JosÃ© Nuno Canongia Lopes

List of Publications by Year
in descending order

225 papers	19,595 citations	17405 63 h-index	11288 136 g-index
235 all docs	235 docs citations	235 times ranked	10180 citing authors

#	Article	IF	Citations
1	Melted and recrystallized holey-graphene-reinforced aluminum composites: Structure, elasticity and strength. Composite Structures, 2022, 292, 115679.	3.1	8
2	Tailoring amphotericin B as an ionic liquid: an upfront strategy to potentiate the biological activity of antifungal drugs. RSC Advances, 2021, 11, 14441-14452.	1.7	7
3	Molecular dynamics simulations of effective interactions among clinker minerals in aqueous solution and the structure and dynamics of the interstitial water. Materials and Structures/Materiaux Et Constructions, 2021, 54, 1.	1.3	1
4	Graphdiyne nanotubes in ionic liquids: Characterization of interfacial interactions by molecular dynamics. Journal of Molecular Liquids, 2021, 342, 116966.	2.3	6
5	The Solubility of Gases in Ionic Liquids: A Chemoinformatic Predictive and Interpretable Approach. ChemPhysChem, 2021, 22, 2190-2200.	1.0	9
6	Water Solubility Trends in Ionic Liquids: The Quantitative Structureâ€“Property Relationship Model versus Molecular Dynamics. Journal of Physical Chemistry B, 2021, 125, 11491-11497.	1.2	5
7	Ionic Liquids and Water: Hydrophobicity vs. Hydrophilicity. Molecules, 2021, 26, 7159.	1.7	19
8	Strength and fracture of graphyne and graphdiyne nanotubes. Computational Materials Science, 2020, 171, 109233.	1.4	22
9	Bio-inspired hydrophilic bistriflimide-based ionic liquids: Molecular dynamics modeling and simulations. Journal of Molecular Liquids, 2020, 301, 112402.	2.3	6
10	C13 â€“ a new empirical force field to characterize the mechanical behavior of carbyne chains. Physical Chemistry Chemical Physics, 2020, 22, 758-771.	1.3	4
11	Solvate ionic liquids based on lithium bis(trifluoromethanesulfonyl)imideâ€“glyme systems: coordination in MD simulations with scaled charges. Physical Chemistry Chemical Physics, 2020, 22, 525-535.	1.3	22
12	Towards the development of nanosprings from confined carbyne chains. Physica E: Low-Dimensional Systems and Nanostructures, 2020, 117, 113831.	1.3	9
13	Tuning the miscibility of water in imide-based ionic liquids. Physical Chemistry Chemical Physics, 2020, 22, 25236-25242.	1.3	6
14	Vapor Pressure Assessment of Sulfolane-Based Eutectic Solvents: Experimental, PC-SAFT, and Molecular Dynamics. Journal of Physical Chemistry B, 2020, 124, 10386-10397.	1.2	12
15	CNT-reinforced iron and titanium nanocomposites: Strength and deformation mechanisms. Composites Part B: Engineering, 2020, 187, 107836.	5.9	22
16	Aluminum composites reinforced by Î³-graphynes: The effect of nanofillers porosity and shape on crystal growth and composite strengthening. Computational Materials Science, 2020, 176, 109538.	1.4	6
17	Photon Upconversion in TTA-Inducing Ionic Liquids: Pinpointing the Role of IL Nanostructured Media Using MD Simulations. Journal of Physical Chemistry B, 2020, 124, 3137-3144.	1.2	3
18	Evidences for a Null Molar Volume Contribution by Hydroxyl Groups in Ammonium Bistriflimide-Based Ionic Liquids. Journal of Chemical & Engineering Data, 2019, 64, 4932-4945.	1.0	3

#	Article	IF	Citations
19	Transferable, Polarizable Force Field for Ionic Liquids. Journal of Chemical Theory and Computation, 2019, 15, 5858-5871.	2.3	108
20	A force field for MD simulations on rhenium organometallic compounds developed from enthalpy of sublimation and X-ray diffraction measurements. Journal of Chemical Thermodynamics, 2019, 133, 60-69.	1.0	5
21	Ionic Liquids in Wonderland: From Electrostatics to Coordination Chemistry. Journal of Physical Chemistry C, 2019, 123, 5804-5811.	1.5	5
22	Adsorption and viscoelastic behaviour of ionic liquid surfactants on gold surfaces. Journal of Molecular Liquids, 2019, 282, 633-641.	2.3	5
23	Neat ionic liquids versus ionic liquid mixtures: a combination of experimental data and molecular simulation. Physical Chemistry Chemical Physics, 2019, 21, 23305-23309.	1.3	12
24	Strength and failure mechanisms of cnt-reinforced copper nanocomposite. Composites Part B: Engineering, 2018, 145, 108-120.	5.9	39
25	Probing the Surface Tension of Ionic Liquids Using the Langmuir Principle. Langmuir, 2018, 34, 4408-4416.	1.6	31
26	Formation of nanocrystalline tobermorite in calcium silicate binders with low C/S ratio. Acta Materialia, 2018, 152, 7-15.	3.8	40
27	Nanoscale organization in the fluorinated room temperature ionic liquid: Tetraethyl ammonium (trifluoromethanesulfonyl)(nonafluorobutylsulfonyl)imide. Journal of Chemical Physics, 2018, 148, 193816.	1.2	19
28	Enhanced dissolution of ibuprofen using ionic liquids as catanionic hydrotropes. Physical Chemistry Chemical Physics, 2018, 20, 2094-2103.	1.3	68
29	Solvation of alcohols in ionic liquids â€“ understanding the effect of the anion and cation. Physical Chemistry Chemical Physics, 2018, 20, 2536-2548.	1.3	17
30	Structure and dynamics of mica-confined films of [C10C1Pyrr][NTf2] ionic liquid. Journal of Chemical Physics, 2018, 148, 193808.	1.2	15
31	Design of task-specific fluorinated ionic liquids: nanosegregation versus hydrogen-bonding ability in aqueous solutions. Chemical Communications, 2018, 54, 3524-3527.	2.2	17
32	ILs through the looking glass: electrostatics and structure probed using charge-inverted ionic liquid pairs. Faraday Discussions, 2018, 206, 203-218.	1.6	4
33	Structure and dynamics of ionic liquids: general discussion. Faraday Discussions, 2018, 206, 291-337.	1.6	8
34	Ionic liquids at interfaces: general discussion. Faraday Discussions, 2018, 206, 549-586.	1.6	0
35	Comparative structural analyses in four ionic liquid systems: the two low-q peaks of IL structure factor functions. Molecular Simulation, 2018, 44, 478-484.	0.9	9
36	Exploring the bulk-phase structure of ionic liquid mixtures using small-angle neutron scattering. Faraday Discussions, 2018, 206, 265-289.	1.6	42

