JosÃ© Nuno Canongia Lopes

List of Publications by Year
in descending order

225 papers	19,595 citations	17440 63 h-index	11308 136 g-index
235 all docs	235 docs citations	235 times ranked	10180 citing authors

#	Article	IF	Citations
1	The distillation and volatility of ionic liquids. Nature, 2006, 439, 831-834.	27.8	1,926
2	Nanostructural Organization in Ionic Liquids. Journal of Physical Chemistry B, 2006, 110, 3330-3335.	2.6	1,693
3	Modeling Ionic Liquids Using a Systematic All-Atom Force Field. Journal of Physical Chemistry B, 2004, 108, 2038-2047.	2.6	1,190
4	Molecular Force Field for Ionic Liquids Composed of Triflate or Bistriflylimide Anions. Journal of Physical Chemistry B, 2004, 108, 16893-16898.	2.6	875
5	Aqueous biphasic systems: a boost brought about by using ionic liquids. Chemical Society Reviews, 2012, 41, 4966.	38.1	726
6	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.	2.6	504
7	On the Critical Temperature, Normal Boiling Point, and Vapor Pressure of Ionic Liquids. Journal of Physical Chemistry B, 2005, 109, 6040-6043.	2.6	475
8	Molecular Solutes in Ionic Liquids: A Structural Perspective. Accounts of Chemical Research, 2007, 40, 1087-1096.	15.6	450
9	Nonpolar, Polar, and Associating Solutes in Ionic Liquids. Journal of Physical Chemistry B, 2006, 110, 16816-16818.	2.6	446
10	Surface tension of ionic liquids and ionic liquid solutions. Chemical Society Reviews, 2012, 41, 829-868.	38.1	375
11	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.	2.0	369
12	Ionic Liquids:Â First Direct Determination of their Cohesive Energy. Journal of the American Chemical Society, 2007, 129, 284-285.	13.7	295
13	Volatility of Aprotic Ionic Liquids â€" A Review. Journal of Chemical & Engineering Data, 2010, 55, 3-12.	1.9	294
14	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.	2.6	286
15	CL&P: A generic and systematic force field for ionic liquids modeling. Theoretical Chemistry Accounts, 2012, 131, 1.	1.4	281
16	Deviations from Ideality in Mixtures of Two Ionic Liquids Containing a Common Ion. Journal of Physical Chemistry B, 2005, 109, 3519-3525.	2.6	246
17	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.	2.6	223
18	Viscosity of (C2â€"C14) 1-alkyl-3-methylimidazolium bis(trifluoromethylsulfonyl)amide ionic liquids in an extended temperature range. Fluid Phase Equilibria, 2011, 301, 22-32.	2.5	220

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19	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.	15.6	213
20	High-performance extraction of alkaloids using aqueous two-phase systems with ionic liquids. Green Chemistry, 2010, 12, 1715.	9.0	213
21	The Nature of Ionic Liquids in the Gas Phase. Journal of Physical Chemistry A, 2007, 111, 6176-6182.	2.5	201
22	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.	2.6	199
23	Systematic Study of the Thermophysical Properties of Imidazolium-Based Ionic Liquids with Cyano-Functionalized Anions. Journal of Physical Chemistry B, 2013, 117, 10271-10283.	2.6	195
24	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.	2.5	171
25	On the Self-Aggregation and Fluorescence Quenching Aptitude of Surfactant Ionic Liquids. Journal of Physical Chemistry B, 2008, 112, 8645-8650.	2.6	168
26	Three commentaries on the nano-segregated structure of ionic liquids. Computational and Theoretical Chemistry, 2010, 946, 70-76.	1.5	156
27	The magic of aqueous solutions of ionic liquids: ionic liquids as a powerful class of catanionic hydrotropes. Green Chemistry, 2015, 17, 3948-3963.	9.0	156
28	Polarity, Viscosity, and Ionic Conductivity of Liquid Mixtures Containing [C₄C₁im][Ntf₂] and a Molecular Component. Journal of Physical Chemistry B, 2011, 115, 6088-6099.	2.6	154
29	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.	2.6	146
30	High-temperature surface tension and density measurements of 1-alkyl-3-methylimidazolium bistriflamide ionic liquids. Fluid Phase Equilibria, 2010, 294, 131-138.	2.5	145
31	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.	2.6	142
32	Compressive behavior of CNT-reinforced aluminum composites using molecular dynamics. Composites Science and Technology, 2014, 90, 16-24.	7.8	134
33	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.	2.6	128
34	Ionic liquid-based aqueous biphasic system for lipase extraction. Green Chemistry, 2011, 13, 390-396.	9.0	120
35	Nano-segregation in ionic liquids: scorpions and vanishing chains. Physical Chemistry Chemical Physics, 2013, 15, 16256.	2.8	119
36	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.	1.9	118

