Eduardo J M Filipe

List of Publications by Year
in descending order

78	1,881	257357 24	276775 41
papers	citations	h-index	g-index

78	78	78	1536
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Optimized all-atom force field for alkynes within the OPLS-AA framework. Fluid Phase Equilibria, 2022, 554, 113314.	1.4	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.	1.2	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.	0.9	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, .	0.8	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.	1.2	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.	2.3	0
7	Solubility of water in n-alkanes: New experimental measurements and molecular dynamics simulations. Fluid Phase Equilibria, 2020, 503, 112322.	1.4	10
8	Preaggregation of Asphaltenes in the Presence of Natural Polymers by Molecular Dynamics Simulation. Energy & Fuels, 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. Journal of Molecular Liquids, 2020, 300, 112294.	2.3	8
10	Solubility of water in perfluoroalkylalkanes surfactants: Evidence of specific interaction between water and the surfactant molecule. Fluid Phase Equilibria, 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. Nanomaterials, 2020, 10, 2257.	1.9	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.	1.0	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.	1.4	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.	1.3	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.	1.4	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.	0.8	2
17	Liquidâ€“liquid interfaces: Waterâ€“perfluoroalkanes and waterâ€“perfluoroalkylalkanes, experimental interfacial tensions and molecular simulation. Journal of Molecular Liquids, 2020, 312, 113385.	2.3	15
18	Polyurethane urea membranes for membrane blood oxygenators: synthesis and gas permeation properties. , 2019, , .		1

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19	Surface crystallization of ionic liquid crystals. Physical Chemistry Chemical Physics, 2019, 21, 17792-17800.	1.3	6
20	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
21	Structure of Langmuir Monolayers of Perfluorinated Fatty Acids: Evidence of a New 2D Smectic C Phase. Molecules, 2019, 24, 3590.	1.7	7
22	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.	1.3	21
23	Evidence of lying molecules in the structure of the most condensed phase of semi-fluorinated alkane monolayers. Nanoscale, 2018, 10, 2310-2316.	2.8	9
24	Understanding the interactions of imidazolium-based ionic liquids with cell membrane models. Physical Chemistry Chemical Physics, 2018, 20, 29764-29777.	1.3	27
25	Alkane Coiling in Perfluoroalkane Solutions: A New Primitive Solvophobic Effect. Langmuir, 2017, 33, 11429-11435.	1.6	28
26	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
27	Crystalline-like structures and multilayering in Langmuir films of ionic liquids at the airâ€“water interface. Chemical Communications, 2016, 52, 5585-5588.	2.2	10
28	Liquid Mixtures Involving Hydrogenated and Fluorinated Alcohols: Thermodynamics, Spectroscopy, and Simulation. Journal of Physical Chemistry B, 2016, 120, 10091-10105.	1.2	27
29	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.	0.8	41
30	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
31	Fluorinated surfactants in solution: Diffusion coefficients of fluorinated alcohols in water. Fluid Phase Equilibria, 2016, 407, 322-333.	1.4	9
32	Vapor Pressure of Perfluoroalkylalkanes: The Role of the Dipole. Journal of Physical Chemistry B, 2015, 119, 1623-1632.	1.2	30
33	High-temperature vapourâ€“liquid equilibrium for ethanolâ€“1-propanol mixtures and modeling with SAFT-VR. Fluid Phase Equilibria, 2015, 398, 5-9.	1.4	4
34	Prediction of diffusion coefficients of chlorophenols in water by computer simulation. Fluid Phase Equilibria, 2015, 396, 9-19.	1.4	20
35	Evidence for Interaction with the Water Subphase As the Origin and Stabilization of Nano-Domain in Semi-Fluorinated Alkanes Monolayer at the Air/Water Interface. Langmuir, 2014, 30, 15193-15199.	1.6	14
36	Cation Alkyl Side Chain Length and Symmetry Effects on the Surface Tension of Ionic Liquids. Langmuir, 2014, 30, 6408-6418.	1.6	75

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37	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
38	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
39	Probing the Structure of Liquids with ¹²⁹Xe NMR Spectroscopy: n-Alkanes, Cycloalkanes, and Branched Alkanes. Journal of Physical Chemistry B, 2013, 117, 9014-9024.	1.2	21
40	Using ¹²⁹Xe NMR to Probe the Structure of Ionic Liquids. Journal of Physical Chemistry Letters, 2013, 4, 2758-2762.	2.1	26
41	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.	1.2	31
42	Viscosity of liquid systems involving hydrogenated and fluorinated substances: Liquid mixtures of (hexane+perfluorohexane). Fluid Phase Equilibria, 2013, 358, 161-165.	1.4	22
43	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.	1.0	11
44	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.	1.4	16
45	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
46	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.	1.2	7
47	Viscosity of Liquid Perfluoroalkanes and Perfluoroalkylalkane Surfactants. Journal of Physical Chemistry B, 2011, 115, 9130-9139.	1.2	42
48	Long-Range Nanometer-Scale Organization of Semifluorinated Alkane Monolayers at the Air/Water Interface. Langmuir, 2011, 27, 13497-13505.	1.6	25
49	On the behaviour of solutions of xenon in liquid cycloalkanes: Solubility of xenon in cyclopentane. Fluid Phase Equilibria, 2011, 303, 193-200.	1.4	2
50	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
51	Highly organized crystalline monolayer of a semi-fluorinated alkane on a solid substrate obtained by spin-coating. Thin Solid Films, 2010, 519, 414-416.	0.8	25
52	On the Behavior of Solutions of Xenon in Liquid n-Alkanes: Solubility of Xenon in n-Pentane and n-Hexane. Journal of Physical Chemistry B, 2010, 114, 15897-15904.	1.2	5
53	Integrated Modeling of Mixture Fluid Phase Equilibrium Experiments Using SAFT-VR Applied to Xenon + Diborane, Xenon + Cyclopropane, Xenon + Boron Trifluoride. Industrial & Engineering Chemistry Research, 2009, 48, 2188-2198.	1.8	2
54	Solution Behavior of Perfluoroalkanes and Perfluoroalkylalkane Surfactants in n-Octane. Journal of Physical Chemistry C, 2007, 111, 15962-15968.	1.5	34