#	Article	IF	Citations
37	Negative Pressure Regimes in Ionic Liquids: Structure and Interactions in Stretched Liquids as Probed by NMR. ECS Transactions, 2018, 86, 141-147.	0.3	1
38	Atomistic Simulations of Carbon Nanotubes: Stiffness, Strength, and Toughness of Locally Buckled CNTs. , 2018, , 259-290.		0
39	Molecular dynamics studies on the structure and interactions of ionic liquids containing amino-acid anions. Physical Chemistry Chemical Physics, 2018, 20, 23864-23872.	1.3	19
40	Designing the ammonium cation to achieve a higher hydrophilicity of bistriflimide-based ionic liquids. Physical Chemistry Chemical Physics, 2018, 20, 19307-19313.	1.3	17
41	Negative Pressure Regimes in Ionic Liquids: Structure and Interactions in Stretched Liquids as Probed by NMR. ECS Meeting Abstracts, 2018, , .	0.0	0
42	Influence of Nanosegregation on the Phase Behavior of Fluorinated Ionic Liquids. Journal of Physical Chemistry C, 2017, 121, 5415-5427.	1.5	46
43	Nanosegregation and Structuring in the Bulk and at the Surface of Ionic-Liquid Mixtures. Journal of Physical Chemistry B, 2017, 121, 6002-6020.	1.2	82
44	Polycyclic aromatic hydrocarbons as model solutes for carbon nanomaterials in ionic liquids. Physical Chemistry Chemical Physics, 2017, 19, 27694-27703.	1.3	11
45	Modeling Halogen Bonds in Ionic Liquids: A Force Field for Imidazolium and Halo-Imidazolium Derivatives. Journal of Chemical Theory and Computation, 2017, 13, 6167-6176.	2.3	10
46	Ionic liquids with anions based on fluorosulfonyl derivatives: from asymmetrical substitutions to a consistent force field model. Physical Chemistry Chemical Physics, 2017, 19, 29617-29624.	1.3	49
47	Structural characterization of the [CnC1im][C4F9SO3] ionic liquid series: Alkyl versus perfluoroalkyl side chains. Journal of Molecular Liquids, 2017, 226, 28-34.	2.3	30
48	Phase behaviour and thermodynamics: general discussion. Faraday Discussions, 2017, 206, 113-139.	1.6	8
49	Li⁺ Local Structure in Liâ€“Tetraglyme Solvate Ionic Liquid Revealed by Neutron Total Scattering Experiments with the ^{6/7}Li Isotopic Substitution Technique. Journal of Physical Chemistry Letters, 2016, 7, 2832-2837.	2.1	44
50	Mechanical behaviour of carbon nanotubes under combined twistingâ€“bending. Mechanics Research Communications, 2016, 73, 19-24.	1.0	16
51	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
52	Novel high-resistance clinkers with 1.10<CaO/SiO2<1.25: production route and preliminary hydration characterization. Cement and Concrete Research, 2016, 85, 39-47.	4.6	9
53	Liquidâ€Crystalline Ionic Liquids as Ordered Reaction Media for the Dielsâ€“Alder Reaction. Chemistry - A European Journal, 2016, 22, 16113-16123.	1.7	35
54	ABS Composed of Ionic Liquids and Inorganic Salts. Green Chemistry and Sustainable Technology, 2016, , 27-35.	0.4	3