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37	Densities and Viscosities of Mixtures of Two Ionic Liquids Containing a Common Cation. Journal of Chemical & Engineering Data, 2016, 61, 2828-2843.	1.9	117
38	New catanionic surfactants based on 1-alkyl-3-methylimidazolium alkylsulfonates, [CnH2n+1mim][CmH2m+1SO3]: mesomorphism and aggregation. Physical Chemistry Chemical Physics, 2009, 11, 4260.	2.8	111
39	Multiresolution calculation of ionic liquids. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2015, 5, 202-214.	14.6	108
40	Transferable, Polarizable Force Field for Ionic Liquids. Journal of Chemical Theory and Computation, 2019, 15, 5858-5871.	5.3	108
41	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
42	Condensed phase behaviour of ionic liquidâ€“benzene mixtures: congruent melting of a [emim][NTf2]Â·C6H6inclusion crystal. Chemical Communications, 2006, , 2445-2447.	4.1	100
43	On the Formation of a Third, Nanostructured Domain in Ionic Liquids. Journal of Physical Chemistry B, 2013, 117, 10826-10833.	2.6	99
44	Salting-Out Effects in Aqueous Ionic Liquid Solutions:Â Cloud-Point Temperature Shiftsâ€. Journal of Physical Chemistry B, 2007, 111, 4737-4741.	2.6	97
45	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.	2.6	97
46	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.	2.6	94
47	Inorganic salts in purely ionic liquid media: the development of high ionicity ionic liquids (HIILs). Chemical Communications, 2012, 48, 3656.	4.1	91
48	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.	2.6	89
49	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.	2.6	86
50	Density, Thermal Expansion and Viscosity of Cholinium–Derived Ionic Liquids. ChemPhysChem, 2012, 13, 1902-1909.	2.1	83
51	Nanosegregation and Structuring in the Bulk and at the Surface of Ionic-Liquid Mixtures. Journal of Physical Chemistry B, 2017, 121, 6002-6020.	2.6	82
52	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.	4.1	81
53	Potential Energy Landscape of Bis(fluorosulfonyl)amide. Journal of Physical Chemistry B, 2008, 112, 9449-9455.	2.6	81
54	Effect of alkyl chain length and hydroxyl group functionalization on the surface properties of imidazolium ionic liquids. Physical Chemistry Chemical Physics, 2011, 13, 13518.	2.8	81

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55	Structural and aggregate analyses of (Li salt + glyme) mixtures: the complex nature of solvate ionic liquids. Physical Chemistry Chemical Physics, 2015, 17, 22321-22335.	2.8	78
56	Binary mixtures of ionic liquids with a common ion revisited: A molecular dynamics simulation study. Journal of Molecular Liquids, 2010, 153, 52-56.	4.9	75
57	Cation Alkyl Side Chain Length and Symmetry Effects on the Surface Tension of Ionic Liquids. Langmuir, 2014, 30, 6408-6418.	3.5	75
58	Mutual Solubility of Water and Structural/Positional Isomers of N-Alkylpyridinium-Based Ionic Liquids. Journal of Physical Chemistry B, 2010, 114, 15925-15934.	2.6	74
59	1-Alkyl-3-methylimidazolium alkanesulfonate ionic liquids, [CnH2n+1mim][CkH2k+1SO3]: synthesis and physicochemical properties. Physical Chemistry Chemical Physics, 2009, 11, 8939.	2.8	70
60	Solubility of inorganic salts in pure ionic liquids. Journal of Chemical Thermodynamics, 2012, 55, 29-36.	2.0	70
61	Pressureâ^'Densityâ^'Temperature (pâ^'Ïâ^'T) Surface of [C₆mim][NTf₂]. Journal of Chemical & Engineering Data, 2008, 53, 867-870.	1.9	69
62	Enhanced dissolution of ibuprofen using ionic liquids as catanionic hydrotropes. Physical Chemistry Chemical Physics, 2018, 20, 2094-2103.	2.8	68
63	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.	2.6	66
64	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.	2.6	65
65	The effect of the cation alkyl chain branching on mutual solubilities with water and toxicities. Physical Chemistry Chemical Physics, 2014, 16, 19952.	2.8	64
66	A thermophysical and structural characterization of ionic liquids with alkyl and perfluoroalkyl side chains. RSC Advances, 2015, 5, 65337-65350.	3.6	63
67	Ionic Liquids in Polyethylene Glycol Aqueous Solutions: Salting-in and Salting-out Effects. Monatshefte FÃ¼r Chemie, 2007, 138, 1153-1157.	1.8	62
68	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.	2.6	56
69	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.	3.2	56
70	Molecular Dynamics Simulations of Charged Dendrimers:â€‰Low-to-Intermediate Half-Generation PAMAMs. Journal of Physical Chemistry B, 2007, 111, 10651-10664.	2.6	54
71	Impact of Self-Aggregation on the Formation of Ionic-Liquid-Based Aqueous Biphasic Systems. Journal of Physical Chemistry B, 2012, 116, 7660-7668.	2.6	54
72	Thermodynamics and Micro Heterogeneity of Ionic Liquids. Topics in Current Chemistry, 2009, 290, 161-183.	4.0	53

