AgÃ-lio A H PÃ¡dua

List of Publications by Year
in descending order

170 papers	15,239 citations	22153 59 h-index	18130 120 g-index
190 all docs	190 docs citations	190 times ranked	9984 citing authors

#	Article	IF	Citations
1	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.	14.6	24
2	Charge transfer and polarisability in ionic liquids: a case study. Physical Chemistry Chemical Physics, 2022, 24, 3144-3162.	2.8	11
3	Enhancement of the solubility of organic dyes in aqueous ionic solvents doped with surfactants. Journal of Molecular Liquids, 2022, 357, 118958.	4.9	4
4	Fluorination effect on the solubility of C60 in a bis(trifluoromethimide based)imide based ionic liquid. Colloids and Surfaces A: Physicochemical and Engineering Aspects, 2022, , 129140.	4.7	1
5	Connecting chloride solvation with hydration in deep eutectic systems. Physical Chemistry Chemical Physics, 2021, 23, 107-111.	2.8	37
6	Improved carbon dioxide absorption in double-charged ionic liquids. Physical Chemistry Chemical Physics, 2021, 23, 23130-23140.	2.8	8
7	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.	5.3	56
8	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.	3.0	13
9	Porous Ionic Liquids: Structure, Stability, and Gas Absorption Mechanisms. Advanced Materials Interfaces, 2021, 8, 2001982.	3.7	32
10	Highâ€Performance Porous Ionic Liquids for Lowâ€Pressure CO₂ Capture**. Angewandte Chemie, 2021, 133, 12986-12992.	2.0	6
11	Highâ€Performance Porous Ionic Liquids for Lowâ€Pressure CO₂ Capture**. Angewandte Chemie - International Edition, 2021, 60, 12876-12882.	13.8	63
12	Screening Ionic Solvents for Enhancing the Solubility of Water-Insoluble Natural Dyes. Industrial & Engineering Chemistry Research, 2021, 60, 8555-8564.	3.7	5
13	Tuning the solvation of indigo in aqueous deep eutectics. Journal of Chemical Physics, 2021, 154, 224502.	3.0	10
14	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.	5.4	94
15	Excess Molar Enthalpies of Water + Primary Alkanolamines with a Common Nâ€“Câ€“Câ€“O Skeleton. Journal of Chemical & Engineering Data, 2021, 66, 4206-4214.	1.9	1
16	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.	2.7	6
17	All-Atom Models of Ionic Liquids. , 2021, , 1-7.		0
18	Kinetic analysis of microwave-enhanced cellulose dissolution in ionic solvents. Physical Chemistry Chemical Physics, 2020, 22, 1003-1010.	2.8	21

