AgÃ-lio A H PÃ¡dua

List of Publications by Year
in descending order

170 papers	15,239 citations	22132 59 h-index	18115 120 g-index
190 all docs	190 docs citations	190 times ranked	9984 citing authors

#	Article	IF	Citations
1	Nanostructural Organization in Ionic Liquids. Journal of Physical Chemistry B, 2006, 110, 3330-3335.	1.2	1,693
2	Modeling Ionic Liquids Using a Systematic All-Atom Force Field. Journal of Physical Chemistry B, 2004, 108, 2038-2047.	1.2	1,190
3	Molecular Force Field for Ionic Liquids Composed of Triflate or Bistriflylimide Anions. Journal of Physical Chemistry B, 2004, 108, 16893-16898.	1.2	875
4	Density and viscosity of several pure and water-saturated ionic liquids. Green Chemistry, 2006, 8, 172-180.	4.6	755
5	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
6	Molecular Solutes in Ionic Liquids: A Structural Perspective. Accounts of Chemical Research, 2007, 40, 1087-1096.	7.6	450
7	Nonpolar, Polar, and Associating Solutes in Ionic Liquids. Journal of Physical Chemistry B, 2006, 110, 16816-16818.	1.2	446
8	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
9	CL&P: A generic and systematic force field for ionic liquids modeling. Theoretical Chemistry Accounts, 2012, 131, 1.	0.5	281
10	Enhancing effect of dimethylamine in sulfuric acid nucleation in the presence of water â€“ a computational study. Atmospheric Chemistry and Physics, 2010, 10, 4961-4974.	1.9	245
11	Improvement of Quality in Publication of Experimental Thermophysical Property Data: Challenges, Assessment Tools, Global Implementation, and Online Support. Journal of Chemical & Engineering Data, 2013, 58, 2699-2716.	1.0	236
12	Prediction of Ionic Liquid Properties. I. Volumetric Properties as a Function of Temperature at 0.1 MPa. Journal of Chemical & Engineering Data, 2008, 53, 716-726.	1.0	233
13	Understanding the role of co-solvents in the dissolution of cellulose in ionic liquids. Green Chemistry, 2014, 16, 2528.	4.6	231
14	Liquid Structure of the Ionic Liquid 1,3-Dimethylimidazolium Bis{(trifluoromethyl)sulfonyl}amide. Journal of Physical Chemistry B, 2006, 110, 12055-12061.	1.2	215
15	Liquid-Phase Exfoliation of Phosphorene: Design Rules from Molecular Dynamics Simulations. ACS Nano, 2015, 9, 8255-8268.	7.3	160
16	Effect of Fluorination and Size of the Alkyl Side-Chain on the Solubility of Carbon Dioxide in 1-Alkyl-3-methylimidazolium Bis(trifluoromethylsulfonyl)amide Ionic Liquids. Journal of Physical Chemistry B, 2010, 114, 3608-3617.	1.2	159
17	Three commentaries on the nano-segregated structure of ionic liquids. Computational and Theoretical Chemistry, 2010, 946, 70-76.	1.5	156
18	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

#	Article	IF	Citations
19	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
20	Self-assembled nanostructures in ionic liquids facilitate charge storage at electrified interfaces. Nature Materials, 2019, 18, 1350-1357.	13.3	144
21	Prediction of Ionic Liquid Properties. II. Volumetric Properties as a Function of Temperature and Pressure. Journal of Chemical & Engineering Data, 2008, 53, 2133-2143.	1.0	139
22	Solvation and Stabilization of Metallic Nanoparticles in Ionic Liquids. Angewandte Chemie - International Edition, 2011, 50, 8683-8687.	7.2	132
23	Organized 3D-alkyl imidazolium ionic liquids could be used to control the size of in situ generated ruthenium nanoparticles?. Journal of Materials Chemistry, 2009, 19, 3624.	6.7	131
24	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