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73	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.	2.1	51
74	Nanostructure of Trialkylmethylammonium Bistriflamide Ionic Liquids Studied by Molecular Dynamics. Journal of Physical Chemistry B, 2010, 114, 15635-15641.	2.6	50
75	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.	2.8	49
76	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.	2.8	49
77	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.	2.6	47
78	Complex Structure of Ionic Liquids. Molecular Dynamics Studies with Different Cationâ€“Anion Combinations. Journal of Chemical & Engineering Data, 2014, 59, 3120-3129.	1.9	47
79	Influence of Nanosegregation on the Phase Behavior of Fluorinated Ionic Liquids. Journal of Physical Chemistry C, 2017, 121, 5415-5427.	3.1	46
80	A Molecular Dynamics Study of the Thermodynamic Properties of Calcium Apatites. 1. Hexagonal Phases. Journal of Physical Chemistry B, 2005, 109, 24473-24479.	2.6	44
81	Solubility of alkanes, alkanols and their fluorinated counterparts in tetraalkylphosphonium ionic liquids. Physical Chemistry Chemical Physics, 2010, 12, 9685.	2.8	44
82	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.	4.6	44
83	Exploring the bulk-phase structure of ionic liquid mixtures using small-angle neutron scattering. Faraday Discussions, 2018, 206, 265-289.	3.2	42
84	Experimental and Molecular Dynamics Simulation Study of the Sublimation and Vaporization Energetics of Iron Metalocenes. Crystal Structures of Fe(Î·⁵-C₅H₄CH₃)₂ and		

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91	Plasma membrane permeabilisation by ionic liquids: a matter of charge. Green Chemistry, 2015, 17, 4587-4598.	9.0	37
92	Additive polarizabilities in ionic liquids. Physical Chemistry Chemical Physics, 2016, 18, 1665-1670.	2.8	37
93	Characteristics of aggregation in aqueous solutions of dialkylpyrrolidinium bromides. Journal of Colloid and Interface Science, 2011, 360, 606-616.	9.4	36
94	An All-Atom Force Field for Metallocenes. Journal of Physical Chemistry A, 2006, 110, 13850-13856.	2.5	35
95	Solubility of fluorinated compounds in a range of ionic liquids. Cloud-point temperature dependence on composition and pressure. Green Chemistry, 2008, 10, 918.	9.0	35
96	Liquidâ€Crystalline Ionic Liquids as Ordered Reaction Media for the Dielsâ€“Alder Reaction. Chemistry - A European Journal, 2016, 22, 16113-16123.	3.3	35
97	Solubility isotope effects in aqueous solutions of methane. Journal of Chemical Physics, 2002, 116, 10816-10824.	3.0	34
98	Raman Spectroscopic Study of the Vapor Phase of 1-Methylimidazolium Ethanoate, a Protic Ionic Liquid. Journal of Physical Chemistry A, 2010, 114, 10834-10841.	2.5	34
99	Liquidâ€“Liquid Equilibrium of Cholinium-Derived Bistriflimide Ionic Liquids with Water and Octanol. Journal of Physical Chemistry B, 2012, 116, 9186-9195.	2.6	34
100	The alternation effect in ionic liquid homologous series. Physical Chemistry Chemical Physics, 2014, 16, 4033-4038.	2.8	34
101	Phase Equilibria in Ionic Liquidâ^'Aromatic Compound Mixtures, Including Benzene Fluorination Effects. Journal of Physical Chemistry B, 2009, 113, 7631-7636.	2.6	33
102	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.	2.5	33
103	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.	2.5	32
104	Probing the Surface Tension of Ionic Liquids Using the Langmuir Principle. Langmuir, 2018, 34, 4408-4416.	3.5	31
105	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.	2.6	30
106	The impact of ionic liquid fluorinated moieties on their thermophysical properties and aqueous phase behaviour. Physical Chemistry Chemical Physics, 2014, 16, 21340-21348.	2.8	30
107	Structural characterization of the [CnC1im][C4F9SO3] ionic liquid series: Alkyl versus perfluoroalkyl side chains. Journal of Molecular Liquids, 2017, 226, 28-34.	4.9	30
108	Phase Behavior and Thermodynamic Properties of Ionic Liquids, Ionic Liquid Mixtures, and Ionic Liquid Solutions. ACS Symposium Series, 2005, , 270-291.	0.5	29