#	Article	IF	Citations
55	Densities and Viscosities of Mixtures of Two Ionic Liquids Containing a Common Cation. Journal of Chemical & Engineering Data, 2016, 61, 2828-2843.	1.0	117
56	Influence of Nanosegregation on the Surface Tension of Fluorinated Ionic Liquids. Langmuir, 2016, 32, 6130-6139.	1.6	38
57	Comparing the structure of different ionic liquid series: Bistriflamide v. hexafluorophosphate; pure v. equimolar mixtures. Fluid Phase Equilibria, 2016, 418, 181-191.	1.4	16
58	Protonic Ammonium Nitrate Ionic Liquids and Their Mixtures: Insights into Their Thermophysical Behavior. Journal of Physical Chemistry B, 2016, 120, 2397-2406.	1.2	39
59	Bulk nanostructure of the prototypical â€˜goodâ€™ and â€˜poorâ€™ solvate ionic liquids [Li(G4)][TFSI] and [Li(G4)][NO₃]. Physical Chemistry Chemical Physics, 2016, 18, 17224-17236.	1.3	49
60	Additive polarizabilities in ionic liquids. Physical Chemistry Chemical Physics, 2016, 18, 1665-1670.	1.3	37
61	Mixtures of the 1-ethyl-3-methylimidazolium acetate ionic liquid with different inorganic salts: insights into their interactions. Physical Chemistry Chemical Physics, 2016, 18, 2756-2766.	1.3	12
62	The magic of aqueous solutions of ionic liquids: ionic liquids as a powerful class of catanionic hydrotropes. Green Chemistry, 2015, 17, 3948-3963.	4.6	156
63	Inter-laminar shear stress in hybrid CFRP/austenitic steel. Frattura Ed Integrita Strutturale, 2015, 9, 67-79.	0.5	2
64	Multiresolution calculation of ionic liquids. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2015, 5, 202-214.	6.2	108
65	Structural and aggregate analyses of (Li salt + glyme) mixtures: the complex nature of solvate ionic liquids. Physical Chemistry Chemical Physics, 2015, 17, 22321-22335.	1.3	78
66	Plasma membrane permeabilisation by ionic liquids: a matter of charge. Green Chemistry, 2015, 17, 4587-4598.	4.6	37
67	From lime to silica and alumina: systematic modeling of cement clinkers using a general force-field. Physical Chemistry Chemical Physics, 2015, 17, 18477-18494.	1.3	16
68	Microstructural control and hydration of novel micro-dendritic clinkers with CaO/SiO 2 = 1.4. Cement and Concrete Research, 2015, 76, 212-221.	4.6	16
69	A thermophysical and structural characterization of ionic liquids with alkyl and perfluoroalkyl side chains. RSC Advances, 2015, 5, 65337-65350.	1.7	63
70	Ionic Liquid Films at the Waterâ€“Air Interface: Langmuir Isotherms of Tetra-alkylphosphonium-Based Ionic Liquids. Langmuir, 2015, 31, 8371-8378.	1.6	12
71	Modeling the structure and thermodynamics of ferrocenium-based ionic liquids. Physical Chemistry Chemical Physics, 2015, 17, 10200-10208.	1.3	10
72	Viscosity minima in binary mixtures of ionic liquids + molecular solvents. Physical Chemistry Chemical Physics, 2015, 17, 13480-13494.	1.3	21

#	Article	IF	Citations
73	Probing the structural features of the 1-alkyl-3-methylimidazolium hexafluorophosphate ionic liquid series using Molecular Dynamics simulations. Journal of Molecular Liquids, 2015, 210, 257-263.	2.3	28
74	Solvent effects on the polar network of ionic liquid solutions. Journal of Physics Condensed Matter, 2015, 27, 194116.	0.7	12
75	Solubility of n-butane and 2-methylpropane (isobutane) in 1-alkyl-3-methylimidazolium-based ionic liquids with linear and branched alkyl side-chains. Physical Chemistry Chemical Physics, 2015, 17, 30328-30342.	1.3	14
76	Refraction Index and Molar Refraction in Ionic Liquid/PEG200 Solutions. Journal of Solution Chemistry, 2015, 44, 431-439.	0.6	11
77	Self-Organization in Ionic Liquids: From Bulk to Interfaces and Films. Journal of the Brazilian Chemical Society, 2015, , .	0.6	12
78	The complex structure of ionic liquids at an atomistic level: from â€œred-and-greensâ€•to charge templates. Pure and Applied Chemistry, 2014, 86, 119-133.	0.9	15
79	Cation Alkyl Side Chain Length and Symmetry Effects on the Surface Tension of Ionic Liquids. Langmuir, 2014, 30, 6408-6418.	1.6	75
80	Structure and Aggregation in the 1-Alkyl-3-Methylimidazolium Bis(trifluoromethylsulfonyl)imide Ionic Liquid Homologous Series. Journal of Physical Chemistry B, 2014, 118, 567-576.	1.2	223
81	Compressive behavior of CNT-reinforced aluminum composites using molecular dynamics. Composites Science and Technology, 2014, 90, 16-24.	3.8	134
82	The impact of ionic liquid fluorinated moieties on their thermophysical properties and aqueous phase behaviour. Physical Chemistry Chemical Physics, 2014, 16, 21340-21348.	1.3	30
83	The alternation effect in ionic liquid homologous series. Physical Chemistry Chemical Physics, 2014, 16, 4033-4038.	1.3	34
84	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
85	The effect of the cation alkyl chain branching on mutual solubilities with water and toxicities. Physical Chemistry Chemical Physics, 2014, 16, 19952.	1.3	64
86	Complex Structure of Ionic Liquids. Molecular Dynamics Studies with Different Cationâ€“Anion Combinations. Journal of Chemical & Engineering Data, 2014, 59, 3120-3129.	1.0	47
87	Structure and Aggregation in the 1,3-Dialkyl-imidazolium Bis(trifluoromethylsulfonyl)imide Ionic Liquid Family: 2. From Single to Double Long Alkyl Side Chains. Journal of Physical Chemistry B, 2014, 118, 6885-6895.	1.2	65
88	Influence of Bond Kinematics on the Rupture of Non-Chiral CNTs under Stretchingâ€“Twisting. Springer Series in Materials Science, 2014, , 275-302.	0.4	0
89	Using ¹²⁹Xe NMR to Probe the Structure of Ionic Liquids. Journal of Physical Chemistry Letters, 2013, 4, 2758-2762.	2.1	26
90	Nano-segregation in ionic liquids: scorpions and vanishing chains. Physical Chemistry Chemical Physics, 2013, 15, 16256.	1.3	119