25	Porous Ionic Liquids or Liquid Metalâ€“Organic Frameworks?. Angewandte Chemie - International Edition, 2018, 57, 11909-11912.	7.2	124
26	Effect of Water on the Carbon Dioxide Absorption by 1-Alkyl-3-methylimidazolium Acetate Ionic Liquids. Journal of Physical Chemistry B, 2012, 116, 14416-14425.	1.2	111
27	Multiresolution calculation of ionic liquids. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2015, 5, 202-214.	6.2	108
28	Transferable, Polarizable Force Field for Ionic Liquids. Journal of Chemical Theory and Computation, 2019, 15, 5858-5871.	2.3	108
29	Density and Viscosity Measurements of 2,2,4-Trimethylpentane (Isooctane) from 198 K to 348 K and up to 100 MPa. Journal of Chemical & Engineering Data, 1996, 41, 1488-1494.	1.0	107
30	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
31	Absorption of Carbon Dioxide, Nitrous Oxide, Ethane and Nitrogen by 1-Alkyl-3-methylimidazolium (C_nmim, n = 2,4,6) Tris(pentafluoroethyl)trifluorophosphate Ionic Liquids (eFAP). Journal of Physical Chemistry B, 2012, 116, 7728-7738.	1.2	95
32	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
33	Are There Magic Compositions in Deep Eutectic Solvents? Effects of Composition and Water Content in Choline Chloride/Ethylene Glycol from Ab Initio Molecular Dynamics. Journal of Physical Chemistry B, 2020, 124, 7433-7443.	1.2	94
34	Systematic Comparison of the Structural and Dynamic Properties of Commonly Used Water Models for Molecular Dynamics Simulations. Journal of Chemical Information and Modeling, 2021, 61, 4521-4536.	2.5	94
35	Molecular Simulation Study of Interactions of Carbon Dioxide and Water with Ionic Liquids. ChemPhysChem, 2004, 5, 1049-1052.	1.0	92
36	Relationship between Viscosity Coefficients and Volumetric Properties Using a Scaling Concept for Molecular and Ionic Liquids. Journal of Physical Chemistry B, 2008, 112, 5563-5574.	1.2	91

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37	Density scaling of the transport properties of molecular and ionic liquids. Journal of Chemical Physics, 2011, 134, 144507.	1.2	91
38	Validation of an accurate vibrating-wire densimeter: Density and viscosity of liquids over wide ranges of temperature and pressure. International Journal of Thermophysics, 1996, 17, 781-802.	1.0	87
39	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
40	Mixing Enthalpy for Binary Mixtures Containing Ionic Liquids. Chemical Reviews, 2016, 116, 6075-6106.	23.0	85
41	Potential Energy Landscape of Bis(fluorosulfonyl)amide. Journal of Physical Chemistry B, 2008, 112, 9449-9455.	1.2	81
42	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
43	Quantitative Modeling of MoS₂â€“Solvent Interfaces: Predicting Contact Angles and Exfoliation Performance using Molecular Dynamics. Journal of Physical Chemistry C, 2017, 121, 9022-9031.	1.5	81
44	Viscosity and density of mixtures of methane and n-decane from 298 to 393 K and up to 75 MPa. Fluid Phase Equilibria, 2004, 216, 235-244.	1.4	80
45	Simultaneous measurement of the solubility of nitrogen and carbon dioxide in polystyrene and of the associated polymer swelling. Journal of Polymer Science, Part B: Polymer Physics, 2001, 39, 2063-2070.	2.4	79
46	Solubility of oxygen in n-hexane and in n-perfluorohexane. Experimental determination and prediction by molecular simulation. Physical Chemistry Chemical Physics, 2003, 5, 543-549.	1.3	76