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19	Ion pair free energy surface as a probe of ionic liquid structure. Journal of Chemical Physics, 2020, 152, 014103.	3.0	7
20	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.	2.6	94
21	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.	2.8	13
22	Self-assembled nanostructures in ionic liquids facilitate charge storage at electrified interfaces. Nature Materials, 2019, 18, 1350-1357.	27.5	144
23	On the Regular Behavior of a Binary Mixture of Ionic Liquids. Journal of Physical Chemistry B, 2019, 123, 6579-6587.	2.6	13
24	Ionic Liquids Can Enable the Recycling of Fluorinated Greenhouse Gases. ACS Sustainable Chemistry and Engineering, 2019, 7, 16900-16906.	6.7	47
25	Transferable, Polarizable Force Field for Ionic Liquids. Journal of Chemical Theory and Computation, 2019, 15, 5858-5871.	5.3	108
26	Strong Microheterogeneity in Novel Deep Eutectic Solvents. ChemPhysChem, 2019, 20, 1786-1792.	2.1	41
27	Dispersion and Stabilization of Exfoliated Graphene in Ionic Liquids. Frontiers in Chemistry, 2019, 7, 223.	3.6	35
28	Using hydrogenated and perfluorinated gases to probe the interactions and structure of fluorinated ionic liquids. Physical Chemistry Chemical Physics, 2019, 21, 8865-8873.	2.8	18
29	Influence of Ionic Liquids on the Morphology of Corn Flour/Polyester Mixtures. Starch/Staerke, 2018, 70, 1700233.	2.1	2
30	Thermal Conductivity of Ionic Liquids and IoNanofluids and Their Feasibility as Heat Transfer Fluids. Industrial & Engineering Chemistry Research, 2018, 57, 6516-6529.	3.7	59
31	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.	4.9	12
32	Ionic liquids at the surface of graphite: Wettability and structure. Journal of Chemical Physics, 2018, 148, 193840.	3.0	37
33	Exfoliation of graphene and fluorographene in molecular and ionic liquids. Faraday Discussions, 2018, 206, 61-75.	3.2	25
34	Structure and dynamics of ionic liquids: general discussion. Faraday Discussions, 2018, 206, 291-337.	3.2	8
35	Ionic liquids at interfaces: general discussion. Faraday Discussions, 2018, 206, 549-586.	3.2	0
36	Porous Ionic Liquids or Liquid Metalâ€“Organic Frameworks?. Angewandte Chemie - International Edition, 2018, 57, 11909-11912.	13.8	124

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37	Porous Ionic Liquids or Liquid Metalâ€“Organic Frameworks?. Angewandte Chemie, 2018, 130, 12085-12088.	2.0	32
38	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.	2.6	23
39	New solvent-stabilized few-layer black phosphorus for antibacterial applications. Nanoscale, 2018, 10, 12543-12553.	5.6	74
40	Molecular understanding of pyridinium ionic liquids as absorbents with water as refrigerant for use in heat pumps. AICHE Journal, 2017, 63, 3523-3531.	3.6	10
41	Can the tricyanomethanide anion improve CO₂ absorption by acetate-based ionic liquids?. Physical Chemistry Chemical Physics, 2017, 19, 12431-12440.	2.8	26
42	Molecular interactions and thermal transport in ionic liquids with carbon nanomaterials. Physical Chemistry Chemical Physics, 2017, 19, 17075-17087.	2.8	35
43	Ab initio molecular dynamics simulations of SO 2 solvation in choline chloride/glycerol deep eutectic solvent. Fluid Phase Equilibria, 2017, 448, 59-68.	2.5	56
44	Quantitative Modeling of MoS₂â€“Solvent Interfaces: Predicting Contact Angles and Exfoliation Performance using Molecular Dynamics. Journal of Physical Chemistry C, 2017, 121, 9022-9031.	3.1	81
45	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.	2.6	44
46	Polycyclic aromatic hydrocarbons as model solutes for carbon nanomaterials in ionic liquids. Physical Chemistry Chemical Physics, 2017, 19, 27694-27703.	2.8	11
47	Experimental Study of the Interactions of Fullerene with Ionic Liquids. ACS Symposium Series, 2017, , 273-281.	0.5	1
48	Structural effects on dynamic and energetic properties of mixtures of ionic liquids and water. Journal of Molecular Liquids, 2017, 242, 204-212.	4.9	19
49	Resolving dispersion and induction components for polarisable molecular simulations of ionic liquids. Journal of Chemical Physics, 2017, 146, 204501.	3.0	45
50	Phase behaviour and thermodynamics: general discussion. Faraday Discussions, 2017, 206, 113-139.	3.2	8
51	Mixing Enthalpy for Binary Mixtures Containing Ionic Liquids. Chemical Reviews, 2016, 116, 6075-6106.	47.7	85
52	Solvation of C₆₀ Fullerene and C₆₀F₄₈ Fluorinated Fullerene in Molecular and Ionic Liquids. Journal of Physical Chemistry C, 2016, 120, 19396-19408.	3.1	11
53	Tailoring the properties of acetate-based ionic liquids using the tricyanomethanide anion. Physical Chemistry Chemical Physics, 2016, 18, 23285-23295.	2.8	28
54	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.	14.6	63