#	Article	IF	Citations
91	Tensionâ€“twisting dependent kinematics of chiral CNTs. Composites Science and Technology, 2013, 74, 211-220.	3.8	21
92	Shifts in the temperature of maximum density (TMD) of ionic liquid aqueous solutions. Physical Chemistry Chemical Physics, 2013, 15, 10960.	1.3	20
93	All-Atom Force Field for Molecular Dynamics Simulations on Organotransition Metal Solids and Liquids. Application to M(CO)_n (MÂ= Cr, Fe, Ni, Mo, Ru, or W) Compounds. Journal of Physical Chemistry A, 2013, 117, 11107-11113.	1.1	32
94	Systematic Study of the Thermophysical Properties of Imidazolium-Based Ionic Liquids with Cyano-Functionalized Anions. Journal of Physical Chemistry B, 2013, 117, 10271-10283.	1.2	195
95	High ionicity ionic liquids (HIILs): comparing the effect of ethylsulfonate and ethylsulfate anions. Physical Chemistry Chemical Physics, 2013, 15, 18138.	1.3	20
96	On the Formation of a Third, Nanostructured Domain in Ionic Liquids. Journal of Physical Chemistry B, 2013, 117, 10826-10833.	1.2	99
97	Unusual LCST-type behaviour found in binary mixtures of choline-based ionic liquids with ethers. RSC Advances, 2013, 3, 10262.	1.7	24
98	Induced anisotropy of chiral carbon nanotubes under combined tension-twisting. Mechanics of Materials, 2013, 58, 97-109.	1.7	20
99	Probing the self-aggregation of ionic liquids in aqueous solutions using density and speed of sound data. Journal of Chemical Thermodynamics, 2013, 59, 43-48.	1.0	16
100	Thermophysical and magnetic studies of two paramagnetic liquid salts: [C4mim][FeCl4] and [P66614][FeCl4]. Fluid Phase Equilibria, 2013, 350, 43-50.	1.4	41
101	Hydrogen-Bonding and the Dissolution Mechanism of Uracil in an Acetate Ionic Liquid: New Insights from NMR Spectroscopy and Quantum Chemical Calculations. Journal of Physical Chemistry B, 2013, 117, 4109-4120.	1.2	27
102	Viscosity Mixing Rules for Binary Systems Containing One Ionic Liquid. ChemPhysChem, 2013, 14, 1956-1968.	1.0	12
103	Probing Ionic Liquid Aqueous Solutions Using Temperature of Maximum Density Isotope Effects. Molecules, 2013, 18, 3703-3711.	1.7	3
104	Inorganic salts in purely ionic liquid media: the development of high ionicity ionic liquids (HIILs). Chemical Communications, 2012, 48, 3656.	2.2	91
105	Partition Coefficients of Alkaloids in Biphasic Ionic-Liquid-Aqueous Systems and their Dependence on the Hofmeister Series. Separation Science and Technology, 2012, 47, 284-291.	1.3	33
106	2D or not 2D: Structural and charge ordering at the solid-liquid interface of the 1-(2-hydroxyethyl)-3-methylimidazolium tetrafluoroborate ionic liquid. Faraday Discussions, 2012, 154, 155-169.	1.6	56
107	Hollow calcite rhombohedra at ionic liquid-stabilized bubbles. CrystEngComm, 2012, 14, 5723.	1.3	3
108	Liquidâ€“Liquid Equilibrium of Cholinium-Derived Bistriflimide Ionic Liquids with Water and Octanol. Journal of Physical Chemistry B, 2012, 116, 9186-9195.	1.2	34