47	Selectivity enhancement in the aqueous acid-catalyzed conversion of glucose to 5-hydroxymethylfurfural induced by choline chloride. Green Chemistry, 2013, 15, 3205.	4.6	74
48	New solvent-stabilized few-layer black phosphorus for antibacterial applications. Nanoscale, 2018, 10, 12543-12553.	2.8	74
49	Thermalized Drude Oscillators with the LAMMPS Molecular Dynamics Simulator. Journal of Chemical Information and Modeling, 2016, 56, 260-268.	2.5	73
50	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
51	A novel stabilisation model for ruthenium nanoparticles in imidazolium ionic liquids: in situ spectroscopic and labelling evidence. Physical Chemistry Chemical Physics, 2010, 12, 4217.	1.3	68
52	Interactions of Carbon Dioxide with Liquid Fluorocarbons. Journal of Physical Chemistry B, 2003, 107, 14020-14024.	1.2	67
53	Nonequilibrium Molecular Simulations of New Ionic Lubricants at Metallic Surfaces: Prediction of the Friction. Journal of Chemical Theory and Computation, 2013, 9, 1600-1610.	2.3	67
54	Molecular Dynamics Simulations of the Liquid Surface of the Ionic Liquid 1-Hexyl-3-methylimidazolium Bis(trifluoromethanesulfonyl)amide: Structure and Surface Tension. Journal of Physical Chemistry B, 2009, 113, 14708-14718.	1.2	66

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55	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
56	Interactions and Ordering of Ionic Liquids at a Metal Surface. Journal of Chemical Theory and Computation, 2012, 8, 3348-3355.	2.3	66
57	Interactions and structure of ionic liquids on graphene and carbon nanotubes surfaces. RSC Advances, 2014, 4, 18017-18024.	1.7	65
58	Dominance of Dispersion Interactions and Entropy over Electrostatics in Determining the Wettability and Friction of Two-Dimensional MoS₂ Surfaces. ACS Nano, 2016, 10, 9145-9155.	7.3	63
59	Highâ€Performance Porous Ionic Liquids for Lowâ€Pressure CO₂ Capture**. Angewandte Chemie - International Edition, 2021, 60, 12876-12882.	7.2	63
60	Simultaneous measurement of density and viscosity of n-pentane from 298 to 383 K and up to 100 MPa using a vibrating-wire instrument. Fluid Phase Equilibria, 2001, 181, 147-161.	1.4	61
61	Thermophysical properties, low pressure solubilities and thermodynamics of solvation of carbon dioxide and hydrogen in two ionic liquids based on the alkylsulfate anion. Green Chemistry, 2008, 10, 944.	4.6	61
62	Thermal Conductivity of Ionic Liquids and IoNanofluids and Their Feasibility as Heat Transfer Fluids. Industrial & Engineering Chemistry Research, 2018, 57, 6516-6529.	1.8	59
63	Torsion Energy Profiles and Force Fields Derived from Ab Initio Calculations for Simulations of Hydrocarbonâ^'Fluorocarbon Diblocks and Perfluoroalkylbromides. Journal of Physical Chemistry A, 2002, 106, 10116-10123.	1.1	57
64	Absorption of carbon dioxide by ionic liquids with carboxylate anions. International Journal of Greenhouse Gas Control, 2013, 17, 78-88.	2.3	57
65	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
66	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
67	Ab initio molecular dynamics simulations of SO 2 solvation in choline chloride/glycerol deep eutectic solvent. Fluid Phase Equilibria, 2017, 448, 59-68.	1.4	56
68	Extension of the CL&Pol Polarizable Force Field to Electrolytes, Protic Ionic Liquids, and Deep Eutectic Solvents. Journal of Chemical Theory and Computation, 2021, 17, 1606-1617.	2.3	56
69	Thermophysical properties of ionic liquid dicyanamide (DCA) nanosystems. Journal of Chemical Thermodynamics, 2014, 79, 248-257.	1.0	55