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109	Ionic liquids and reactive azeotropes: the continuity of the aprotic and protic classes. Physical Chemistry Chemical Physics, 2010, 12, 1948.	2.8	29
110	A molecular dynamics study on the thickness and post-critical strength of carbon nanotubes. Composite Structures, 2012, 94, 1352-1358.	5.8	29
111	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.	4.9	28
112	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.	2.6	27
113	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.	2.6	27
114	Using ¹²⁹Xe NMR to Probe the Structure of Ionic Liquids. Journal of Physical Chemistry Letters, 2013, 4, 2758-2762.	4.6	26
115	Phase Equilibria of Haloalkanes Dissolved in Ethylsulfate- or Ethylsulfonate-Based Ionic Liquids. Journal of Physical Chemistry B, 2010, 114, 7329-7337.	2.6	24
116	Liquid- or Solid-Like Behavior of [omim][BF₄] at a Solid Interface?. Journal of Physical Chemistry Letters, 2011, 2, 1551-1555.	4.6	24
117	Unusual LCST-type behaviour found in binary mixtures of choline-based ionic liquids with ethers. RSC Advances, 2013, 3, 10262.	3.6	24
118	Molecular Dynamics Study of the Thermodynamic Properties of Calcium Apatites. 2. Monoclinic Phases. Journal of Physical Chemistry B, 2006, 110, 4387-4392.	2.6	23
119	Vaporisation of a Dicationic Ionic Liquid Revisited. ChemPhysChem, 2010, 11, 3673-3677.	2.1	23
120	Strength and fracture of graphyne and graphdiyne nanotubes. Computational Materials Science, 2020, 171, 109233.	3.0	22
121	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.	2.8	22
122	CNT-reinforced iron and titanium nanocomposites: Strength and deformation mechanisms. Composites Part B: Engineering, 2020, 187, 107836.	12.0	22
123	Phase equilibra in binary Lennard-Jones mixtures: phase diagram simulation. Molecular Physics, 1999, 96, 1649-1658.	1.7	21
124	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.	3.0	21
125	Tensionâ€“twisting dependent kinematics of chiral CNTs. Composites Science and Technology, 2013, 74, 211-220.	7.8	21
126	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