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55	Thermodynamic Properties of Selected Homologous Series of Ionic Liquids Calculated Using Molecular Dynamics. Journal of Physical Chemistry B, 2016, 120, 2362-2371.	2.6	37
56	Thermalized Drude Oscillators with the LAMMPS Molecular Dynamics Simulator. Journal of Chemical Information and Modeling, 2016, 56, 260-268.	5.4	73
57	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.	2.0	9
58	Multiresolution calculation of ionic liquids. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2015, 5, 202-214.	14.6	108
59	Thermodynamics of cellulose dissolution in an imidazolium acetate ionic liquid. Chemical Communications, 2015, 51, 4485-4487.	4.1	47
60	Liquid-Phase Exfoliation of Phosphorene: Design Rules from Molecular Dynamics Simulations. ACS Nano, 2015, 9, 8255-8268.	14.6	160
61	Self-Organization in Ionic Liquids: From Bulk to Interfaces and Films. Journal of the Brazilian Chemical Society, 2015, , .	0.6	12
62	Solvation of a Cellulose Microfibril in Imidazolium Acetate Ionic Liquids: Effect of a Cosolvent. Journal of Physical Chemistry B, 2014, 118, 141211094045002.	2.6	39
63	Glass transition of ionic liquids under high pressure. Journal of Chemical Physics, 2014, 140, 244514.	3.0	37
64	Equations of states for an ionic liquid under high pressure: A molecular dynamics simulation study. Journal of Chemical Thermodynamics, 2014, 74, 39-42.	2.0	10
65	Interactions and structure of ionic liquids on graphene and carbon nanotubes surfaces. RSC Advances, 2014, 4, 18017-18024.	3.6	65
66	Understanding the role of co-solvents in the dissolution of cellulose in ionic liquids. Green Chemistry, 2014, 16, 2528.	9.0	231
67	Interactions of Alkanolamines with Water: Excess Enthalpies and Hydrogen Bonding. Journal of Chemical Theory and Computation, 2014, 10, 2471-2478.	5.3	5
68	Bulk and Liquidâ€“Vapor Interface of Pyrrolidinium-Based Ionic Liquids: A Molecular Simulation Study. Journal of Physical Chemistry B, 2014, 118, 731-742.	2.6	51
69	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.	3.7	29
70	Thermophysical properties of ionic liquid dicyanamide (DCA) nanosystems. Journal of Chemical Thermodynamics, 2014, 79, 248-257.	2.0	55
71	Absorption of carbon dioxide by ionic liquids with carboxylate anions. International Journal of Greenhouse Gas Control, 2013, 17, 78-88.	4.6	57
72	Selectivity enhancement in the aqueous acid-catalyzed conversion of glucose to 5-hydroxymethylfurfural induced by choline chloride. Green Chemistry, 2013, 15, 3205.	9.0	74