70	Density and Viscosity Measurements of 1,1,1,2-Tetrafluoroethane (HFC-134a) from 199 K to 298 K and up to 100 MPa. Journal of Chemical & Engineering Data, 1996, 41, 731-735.	1.0	54
71	Electromechanical model for vibrating-wire instruments. Review of Scientific Instruments, 1998, 69, 2392-2399.	0.6	54
72	Viscosity and density measurements for carbon dioxide+pentaerythritol ester lubricant mixtures at low lubricant concentration. Journal of Supercritical Fluids, 2008, 44, 172-185.	1.6	53

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73	Thermodynamics and Micro Heterogeneity of Ionic Liquids. Topics in Current Chemistry, 2009, 290, 161-183.	4.0	53
74	Interaction Energies of Ionic Liquids with Metallic Nanoparticles: Solvation and Stabilization Effects. Journal of Physical Chemistry C, 2013, 117, 3537-3547.	1.5	53
75	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
76	Bulk and Liquidâ€“Vapor Interface of Pyrrolidinium-Based Ionic Liquids: A Molecular Simulation Study. Journal of Physical Chemistry B, 2014, 118, 731-742.	1.2	51
77	Nanostructure of Trialkylmethylammonium Bistriflamide Ionic Liquids Studied by Molecular Dynamics. Journal of Physical Chemistry B, 2010, 114, 15635-15641.	1.2	50
78	Diffusion Coefficients of 1-Alkyl-3-methylimidazolium Ionic Liquids in Water, Methanol, and Acetonitrile at Infinite Dilution. Journal of Chemical & Engineering Data, 2009, 54, 2389-2394.	1.0	48
79	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
80	Thermodynamics of cellulose dissolution in an imidazolium acetate ionic liquid. Chemical Communications, 2015, 51, 4485-4487.	2.2	47
81	Ionic Liquids Can Enable the Recycling of Fluorinated Greenhouse Gases. ACS Sustainable Chemistry and Engineering, 2019, 7, 16900-16906.	3.2	47
82	Resolving dispersion and induction components for polarisable molecular simulations of ionic liquids. Journal of Chemical Physics, 2017, 146, 204501.	1.2	45
83	Influence of Fluorination on the Solubilities of Carbon Dioxide, Ethane, and Nitrogen in 1-n-Fluoro-alkyl-3-methylimidazolium Bis(n-fluoroalkylsulfonyl)amide Ionic Liquids. Journal of Physical Chemistry B, 2017, 121, 426-436.	1.2	44
84	Calorimetric and Volumetric Study on Binary Mixtures 2,2,2-Trifluoroethanol + (1-Butyl-3-methylimidazolium Tetrafluoroborate or 1-Ethyl-3-methylimidazolium Tetrafluoroborate). Journal of Chemical & Engineering Data, 2010, 55, 5504-5512.	1.0	43
85	Ruthenium nanoparticles in ionic liquids: structural and stability effects of polar solutes. Physical Chemistry Chemical Physics, 2011, 13, 13527.	1.3	42
86	Strong Microheterogeneity in Novel Deep Eutectic Solvents. ChemPhysChem, 2019, 20, 1786-1792.	1.0	41
87	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
88	Gasâ€“liquid interactions in solution. Pure and Applied Chemistry, 2005, 77, 653-665.	0.9	40
89	Solvation of a Cellulose Microfibril in Imidazolium Acetate Ionic Liquids: Effect of a Cosolvent. Journal of Physical Chemistry B, 2014, 118, 141211094045002.	1.2	39
90	Using ethane and butane as probes to the molecular structure of 1-alkyl-3-methylimidazolium bis[(trifluoromethyl)sulfonyl]imide ionic liquids. Faraday Discussions, 2012, 154, 41-52.	1.6	38

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91	Glass transition of ionic liquids under high pressure. Journal of Chemical Physics, 2014, 140, 244514.	1.2	37
92	Thermodynamic Properties of Selected Homologous Series of Ionic Liquids Calculated Using Molecular Dynamics. Journal of Physical Chemistry B, 2016, 120, 2362-2371.	1.2	37