#	Article	IF	Citations
109	Solubility of inorganic salts in pure ionic liquids. Journal of Chemical Thermodynamics, 2012, 55, 29-36.	1.0	70
110	Aqueous biphasic systems: a boost brought about by using ionic liquids. Chemical Society Reviews, 2012, 41, 4966.	18.7	726
111	Impact of Self-Aggregation on the Formation of Ionic-Liquid-Based Aqueous Biphasic Systems. Journal of Physical Chemistry B, 2012, 116, 7660-7668.	1.2	54
112	Polymorphism in 4â€²-Hydroxyacetophenone: A Molecular Dynamics Simulation Study. Journal of Physical Chemistry B, 2012, 116, 5179-5184.	1.2	14
113	Surface tension of ionic liquids and ionic liquid solutions. Chemical Society Reviews, 2012, 41, 829-868.	18.7	375
114	Density, Thermal Expansion and Viscosity of Cholinium–Derived Ionic Liquids. ChemPhysChem, 2012, 13, 1902-1909.	1.0	83
115	CL&P: A generic and systematic force field for ionic liquids modeling. Theoretical Chemistry Accounts, 2012, 131, 1.	0.5	281
116	A molecular dynamics study on the thickness and post-critical strength of carbon nanotubes. Composite Structures, 2012, 94, 1352-1358.	3.1	29
117	Wetting Films of Two Ionic Liquids: [C₈mim][BF4] and [C₂OHmim][BF₄]. Journal of Physical Chemistry C, 2011, 115, 16116-16123.	1.5	16
118	High-Accuracy Vapor Pressure Data of the Extended [C_nC₁im][Ntf₂] Ionic Liquid Series: Trend Changes and Structural Shifts. Journal of Physical Chemistry B, 2011, 115, 10919-10926.	1.2	199
119	Polarity, Viscosity, and Ionic Conductivity of Liquid Mixtures Containing [C₄C₁im][Ntf₂] and a Molecular Component. Journal of Physical Chemistry B, 2011, 115, 6088-6099.	1.2	154
120	Mixtures of Pyridine and Nicotine with Pyridinium-Based Ionic Liquids. Journal of Chemical & Engineering Data, 2011, 56, 4356-4363.	1.0	13
121	Effect of alkyl chain length and hydroxyl group functionalization on the surface properties of imidazolium ionic liquids. Physical Chemistry Chemical Physics, 2011, 13, 13518.	1.3	81
122	Liquid- or Solid-Like Behavior of [omim][BF₄] at a Solid Interface?. Journal of Physical Chemistry Letters, 2011, 2, 1551-1555.	2.1	24
123	The Structure of Aqueous Solutions of a Hydrophilic Ionic Liquid: The Full Concentration Range of 1-Ethyl-3-methylimidazolium Ethylsulfate and Water. Journal of Physical Chemistry B, 2011, 115, 2067-2074.	1.2	142
124	Ionic liquid-based aqueous biphasic system for lipase extraction. Green Chemistry, 2011, 13, 390-396.	4.6	120
125	Interaction diagrams for carbon nanotubes under combined shortening–twisting. Composites Science and Technology, 2011, 71, 1811-1818.	3.8	17
126	Viscosity of (C2–C14) 1-alkyl-3-methylimidazolium bis(trifluoromethylsulfonyl)amide ionic liquids in an extended temperature range. Fluid Phase Equilibria, 2011, 301, 22-32.	1.4	220

#	Article	IF	Citations
127	Effect of alkyl chain length on the adsorption and frictional behaviour of 1-alkyl-3-methylimidazolium chloride ionic liquid surfactants on gold surfaces. Colloids and Surfaces A: Physicochemical and Engineering Aspects, 2011, 377, 361-366.	2.3	15
128	Characteristics of aggregation in aqueous solutions of dialkylpyrrolidinium bromides. Journal of Colloid and Interface Science, 2011, 360, 606-616.	5.0	36
129	Three commentaries on the nano-segregated structure of ionic liquids. Computational and Theoretical Chemistry, 2010, 946, 70-76.	1.5	156
130	Vaporisation of a Dicationic Ionic Liquid Revisited. ChemPhysChem, 2010, 11, 3673-3677.	1.0	23
131	Binary mixtures of ionic liquids with a common ion revisited: A molecular dynamics simulation study. Journal of Molecular Liquids, 2010, 153, 52-56.	2.3	75
132	High-temperature surface tension and density measurements of 1-alkyl-3-methylimidazolium bistriflamide ionic liquids. Fluid Phase Equilibria, 2010, 294, 131-138.	1.4	145
133	Studies on the density, heat capacity, surface tension and infinite dilution diffusion with the ionic liquids [C4mim][NTf2], [C4mim][dca], [C2mim][EtOSO3] and [Aliquat][dca]. Fluid Phase Equilibria, 2010, 294, 157-179.	1.4	171
134	Assessing the Dispersive and Electrostatic Components of the Cohesive Energy of Ionic Liquids Using Molecular Dynamics Simulations and Molar Refraction Data. Journal of Physical Chemistry B, 2010, 114, 5831-5834.	1.2	89
135	New Insight into Phase Equilibria Involving Imidazolium Bistriflamide Ionic Liquids and Their Mixtures with Alcohols and Water. Journal of Physical Chemistry B, 2010, 114, 8978-8985.	1.2	15
136	Volatility of Aprotic Ionic Liquids â€" A Review. Journal of Chemical & Engineering Data, 2010, 55, 3-12.	1.0	294
137	Solubility of alkanes, alkanols and their fluorinated counterparts in tetraalkylphosphonium ionic liquids. Physical Chemistry Chemical Physics, 2010, 12, 9685.	1.3	44
138	Nanostructure of Trialkylmethylammonium Bistriflamide Ionic Liquids Studied by Molecular Dynamics. Journal of Physical Chemistry B, 2010, 114, 15635-15641.	1.2	50
139	Raman Spectroscopic Study of the Vapor Phase of 1-Methylimidazolium Ethanoate, a Protic Ionic Liquid. Journal of Physical Chemistry A, 2010, 114, 10834-10841.	1.1	34
140	Energetics of Aqueous Solutions of the Ionic Liquid 1-Ethyl-3-methylimidazolium Ethylsulfate. Journal of Physical Chemistry B, 2010, 114, 13179-13188.	1.2	18
141	Phase Equilibria of Haloalkanes Dissolved in Ethylsulfate- or Ethylsulfonate-Based Ionic Liquids. Journal of Physical Chemistry B, 2010, 114, 7329-7337.	1.2	24
142	The Nature of Protic Ionic Liquids in the Gas Phase Revisited: Fourier Transform Ion Cyclotron Resonance Mass Spectrometry Study of 1,1,3,3-Tetramethylguanidinium Chloride. Journal of Physical Chemistry B, 2010, 114, 8905-8909.	1.2	30
143	High-performance extraction of alkaloids using aqueous two-phase systems with ionic liquids. Green Chemistry, 2010, 12, 1715.	4.6	213
144	Rationalizing the Diverse Solidâ"Liquid Equilibria of Binary Mixtures of Benzene and Its Fluorinated Derivatives. Journal of Physical Chemistry B, 2010, 114, 12589-12596.	1.2	3