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73	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.	1.9	236
74	Novel ionic lubricants for amorphous carbon surfaces: molecular modeling of the structure and friction. Soft Matter, 2013, 9, 10606.	2.7	19
75	Preparation of microfibers from wood/ionic liquid solutions. Carbohydrate Polymers, 2013, 92, 214-217.	10.2	24
76	Nonequilibrium Molecular Simulations of New Ionic Lubricants at Metallic Surfaces: Prediction of the Friction. Journal of Chemical Theory and Computation, 2013, 9, 1600-1610.	5.3	67
77	Effect of Unsaturation on the Absorption of Ethane and Ethylene in Imidazolium-Based Ionic Liquids. Journal of Physical Chemistry B, 2013, 117, 7416-7425.	2.6	36
78	Interaction Energies of Ionic Liquids with Metallic Nanoparticles: Solvation and Stabilization Effects. Journal of Physical Chemistry C, 2013, 117, 3537-3547.	3.1	53
79	Surface Composition/Organization of Ionic Liquids with Au Nanoparticles Revealed by High-Sensitivity Low-Energy Ion Scattering. Langmuir, 2013, 29, 14301-14306.	3.5	34
80	Pressure effect on vibrational frequency and dephasing of 1-alkyl-3-methylimidazolium hexafluorophosphate ionic liquids. Journal of Chemical Physics, 2013, 139, 054510.	3.0	15
81	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.	1.8	10
82	Molecular Simulations of Primary Alkanolamines Using an Extendable Force Field. ChemPhysChem, 2012, 13, 3866-3874.	2.1	21
83	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.	3.2	38
84	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
85	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.	2.6	111
86	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.	2.6	31
87	Ligand effect on the catalytic activity of ruthenium nanoparticles in ionic liquids. Dalton Transactions, 2012, 41, 13919.	3.3	19
88	Interactions and Ordering of Ionic Liquids at a Metal Surface. Journal of Chemical Theory and Computation, 2012, 8, 3348-3355.	5.3	66
89	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.	2.6	95
90	Glycine in 1â€Butylâ€3â€Methylimidazolium Acetate and Trifluoroacetate Ionic Liquids: Effect of Fluorination and Hydrogen Bonding. ChemPhysChem, 2012, 13, 1753-1763.	2.1	18

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91	CL&P: A generic and systematic force field for ionic liquids modeling. Theoretical Chemistry Accounts, 2012, 131, 1.	1.4	281
92	Ruthenium nanoparticles in ionic liquids: structural and stability effects of polar solutes. Physical Chemistry Chemical Physics, 2011, 13, 13527.	2.8	42
93	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.	2.6	18
94	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
95	Density scaling of the transport properties of molecular and ionic liquids. Journal of Chemical Physics, 2011, 134, 144507.	3.0	91
96	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.	2.6	30
97	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
98	Quantum chemical studies on peroxodisulfuric acidâ€“sulfuric acidâ€“water clusters. Computational and Theoretical Chemistry, 2011, 967, 219-225.	2.5	1
99	Solvation and Stabilization of Metallic Nanoparticles in Ionic Liquids. Angewandte Chemie - International Edition, 2011, 50, 8683-8687.	13.8	132
100	Characteristics of aggregation in aqueous solutions of dialkylpyrrolidinium bromides. Journal of Colloid and Interface Science, 2011, 360, 606-616.	9.4	36
101	Three commentaries on the nano-segregated structure of ionic liquids. Computational and Theoretical Chemistry, 2010, 946, 70-76.	1.5	156
102	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.	4.9	245
103	Nanostructure of Trialkylmethylammonium Bistriflamide Ionic Liquids Studied by Molecular Dynamics. Journal of Physical Chemistry B, 2010, 114, 15635-15641.	2.6	50
104	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.	1.9	43
105	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.	2.6	159
106	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.	2.6	31
107	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
108	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

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109	A novel stabilisation model for ruthenium nanoparticles in imidazolium ionic liquids: in situ spectroscopic and labelling evidence. Physical Chemistry Chemical Physics, 2010, 12, 4217.	2.8	68
110	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
111	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
112	Phase Equilibria in Ionic Liquidâ^'Aromatic Compound Mixtures, Including Benzene Fluorination Effects. Journal of Physical Chemistry B, 2009, 113, 7631-7636.	2.6	33
113	Joint Statement of Editors of Journals Publishing Thermophysical Property Data. Journal of Chemical & Engineering Data, 2009, 54, 2-3.	1.9	18
114	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
115	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.	1.9	48
116	Thermodynamics and Micro Heterogeneity of Ionic Liquids. Topics in Current Chemistry, 2009, 290, 161-183.	4.0	53
117	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
118	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.	2.6	66
119	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
120	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
121	Highâ€pressure viscosity and density of carbon dioxide + pentaerythritol ester mixtures: Measurements and modeling. AICHE Journal, 2008, 54, 1625-1636.	3.6	18
122	Viscosity and density measurements for carbon dioxide+pentaerythritol ester lubricant mixtures at low lubricant concentration. Journal of Supercritical Fluids, 2008, 44, 172-185.	3.2	53
123	Prediction of Ionic Liquid Properties. II. Volumetric Properties as a Function of Temperature and Pressure. Journal of Chemical & Engineering Data, 2008, 53, 2133-2143.	1.9	139
124	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.	1.9	233
125	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.	9.0	61
126	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