93	Ionic liquids at the surface of graphite: Wettability and structure. Journal of Chemical Physics, 2018, 148, 193840.	1.2	37
94	Connecting chloride solvation with hydration in deep eutectic systems. Physical Chemistry Chemical Physics, 2021, 23, 107-111.	1.3	37
95	Characteristics of aggregation in aqueous solutions of dialkylpyrrolidinium bromides. Journal of Colloid and Interface Science, 2011, 360, 606-616.	5.0	36
96	Effect of Unsaturation on the Absorption of Ethane and Ethylene in Imidazolium-Based Ionic Liquids. Journal of Physical Chemistry B, 2013, 117, 7416-7425.	1.2	36
97	Molecular interactions and thermal transport in ionic liquids with carbon nanomaterials. Physical Chemistry Chemical Physics, 2017, 19, 17075-17087.	1.3	35
98	Dispersion and Stabilization of Exfoliated Graphene in Ionic Liquids. Frontiers in Chemistry, 2019, 7, 223.	1.8	35
99	Solubility isotope effects in aqueous solutions of methane. Journal of Chemical Physics, 2002, 116, 10816-10824.	1.2	34
100	Surface Composition/Organization of Ionic Liquids with Au Nanoparticles Revealed by High-Sensitivity Low-Energy Ion Scattering. Langmuir, 2013, 29, 14301-14306.	1.6	34
101	Phase Equilibria in Ionic Liquidâ^'Aromatic Compound Mixtures, Including Benzene Fluorination Effects. Journal of Physical Chemistry B, 2009, 113, 7631-7636.	1.2	33
102	A vibrating-wire densimeter for liquids at high pressures: The density of 2,2,4-trimethylpentane from 298.15 to 348.15 K and up to 100 MPa. International Journal of Thermophysics, 1994, 15, 229-243.	1.0	32
103	Porous Ionic Liquids or Liquid Metalâ€“Organic Frameworks?. Angewandte Chemie, 2018, 130, 12085-12088.	1.6	32
104	Porous Ionic Liquids: Structure, Stability, and Gas Absorption Mechanisms. Advanced Materials Interfaces, 2021, 8, 2001982.	1.9	32
105	Perfluoroalkanes in Water:â€‰ Experimental Henry's Law Coefficients for Hexafluoroethane and Computer Simulations for Tetrafluoromethane and Hexafluoroethane. Journal of Physical Chemistry B, 2001, 105, 8403-8409.	1.2	31
106	Solubility of oxygen, carbon dioxide and water in semifluorinated alkanes and in perfluorooctylbromide by molecular simulation. Journal of Fluorine Chemistry, 2004, 125, 409-413.	0.9	31
107	How do Physicalâ^'Chemical Parameters Influence the Catalytic Hydrogenation of 1,3-Cyclohexadiene in Ionic Liquids?. Journal of Physical Chemistry B, 2010, 114, 8156-8165.	1.2	31
108	Using Molecular Simulation to Understand the Structure of [C₂C₁im]⁺â€“Alkylsulfate Ionic Liquids: Bulk and Liquidâ€“Vapor Interfaces. Journal of Physical Chemistry B, 2012, 116, 14159-14170.	1.2	31

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109	The viscosity of liquid carbon dioxide. International Journal of Thermophysics, 1994, 15, 767-777.	1.0	30
110	Influence of Ester Functional Groups on the Liquid-Phase Structure and Solvation Properties of Imidazolium-Based Ionic Liquids. Journal of Physical Chemistry B, 2011, 115, 3942-3948.	1.2	30
111	Density and Viscosity of Mixtures of n-Hexane and 1-Hexanol from 303 to 423 K up to 50 MPa. International Journal of Thermophysics, 2002, 23, 1537-1550.	1.0	29
112	High-Pressure Densities of 2,2,2-Trifluoroethanol + Ionic Liquid Mixtures Useful for Possible Applications in Absorption Cycles. Industrial & Engineering Chemistry Research, 2014, 53, 10791-10802.	1.8	29
113	Tailoring the properties of acetate-based ionic liquids using the tricyanomethanide anion. Physical Chemistry Chemical Physics, 2016, 18, 23285-23295.	1.3	28