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55	Liquid Phase Behavior of Perfluoroalkylalkane Surfactants. Journal of Physical Chemistry B, 2007, 111, 2856-2863.	1.2	52
56	Liquid Mixtures of Xenon with Fluorinated Species:Â Xenon + Sulfur Hexafluoride. Journal of Physical Chemistry B, 2007, 111, 5284-5289.	1.2	8
57	On the Critical Temperature, Normal Boiling Point, and Vapor Pressure of Ionic Liquids. Journal of Physical Chemistry B, 2005, 109, 6040-6043.	1.2	475
58	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.	1.4	53
59	Thermodynamics of Liquid (Xenon + Methane) Mixtures. Journal of Physical Chemistry B, 2004, 108, 7377-7381.	1.2	21
60	Liquidâ€“vapour equilibrium of {xBF3 + (1 â^' x)n-butane} at 195.49 K. Fluid Phase Equilibria, 2003, 205, 163-170.	1.4	18
61	Predicting the solubility of xenon in n-hexane and n-perfluorohexane: a simulation and theoretical study. Molecular Physics, 2002, 100, 2547-2553.	0.8	40
62	Nanoscale Pattern Formation in Langmuirâ^'Blodgett Films of a Semifluorinated Alkane and a Polystyreneâ^'Poly(Ethylene Oxide) Diblock Copolymer. Nano Letters, 2002, 2, 1083-1086.	4.5	54
63	Thermodynamics of Liquid (Xenon + Diborane). Journal of Physical Chemistry B, 2002, 106, 1741-1745.	1.2	4
64	Is xenon an â€œennobledâ€•alkane?. Physical Chemistry Chemical Physics, 2002, 4, 1618-1621.	1.3	28
65	Thermodynamics of liquid (nitrogen + ethane). Journal of Chemical Thermodynamics, 2002, 34, 669-678.	1.0	15
66	Solubility of xenon in n-hexane between 257 and 333 K. Fluid Phase Equilibria, 2002, 193, 41-51.	1.4	17
67	On the liquid mixtures of xenon, alkanes and perfluorinated compounds. Physical Chemistry Chemical Physics, 2001, 3, 2852-2855.	1.3	24
68	Liquid Mixtures Involving Cyclic Molecules. 2:Â Xenon + Cyclobutane. Journal of Physical Chemistry B, 2001, 105, 10936-10941.	1.2	9
69	Thermodynamics of Liquid Mixtures of Xenon with Alkanes:â€‰ (Xenon + n-Butane) and (Xenon +) Tj ETQq1 1 0.784314 rgBT /Overl	1.2	53
70	Thermodynamics of Liquid Mixtures of Xenon with Alkanes:â€‰ (Xenon + Ethane) and (Xenon + Propane). Journal of Physical Chemistry B, 2000, 104, 1315-1321.	1.2	62
71	Liquid mixtures involving triangular molecules: (vapour + liquid) equilibria of (xenon +) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50	1.0	6
72	Shape Effects in Molecular Liquids:Â Phase Equilibria of Binary Mixtures Involving Cyclic Molecules. Journal of Physical Chemistry B, 1997, 101, 11243-11248.	1.2	8

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73	Liquid Mixtures Involving Cyclic Molecules:Â Xenon + Cyclopropane. Journal of Physical Chemistry B, 1997, 101, 7135-7138.	1.2	11
74	Thermodynamics of liquid propane + cyclopropane. Fluid Phase Equilibria, 1997, 135, 249-257.	1.4	3
75	The vapour pressure of liquid cyclopropane. Journal of Chemical Thermodynamics, 1997, 29, 1435-1438.	1.0	3
76	Thermodynamic studies of triangular molecules: liquid mixtures of xenon and the boron halides, BF3 and BCl3. Journal of the Chemical Society, Faraday Transactions, 1996, 92, 215.	1.7	7
77	Liquid mixtures involving cyclic molecules: (vapour + liquid) equilibria of (xenon + ethylene oxide). Journal of Chemical Thermodynamics, 1996, 28, 201-207.	1.0	11
78	The Stabilization of Asphaltenes in Different Crude Fractions: A Molecular Approach. Journal of the Brazilian Chemical Society, 0, , .	0.6	4