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127	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.	2.6	13
128	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
129	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.	2.6	91
130	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
131	Potential Energy Landscape of Bis(fluorosulfonyl)amide. Journal of Physical Chemistry B, 2008, 112, 9449-9455.	2.6	81
132	Molecular Solutes in Ionic Liquids: A Structural Perspective. Accounts of Chemical Research, 2007, 40, 1087-1096.	15.6	450
133	Intra- and Intermodular Structure of Ionic Liquids: From Conformers to Nanostructures. ACS Symposium Series, 2007, , 86-101.	0.5	8
134	Effect of bromine substitution on the solubility of gases in hydrocarbons and fluorocarbons. Fluid Phase Equilibria, 2007, 251, 128-136.	2.5	7
135	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.	2.0	27
136	Chapter 10. Solubility and Molecular Modelling. , 2007, , 153-170.		3
137	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
138	Interactions of Nitrous Oxide with Fluorinated Liquids. Journal of Physical Chemistry B, 2006, 110, 18566-18572.	2.6	9
139	Liquid Structure of the Ionic Liquid 1,3-Dimethylimidazolium Bis{(trifluoromethyl)sulfonyl}amide. Journal of Physical Chemistry B, 2006, 110, 12055-12061.	2.6	215
140	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
141	Nonpolar, Polar, and Associating Solutes in Ionic Liquids. Journal of Physical Chemistry B, 2006, 110, 16816-16818.	2.6	446
142	Density and viscosity of several pure and water-saturated ionic liquids. Green Chemistry, 2006, 8, 172-180.	9.0	755
143	Nanostructural Organization in Ionic Liquids. Journal of Physical Chemistry B, 2006, 110, 3330-3335.	2.6	1,693
144	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

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145	Interactions of Gases with Ionic Liquids: Molecular Simulation. ACS Symposium Series, 2005, , 150-158.	0.5	14
146	Gasâ€“liquid interactions in solution. Pure and Applied Chemistry, 2005, 77, 653-665.	1.9	40
147	Molecular Force Field for Ionic Liquids Composed of Triflate or Bistriflylimide Anions. Journal of Physical Chemistry B, 2004, 108, 16893-16898.	2.6	875
148	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.	2.5	80
149	Molecular Simulation Study of Interactions of Carbon Dioxide and Water with Ionic Liquids. ChemPhysChem, 2004, 5, 1049-1052.	2.1	92
150	Solubility of oxygen, carbon dioxide and water in semifluorinated alkanes and in perfluorooctylbromide by molecular simulation. Journal of Fluorine Chemistry, 2004, 125, 409-413.	1.7	31
151	Modeling Ionic Liquids Using a Systematic All-Atom Force Field. Journal of Physical Chemistry B, 2004, 108, 2038-2047.	2.6	1,190
152	Interactions of Carbon Dioxide with Liquid Fluorocarbons. Journal of Physical Chemistry B, 2003, 107, 14020-14024.	2.6	67
153	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.	2.8	76
154	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
155	Solubility isotope effects in aqueous solutions of methane. Journal of Chemical Physics, 2002, 116, 10816-10824.	3.0	34
156	Predicting the solubility of xenon in n-hexane and n-perfluorohexane: a simulation and theoretical study. Molecular Physics, 2002, 100, 2547-2553.	1.7	40
157	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.	2.5	57
158	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.	2.1	29
159	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.	2.6	31
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