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127	Viscosity minima in binary mixtures of ionic liquids + molecular solvents. Physical Chemistry Chemical Physics, 2015, 17, 13480-13494.	2.8	21
128	The excess thermodynamic properties of liquid (CH4+CD4). Journal of Chemical Physics, 1994, 100, 4582-4590.	3.0	20
129	Shifts in the temperature of maximum density (TMD) of ionic liquid aqueous solutions. Physical Chemistry Chemical Physics, 2013, 15, 10960.	2.8	20
130	High ionicity ionic liquids (HIILs): comparing the effect of ethylsulfonate and ethylsulfate anions. Physical Chemistry Chemical Physics, 2013, 15, 18138.	2.8	20
131	Induced anisotropy of chiral carbon nanotubes under combined tension-twisting. Mechanics of Materials, 2013, 58, 97-109.	3.2	20
132	Nanoscale organization in the fluorinated room temperature ionic liquid: Tetraethyl ammonium (trifluoromethanesulfonyl)(nonafluorobutylsulfonyl)imide. Journal of Chemical Physics, 2018, 148, 193816.	3.0	19
133	Molecular dynamics studies on the structure and interactions of ionic liquids containing amino-acid anions. Physical Chemistry Chemical Physics, 2018, 20, 23864-23872.	2.8	19
134	Ionic Liquids and Water: Hydrophobicity vs. Hydrophilicity. Molecules, 2021, 26, 7159.	3.8	19
135	Energetics of Aqueous Solutions of the Ionic Liquid 1-Ethyl-3-methylimidazolium Ethylsulfate. Journal of Physical Chemistry B, 2010, 114, 13179-13188.	2.6	18
136	Experimental and Molecular Dynamics Simulation Study of the Sublimation Energetics of Cyclopentadienyltricarbonylmanganese (Cymantrene). Journal of Physical Chemistry A, 2008, 112, 10429-10434.	2.5	17
137	Interaction diagrams for carbon nanotubes under combined shorteningâ€“twisting. Composites Science and Technology, 2011, 71, 1811-1818.	7.8	17
138	Solvation of alcohols in ionic liquids â€“ understanding the effect of the anion and cation. Physical Chemistry Chemical Physics, 2018, 20, 2536-2548.	2.8	17
139	Design of task-specific fluorinated ionic liquids: nanosegregation versus hydrogen-bonding ability in aqueous solutions. Chemical Communications, 2018, 54, 3524-3527.	4.1	17
140	Designing the ammonium cation to achieve a higher hydrophilicity of bistriflimide-based ionic liquids. Physical Chemistry Chemical Physics, 2018, 20, 19307-19313.	2.8	17
141	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
142	Wetting Films of Two Ionic Liquids: [C₈mim][BF4] and [C₂OHmim][BF₄]. Journal of Physical Chemistry C, 2011, 115, 16116-16123.	3.1	16
143	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.	2.0	16
144	From lime to silica and alumina: systematic modeling of cement clinkers using a general force-field. Physical Chemistry Chemical Physics, 2015, 17, 18477-18494.	2.8	16

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145	Microstructural control and hydration of novel micro-dendritic clinkers with CaO/SiO 2 = 1.4. Cement and Concrete Research, 2015, 76, 212-221.	11.0	16
146	Mechanical behaviour of carbon nanotubes under combined twistingâ€“bending. Mechanics Research Communications, 2016, 73, 19-24.	1.8	16
147	Comparing the structure of different ionic liquid series: Bistriflamide v. hexafluorophosphate; pure v. equimolar mixtures. Fluid Phase Equilibria, 2016, 418, 181-191.	2.5	16
148	Nicotine:Â On the Potential Role of Ionic Liquids for Its Processing and Purification. Journal of Physical Chemistry B, 2007, 111, 7934-7937.	2.6	15
149	Molecular Dynamics Simulations of Porphyrinâ˜Dendrimer Systems: Toward Modeling Electron Transfer in Solution. Journal of Physical Chemistry B, 2008, 112, 14779-14792.	2.6	15
150	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.	2.6	15
151	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.	4.7	15
152	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.	1.9	15
153	Structure and dynamics of mica-confined films of [C10C1Pyrr][NTf2] ionic liquid. Journal of Chemical Physics, 2018, 148, 193808.	3.0	15
154	Molecular dynamics simulations of molten calcium hydroxyapatite. Fluid Phase Equilibria, 2006, 241, 51-58.	2.5	14
155	Polymorphism in 4â€²-Hydroxyacetophenone: A Molecular Dynamics Simulation Study. Journal of Physical Chemistry B, 2012, 116, 5179-5184.	2.6	14
156	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.	2.8	14
157	Mixtures of Pyridine and Nicotine with Pyridinium-Based Ionic Liquids. Journal of Chemical & Engineering Data, 2011, 56, 4356-4363.	1.9	13
158	Viscosity Mixing Rules for Binary Systems Containing One Ionic Liquid. ChemPhysChem, 2013, 14, 1956-1968.	2.1	12
159	Ionic Liquid Films at the Waterâ€“Air Interface: Langmuir Isotherms of Tetra-alkylphosphonium-Based Ionic Liquids. Langmuir, 2015, 31, 8371-8378.	3.5	12
160	Solvent effects on the polar network of ionic liquid solutions. Journal of Physics Condensed Matter, 2015, 27, 194116.	1.8	12
161	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.	2.8	12
162	Neat ionic liquids versus ionic liquid mixtures: a combination of experimental data and molecular simulation. Physical Chemistry Chemical Physics, 2019, 21, 23305-23309.	2.8	12

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