114	Low pressure solubility and thermodynamics of solvation of oxygen, carbon dioxide, and carbon monoxide in fluorinated liquids. Journal of Chemical Thermodynamics, 2007, 39, 847-854.	1.0	27
115	Can the tricyanomethanide anion improve CO₂ absorption by acetate-based ionic liquids?. Physical Chemistry Chemical Physics, 2017, 19, 12431-12440.	1.3	26
116	Exfoliation of graphene and fluorographene in molecular and ionic liquids. Faraday Discussions, 2018, 206, 61-75.	1.6	25
117	Preparation of microfibers from wood/ionic liquid solutions. Carbohydrate Polymers, 2013, 92, 214-217.	5.1	24
118	The <scp>CL</scp>&Pol polarizable force field for the simulation of ionic liquids and eutectic solvents. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2022, 12, e1572.	6.2	24
119	Investigation of Li+ Cation Coordination and Transportation, by Molecular Modeling and NMR Studies, in a LiNTf2-Doped Ionic Liquidâ€“Vinylene Carbonate Mixture. Journal of Physical Chemistry B, 2018, 122, 8560-8569.	1.2	23
120	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
121	Molecular Simulations of Primary Alkanolamines Using an Extendable Force Field. ChemPhysChem, 2012, 13, 3866-3874.	1.0	21
122	Kinetic analysis of microwave-enhanced cellulose dissolution in ionic solvents. Physical Chemistry Chemical Physics, 2020, 22, 1003-1010.	1.3	21
123	Ligand effect on the catalytic activity of ruthenium nanoparticles in ionic liquids. Dalton Transactions, 2012, 41, 13919.	1.6	19
124	Novel ionic lubricants for amorphous carbon surfaces: molecular modeling of the structure and friction. Soft Matter, 2013, 9, 10606.	1.2	19
125	Structural effects on dynamic and energetic properties of mixtures of ionic liquids and water. Journal of Molecular Liquids, 2017, 242, 204-212.	2.3	19
126	Highâ€pressure viscosity and density of carbon dioxide + pentaerythritol ester mixtures: Measurements and modeling. AICHE Journal, 2008, 54, 1625-1636.	1.8	18

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127	Joint Statement of Editors of Journals Publishing Thermophysical Property Data. Journal of Chemical & Engineering Data, 2009, 54, 2-3.	1.0	18
128	Influence of Ionic Association, Transport Properties, and Solvation on the Catalytic Hydrogenation of 1,3-Cyclohexadiene in Ionic Liquids. Journal of Physical Chemistry B, 2011, 115, 12150-12159.	1.2	18
129	Glycine in 1â€Butylâ€3â€Methylimidazolium Acetate and Trifluoroacetate Ionic Liquids: Effect of Fluorination and Hydrogen Bonding. ChemPhysChem, 2012, 13, 1753-1763.	1.0	18
130	Using hydrogenated and perfluorinated gases to probe the interactions and structure of fluorinated ionic liquids. Physical Chemistry Chemical Physics, 2019, 21, 8865-8873.	1.3	18
131	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
132	Pressure effect on vibrational frequency and dephasing of 1-alkyl-3-methylimidazolium hexafluorophosphate ionic liquids. Journal of Chemical Physics, 2013, 139, 054510.	1.2	15
133	Interactions of Gases with Ionic Liquids: Molecular Simulation. ACS Symposium Series, 2005, , 150-158.	0.5	14
134	Solvation of Halogens in Fluorous Phases. Experimental and Simulation Data for F2, Cl2, and Br2 in Several Fluorinated Liquids. Journal of Physical Chemistry B, 2008, 112, 6653-6664.	1.2	13
135	On the Regular Behavior of a Binary Mixture of Ionic Liquids. Journal of Physical Chemistry B, 2019, 123, 6579-6587.	1.2	13