#	Article	IF	Citations
145	Structural and Positional Isomerism Influence in the Physical Properties of Pyridinium NTf₂-Based Ionic Liquids: Pure and Water-Saturated Mixtures. Journal of Chemical & Engineering Data, 2010, 55, 4514-4520.	1.0	118
146	Dependence of the Conformational Isomerism in 1-n-Butyl-3-methylimidazolium Ionic Liquids on the Nature of the Halide Anion. Journal of Physical Chemistry B, 2010, 114, 11715-11724.	1.2	66
147	Mutual Solubility of Water and Structural/Positional Isomers of N-Alkylpyridinium-Based Ionic Liquids. Journal of Physical Chemistry B, 2010, 114, 15925-15934.	1.2	74
148	Molecular Force Field for Ionic Liquids V: Hydroxyethylimidazolium, Dimethoxy-2- Methylimidazolium, and Fluoroalkylimidazolium Cations and Bis(Fluorosulfonyl)Amide, Perfluoroalkanesulfonylamide, and Fluoroalkylfluorophosphate Anions. Journal of Physical Chemistry B, 2010, 114, 3592-3600.	1.2	146
149	Ionic liquids and reactive azeotropes: the continuity of the aprotic and protic classes. Physical Chemistry Chemical Physics, 2010, 12, 1948.	1.3	29
150	What Farâ€Infrared Spectra Can Contribute to the Development of Force Fields for Ionic Liquids Used in Molecular Dynamics Simulations. ChemPhysChem, 2009, 10, 1181-1186.	1.0	51
151	Densities and refractive indices of imidazolium- and phosphonium-based ionic liquids: Effect of temperature, alkyl chain length, and anion. Journal of Chemical Thermodynamics, 2009, 41, 790-798.	1.0	369
152	On the Role of the Dipole and Quadrupole Moments of Aromatic Compounds in the Solvation by Ionic Liquids. Journal of Physical Chemistry B, 2009, 113, 9894-9900.	1.2	86
153	Bridging the Gap between Ionic Liquids and Molten Salts: Group 1 Metal Salts of the Bistriflamide Anion in the Gas Phase. Journal of Physical Chemistry B, 2009, 113, 3491-3498.	1.2	27
154	Phase Equilibria in Ionic Liquidâ^'Aromatic Compound Mixtures, Including Benzene Fluorination Effects. Journal of Physical Chemistry B, 2009, 113, 7631-7636.	1.2	33
155	Raman Spectroscopic Study, DFT Calculations and MD Simulations on the Conformational Isomerism of N-Alkyl-N-methylpyrrolidinium Bis-(trifluoromethanesulfonyl) Amide Ionic Liquids. Journal of Physical Chemistry B, 2009, 113, 4338-4346.	1.2	56
156	Thermodynamics and Micro Heterogeneity of Ionic Liquids. Topics in Current Chemistry, 2009, 290, 161-183.	4.0	53
157	1-Alkyl-3-methylimidazolium alkanesulfonate ionic liquids, [CnH2n+1mim][CkH2k+1SO3]: synthesis and physicochemical properties. Physical Chemistry Chemical Physics, 2009, 11, 8939.	1.3	70
158	New catanionic surfactants based on 1-alkyl-3-methylimidazolium alkylsulfonates, [CnH2n+1mim][CmH2m+1SO3]: mesomorphism and aggregation. Physical Chemistry Chemical Physics, 2009, 11, 4260.	1.3	111
159	Interaction between the Ï€-System of Toluene and the Imidazolium Ring of Ionic Liquids: A Combined NMR and Molecular Simulation Study. Journal of Physical Chemistry B, 2009, 113, 170-177.	1.2	97
160	On the Self-Aggregation and Fluorescence Quenching Aptitude of Surfactant Ionic Liquids. Journal of Physical Chemistry B, 2008, 112, 8645-8650.	1.2	168
161	Solubility of fluorinated compounds in a range of ionic liquids. Cloud-point temperature dependence on composition and pressure. Green Chemistry, 2008, 10, 918.	4.6	35
162	Experimental and Molecular Dynamics Simulation Study of the Sublimation and Vaporization Energetics of Iron Metalocenes. Crystal Structures of Fe(Î·⁵-C₅H₄CH₃)₂ and		

