid Phase Equilibria</i> , 2020, 522, 112754.	1.4	4
11	Langmuir Films of Perfluorinated Fatty Alcohols: Evidence of Spontaneous Formation of Solid Aggregates at Zero Surface Pressure and Very Low Surface Density. <i>Nanomaterials</i> , 2020, 10, 2257.	1.9	5
12	Modeling the Fluid-Phase Equilibria of Semifluorinated Alkanes and Mixtures of (n-Alkanes +) <i>Engineering Data</i> , 2020, 65, 5909-5919.	1.0	4
13	Towards Aqueous "Fluorous" Hydrogenous emulsions: Phase equilibria and liquid structure of (water + 1H,1H-Perfluorobutanol + 1-butanol) ternary mixture. <i>Fluid Phase Equilibria</i> , 2020, 522, 112737.	1.4	7
14	From nano-segregation to mesophases: probing the liquid structure of perfluoroalkylalkanes with ^{129}Xe NMR spectroscopy. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 14736-14747.	1.3	16
15	Sorption/Diffusion Contributions to the Gas Permeation Properties of Bi-Soft Segment Polyurethane/Polycaprolactone Membranes for Membrane Blood Oxygenators. <i>Membranes</i> , 2020, 10, 8.	1.4	9
16	Modelling the thermodynamic properties and fluid-phase equilibria of n-perfluoroalkanes and their binary mixtures with the SAFT- λ^3 Mie group contribution equation of state. <i>Molecular Physics</i> , 2020, 118, e1722270.	0.8	2
17	Liquid-liquid interfaces: Water-perfluoroalkanes and water-perfluoroalkylalkanes, experimental interfacial tensions and molecular simulation. <i>Journal of Molecular Liquids</i> , 2020, 312, 113385.	2.3	15
18	Surface crystallization of ionic liquid crystals. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 17792-17800.	1.3	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.	3.3	34
20	Structure of Langmuir Monolayers of Perfluorinated Fatty Acids: Evidence of a New 2D Smectic C Phase. Molecules, 2019, 24, 3590.	1.7	7
21	From nano-emulsions to phase separation: evidence of nano-segregation in (alkane + perfluoroalkane) mixtures using ¹²⁹ Xe NMR Spectroscopy. Physical Chemistry Chemical Physics, 2019, 21, 3742-3751.	1.3	21
22	Understanding the interactions of imidazolium-based ionic liquids with cell membrane models. Physical Chemistry Chemical Physics, 2018, 20, 29764-29777.	1.3	27
23	Alkane Coiling in Perfluoroalkane Solutions: A New Primitive Solvophobic Effect. Langmuir, 2017, 33, 11429-11435.	1.6	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.	1.2	16
25	Crystalline-like structures and multilayering in Langmuir films of ionic liquids at the air-water interface. Chemical Communications, 2016, 52, 5585-5588.	2.2	10
26	Liquid Mixtures Involving Hydrogenated and Fluorinated Alcohols: Thermodynamics, Spectroscopy, and Simulation. Journal of Physical Chemistry B, 2016, 120, 10091-10105.	1.2	27
27	SAFT- γ force field for the simulation of molecular fluids: 8. Hetero-segmented coarse-grained models of perfluoroalkylalkanes assessed with new vapour-liquid interfacial tension data. Molecular Physics, 2016, 114, 2597-2614.	0.8	41
28	Vapor pressure and liquid density of fluorinated alcohols: Experimental, simulation and GC-SAFT-VR predictions. Fluid Phase Equilibria, 2016, 425, 297-304.	1.4	17
29	Fluorinated surfactants in solution: Diffusion coefficients of fluorinated alcohols in water. Fluid Phase Equilibria, 2016, 407, 322-333.	1.4	9
30	Vapor Pressure of Perfluoroalkylalkanes: The Role of the Dipole. Journal of Physical Chemistry B, 2015, 119, 1623-1632.	1.2	30
31	High-temperature vapour-liquid equilibrium for ethanol-1-propanol mixtures and modeling with SAFT-VR. Fluid Phase Equilibria, 2015, 398, 5-9.	1.4	4
32	Prediction of diffusion coefficients of chlorophenols in water by computer simulation. Fluid Phase Equilibria, 2015, 396, 9-19.	1.4	20
33	Cation Alkyl Side Chain Length and Symmetry Effects on the Surface Tension of Ionic Liquids. Langmuir, 2014, 30, 6408-6418.	1.6	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.	1.2	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.	1.0	31
36	Probing the Structure of Liquids with ¹²⁹ Xe NMR Spectroscopy: <i>n</i> -Alkanes, Cycloalkanes, and Branched Alkanes. Journal of Physical Chemistry B, 2013, 117, 9014-9024.	1.2	21

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37	Using ¹²⁹ Xe NMR to Probe the Structure of Ionic Liquids. Journal of Physical Chemistry Letters, 2013, 4, 2758-2762.	2.1	26
38	Liquid Mixtures Involving Hydrogenated and Fluorinated Chains: (<i>p</i> , <i>T</i> , <i>x</i>) Surface of (Ethanol + 2,2,2-Trifluoroethanol), Experimental and Simulation. Journal of Physical Chemistry B, 2013, 117, 9709-9717.	1.2	31
39	Viscosity of liquid systems involving hydrogenated and fluorinated substances: Liquid mixtures of (hexane+perfluorohexane). Fluid Phase Equilibria, 2013, 358, 161-165.	1.4	22
40	High-temperature vapour-liquid equilibrium for the (water+alcohol) systems and modelling with SAFT-VR: 2. Water-1-propanol. Journal of Chemical Thermodynamics, 2013, 60, 15-18.	1.0	11
41	High-temperature vapour-liquid equilibrium for the water-alcohol systems and modeling with SAFT-VR: 1. Water-ethanol. Fluid Phase Equilibria, 2013, 341, 48-53.	1.4	16
42	Systems Involving Hydrogenated and Fluorinated Chains: Volumetric Properties of Perfluoroalkanes and Perfluoroalkylalkane Surfactants. Journal of Physical Chemistry B, 2011, 115, 15013-15023.	1.2	34
43	Viscosity of Liquid Perfluoroalkanes and Perfluoroalkylalkane Surfactants. Journal of Physical Chemistry B, 2011, 115, 9130-9139.	1.2	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.	1.4	28
45	Solution Behavior of Perfluoroalkanes and Perfluoroalkylalkane Surfactants in <i>n</i> -Octane. Journal of Physical Chemistry C, 2007, 111, 15962-15968.	1.5	34
46	Liquid Phase Behavior of Perfluoroalkylalkane Surfactants. Journal of Physical Chemistry B, 2007, 111, 2856-2863.	1.2	52
47	Fluid-Phase Behavior of {1-Hexyl-3-methylimidazolium Bis(trifluoromethylsulfonyl) Imide, [C6mim][NTf2], + C ₂ ~C ₈ -Alcohol} Mixtures: Liquid-Liquid Equilibrium and Excess Volumes. Journal of Chemical & Engineering Data, 2006, 51, 2215-2221.	1.0	104
48	Predicting the Phase Behavior of Nitrogen +n-Alkanes for Enhanced Oil Recovery from the SAFT-VR Approach: Examining the Effect of the Quadrupole Moment. Journal of Physical Chemistry B, 2006, 110, 24083-24092.	1.2	43
49	Modelling the phase behaviour and excess properties of alkane + perfluoroalkane binary mixtures with the SAFT-VR approach. Fluid Phase Equilibria, 2005, 228-229, 389-393.	1.4	53