136	Sodium diffusion in ionic liquid-based electrolytes for Na-ion batteries: the effect of polarizable force fields. Physical Chemistry Chemical Physics, 2020, 22, 20114-20122.	1.3	13
137	Effect of side chain modifications in imidazolium ionic liquids on the properties of the electrical double layer at a molybdenum disulfide electrode. Journal of Chemical Physics, 2021, 154, 084504.	1.2	13
138	Cosolvent effect on physical properties of 1,3-dimethyl imidazolium dimethyl phosphate and some theoretical insights on cellulose dissolution. Journal of Molecular Liquids, 2018, 265, 114-120.	2.3	12
139	Self-Organization in Ionic Liquids: From Bulk to Interfaces and Films. Journal of the Brazilian Chemical Society, 2015, , .	0.6	12
140	Solvation of C₆₀ Fullerene and C₆₀F₄₈ Fluorinated Fullerene in Molecular and Ionic Liquids. Journal of Physical Chemistry C, 2016, 120, 19396-19408.	1.5	11
141	Polycyclic aromatic hydrocarbons as model solutes for carbon nanomaterials in ionic liquids. Physical Chemistry Chemical Physics, 2017, 19, 27694-27703.	1.3	11
142	Charge transfer and polarisability in ionic liquids: a case study. Physical Chemistry Chemical Physics, 2022, 24, 3144-3162.	1.3	11
143	Predicting thermophysical properties of ionic liquids as a function of temperature and pressure. Proceedings of the Institution of Mechanical Engineers, Part J: Journal of Engineering Tribology, 2012, 226, 965-976.	1.0	10
144	Equations of states for an ionic liquid under high pressure: A molecular dynamics simulation study. Journal of Chemical Thermodynamics, 2014, 74, 39-42.	1.0	10

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145	Molecular understanding of pyridinium ionic liquids as absorbents with water as refrigerant for use in heat pumps. AIChE Journal, 2017, 63, 3523-3531.	1.8	10
146	Tuning the solvation of indigo in aqueous deep eutectics. Journal of Chemical Physics, 2021, 154, 224502.	1.2	10
147	Interactions of Nitrous Oxide with Fluorinated Liquids. Journal of Physical Chemistry B, 2006, 110, 18566-18572.	1.2	9
148	Isobutane as a probe of the structure of 1-alkyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide ionic liquids. Journal of Chemical Thermodynamics, 2015, 89, 98-103.	1.0	9
149	Intra- and Intermodular Structure of Ionic Liquids: From Conformers to Nanostructures. ACS Symposium Series, 2007, , 86-101.	0.5	8
150	Structure and dynamics of ionic liquids: general discussion. Faraday Discussions, 2018, 206, 291-337.	1.6	8
151	Phase behaviour and thermodynamics: general discussion. Faraday Discussions, 2017, 206, 113-139.	1.6	8
152	Improved carbon dioxide absorption in double-charged ionic liquids. Physical Chemistry Chemical Physics, 2021, 23, 23130-23140.	1.3	8
153	Effect of bromine substitution on the solubility of gases in hydrocarbons and fluorocarbons. Fluid Phase Equilibria, 2007, 251, 128-136.	1.4	7
154	Ion pair free energy surface as a probe of ionic liquid structure. Journal of Chemical Physics, 2020, 152, 014103.	1.2	7
155	Highâ€Performance Porous Ionic Liquids for Lowâ€Pressure CO₂ Capture**. Angewandte Chemie, 2021, 133, 12986-12992.	1.6	6
156	Ambient energy dispersion and long-term stabilisation of large graphene sheets from graphite using a surface energy matched ionic liquidâ€. Journal of Ionic Liquids, 2021, 1, 100001.	1.0	6
157	Interactions of Alkanolamines with Water: Excess Enthalpies and Hydrogen Bonding. Journal of Chemical Theory and Computation, 2014, 10, 2471-2478.	2.3	5
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