#	Article	IF	Citations
163	Pressureâ^'Densityâ^'Temperature (pâ^'Ïâ^'T) Surface of [C₆mim][NTf₂]. Journal of Chemical & Engineering Data, 2008, 53, 867-870.	1.0	69
164	Interactions of Fluorinated Gases with Ionic Liquids: Solubility of CF₄, C₂F₆, and C₃F₈ in Trihexyltetradecylphosphonium Bis(trifluoromethylsulfonyl)amide. Journal of Physical Chemistry B, 2008, 112, 12394-12400.	1.2	47
165	Molecular Dynamics Simulations of Porphyrinâ^'Dendrimer Systems: Toward Modeling Electron Transfer in Solution. Journal of Physical Chemistry B, 2008, 112, 14779-14792.	1.2	15
166	Experimental and Molecular Dynamics Simulation Study of the Sublimation Energetics of Cyclopentadienyltricarbonylmanganese (Cymantrene). Journal of Physical Chemistry A, 2008, 112, 10429-10434.	1.1	17
167	A Tale of Two Ions:â€‰ The Conformational Landscapes of Bis(trifluoromethanesulfonyl)amide and N,N-Dialkylpyrrolidinium. Journal of Physical Chemistry B, 2008, 112, 1465-1472.	1.2	128
168	Molecular Force Field for Ionic Liquids IV:â€‰ Trialkylimidazolium and Alkoxycarbonyl-Imidazolium Cations; Alkylsulfonate and Alkylsulfate Anions. Journal of Physical Chemistry B, 2008, 112, 5039-5046.	1.2	286
169	Potential Energy Landscape of Bis(fluorosulfonyl)amide. Journal of Physical Chemistry B, 2008, 112, 9449-9455.	1.2	81
170	Molecular Solutes in Ionic Liquids: A Structural Perspective. Accounts of Chemical Research, 2007, 40, 1087-1096.	7.6	450
171	Salting-out in Aqueous Solutions of Ionic Liquids and K3PO4: Aqueous Biphasic Systems and Salt Precipitation. International Journal of Molecular Sciences, 2007, 8, 736-748.	1.8	81
172	Accounting for the Unique, Doubly Dual Nature of Ionic Liquids from a Molecular Thermodynamic and Modeling Standpoint. Accounts of Chemical Research, 2007, 40, 1114-1121.	7.6	213
173	Ionic Liquids:Â First Direct Determination of their Cohesive Energy. Journal of the American Chemical Society, 2007, 129, 284-285.	6.6	295
174	Molecular Dynamics Simulations of Charged Dendrimers:â€‰ Low-to-Intermediate Half-Generation PAMAMs. Journal of Physical Chemistry B, 2007, 111, 10651-10664.	1.2	54
175	Salting-Out Effects in Aqueous Ionic Liquid Solutions:Â Cloud-Point Temperature Shiftsâ€. Journal of Physical Chemistry B, 2007, 111, 4737-4741.	1.2	97
176	Nicotine:Â On the Potential Role of Ionic Liquids for Its Processing and Purification. Journal of Physical Chemistry B, 2007, 111, 7934-7937.	1.2	15
177	The Nature of Ionic Liquids in the Gas Phase. Journal of Physical Chemistry A, 2007, 111, 6176-6182.	1.1	201
178	Molecular dynamics simulations of monoclinic calcium apatites: A universal equation of state. Fluid Phase Equilibria, 2007, 253, 142-146.	1.4	6
179	Ionic Liquids in Polyethylene Glycol Aqueous Solutions: Salting-in and Salting-out Effects. Monatshefte FÃ¼r Chemie, 2007, 138, 1153-1157.	0.9	62
180	Using Spectroscopic Data on Imidazolium Cation Conformations To Test a Molecular Force Field for Ionic Liquids. Journal of Physical Chemistry B, 2006, 110, 7485-7489.	1.2	94

#	Article	IF	Citations
181	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.	1.0	104
182	An All-Atom Force Field for Metallocenes. Journal of Physical Chemistry A, 2006, 110, 13850-13856.	1.1	35
183	Molecular Force Field for Ionic Liquids III:â€‰ Imidazolium, Pyridinium, and Phosphonium Cations; Chloride, Bromide, and Dicyanamide Anions. Journal of Physical Chemistry B, 2006, 110, 19586-19592.	1.2	504
184	Nonpolar, Polar, and Associating Solutes in Ionic Liquids. Journal of Physical Chemistry B, 2006, 110, 16816-16818.	1.2	446
185	Energetics of the Thermal Dimerization of Acenaphthylene to Heptacyclene. Journal of Physical Chemistry A, 2006, 110, 2299-2307.	1.1	9
186	Molecular Dynamics Study of the Thermodynamic Properties of Calcium Apatites. 2. Monoclinic Phases. Journal of Physical Chemistry B, 2006, 110, 4387-4392.	1.2	23
187	The distillation and volatility of ionic liquids. Nature, 2006, 439, 831-834.	13.7	1,926
188	Condensed phase behaviour of ionic liquidâ€“benzene mixtures: congruent melting of a [emim][NTf2]Â·C6H6inclusion crystal. Chemical Communications, 2006, , 2445-2447.	2.2	100
189	Nanostructural Organization in Ionic Liquids. Journal of Physical Chemistry B, 2006, 110, 3330-3335.	1.2	1,693
190	Molecular dynamics simulations of molten calcium hydroxyapatite. Fluid Phase Equilibria, 2006, 241, 51-58.	1.4	14
191	Phase Behavior and Thermodynamic Properties of Ionic Liquids, Ionic Liquid Mixtures, and Ionic Liquid Solutions. ChemInform, 2006, 37, no.	0.1	0
192	Modeling Ionic Liquids of the 1-Alkyl-3-methylimidazolium Family Using an All-Atom Force Field. ACS Symposium Series, 2005, , 134-149.	0.5	16
193	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
194	Deviations from Ideality in Mixtures of Two Ionic Liquids Containing a Common Ion. Journal of Physical Chemistry B, 2005, 109, 3519-3525.	1.2	246
195	Phase Behavior and Thermodynamic Properties of Ionic Liquids, Ionic Liquid Mixtures, and Ionic Liquid Solutions. ACS Symposium Series, 2005, , 270-291.	0.5	29
196	A Molecular Dynamics Study of the Thermodynamic Properties of Calcium Apatites. 1. Hexagonal Phases. Journal of Physical Chemistry B, 2005, 109, 24473-24479.	1.2	44
197	Molecular Force Field for Ionic Liquids Composed of Triflate or Bistriflylimide Anions. Journal of Physical Chemistry B, 2004, 108, 16893-16898.	1.2	875
198	Analysis of structural properties in isotopic mixtures: molecular dynamics methods and Kirkwoodâ€“Buff integrals. Journal of Molecular Liquids, 2004, 112, 147-152.	2.3	4

#	Article	IF	Citations
199	On the classification and representation of ternary phase diagrams: The yin and yang of a Tâ€“x approach. Physical Chemistry Chemical Physics, 2004, 6, 2314-2319.	1.3	7
200	Modeling Ionic Liquids Using a Systematic All-Atom Force Field. Journal of Physical Chemistry B, 2004, 108, 2038-2047.	1.2	1,190
201	Calculation of vapor pressure isotope effects in the rare gases and their mixtures using an integral equation theory. Journal of Chemical Physics, 2003, 118, 5028-5037.	1.2	21
202	Solubility isotope effects in aqueous solutions of methane. Journal of Chemical Physics, 2002, 116, 10816-10824.	1.2	34
203	Isotopic krypton mixtures revisited: Vapor pressure isotope effects. Journal of Chemical Physics, 2002, 117, 8836-8841.	1.2	2
204	Microphase separation in mixtures of Lennard-Jones particles. Physical Chemistry Chemical Physics, 2002, 4, 949-954.	1.3	11
205	Deviations from ideal behavior in isotopic mixtures of ammonia. Journal of Chemical Physics, 2001, 115, 5546-5553.	1.2	3
206	Three-phase osmotic equilibria using the Gibbs ensemble simulation method. Molecular Physics, 2000, 98, 769-772.	0.8	3
207	Evidence for nonideality in the fundamental liquid mixture (36Ar+40Ar). Journal of Chemical Physics, 2000, 113, 8706-8716.	1.2	6
208	Non-ideality of an â€œidealâ€™' liquid mixture: (36Ar + 40Ar). Physical Chemistry Chemical Physics, 2000, 2, 1095-1097.	1.3	8
209	Vapor Pressure and Related Thermodynamic Properties of36Ar. Journal of Physical Chemistry B, 2000, 104, 8735-8742.	1.2	8
210	Three-phase osmotic equilibria using the Gibbs ensemble simulation method. Molecular Physics, 2000, 98, 769-772.	0.8	1
211	Phase equilibra in binary Lennard-Jones mixtures: phase diagram simulation. Molecular Physics, 1999, 96, 1649-1658.	0.8	21
212	The building-up of phase diagrams. Pure and Applied Chemistry, 1999, 71, 1183-1196.	0.9	8
213	Thermodynamics of binary liquid mixtures of partially deuterated methanes with CH4 or CD4. Journal of Chemical Physics, 1997, 106, 8799-8805.	1.2	5
214	Vapor pressure of partially deuterated methanes (CH3D, CH2D2, and CHD3). Journal of Chemical Physics, 1997, 106, 8792-8798.	1.2	9
215	Multiphase equilibria using the Gibbs ensemble Monte Carlo method. Molecular Physics, 1997, 92, 187-196.	0.8	39
216	Liquid Mixtures Involving Cyclic Molecules:Â Xenon + Cyclopropane. Journal of Physical Chemistry B, 1997, 101, 7135-7138.	1.2	11

#	Article	IF	Citations
217	Thermodynamics of liquid propane + cyclopropane. Fluid Phase Equilibria, 1997, 135, 249-257.	1.4	3
218	The vapour pressure of liquid cyclopropane. Journal of Chemical Thermodynamics, 1997, 29, 1435-1438.	1.0	3
219	Vapour pressure of liquid deuterium sulphide. Journal of Chemical Thermodynamics, 1996, 28, 1395-1401.	1.0	4
220	The excess thermodynamic properties of liquid (CH4+CD4). Journal of Chemical Physics, 1994, 100, 4582-4590.	1.2	20
221	Vapour pressure isotope effects in liquid hydrogen chloride. Journal of Physics Condensed Matter, 1992, 4, 6691-6702.	0.7	6
222	Vapour pressure of trideuterioammonia. Journal of Chemical Thermodynamics, 1992, 24, 993-1000.	1.0	6
223	On the pseudo-GrÃ¼neisen parameters of molecular liquids. Journal of Molecular Liquids, 1992, 54, 115-124.	2.3	11
224	The building-up of phase diagrams. , 0, .		1
225	Phase equilibra in binary Lennard-Jones mixtures: phase diagram simulation. , 0, .		4