Aglio A H Pdua

List of Publications by Year in Descending Order

168 papers	12,939 citations	56 h-index	111 g-index
190 ext. papers	14,100 ext. citations	4.8 avg, IF	6.77 L-index

#	Paper	IF	Citations
168	Enhancement of the solubility of organic dyes in aqueous ionic solvents doped with surfactants. *Journal of Molecular Liquids*, **2022**, 357, 118958	6	0
167	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	5.1	
166	Porous Ionic Liquids: Structure, Stability, and Gas Absorption Mechanisms. *Advanced Materials Interfaces*, **2021**, 8, 2001982	4.6	8
165	High-Performance Porous Ionic Liquids for Low-Pressure CO2 Capture**. *Angewandte Chemie*, **2021**, 133, 12986-12992	3.6	0
164	High-Performance Porous Ionic Liquids for Low-Pressure CO Capture*. *Angewandte Chemie - International Edition*, **2021**, 60, 12876-12882	16.4	17
163	Screening Ionic Solvents for Enhancing the Solubility of Water-Insoluble Natural Dyes. *Industrial & Engineering Chemistry Research*, **2021**, 60, 8555-8564	3.9	3
162	Tuning the solvation of indigo in aqueous deep eutectics. *Journal of Chemical Physics*, **2021**, 154, 224502	3.9	2
161	Connecting chloride solvation with hydration in deep eutectic systems. *Physical Chemistry Chemical Physics*, **2021**, 23, 107-111	3.6	19
160	Improved carbon dioxide absorption in double-charged ionic liquids. *Physical Chemistry Chemical Physics*, **2021**, 23, 23130-23140	3.6	1
159	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	6.4	20
158	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	3.9	3
157	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	6.1	14
156	Ambient energy dispersion and long-term stabilisation of large graphene sheets from graphite using a surface energy matched ionic liquid *Journal of Ionic Liquids*, **2021**, 1, 100001		1
155	Kinetic analysis of microwave-enhanced cellulose dissolution in ionic solvents. *Physical Chemistry Chemical Physics*, **2020**, 22, 1003-1010	3.6	14
154	Ion pair free energy surface as a probe of ionic liquid structure. *Journal of Chemical Physics*, **2020**, 152, 014103	3.9	4
153	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	3.4	45
152	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	3.6	3

151	Ionic Liquids Can Enable the Recycling of Fluorinated Greenhouse Gases. *ACS Sustainable Chemistry and Engineering*, **2019**, 7, 16900-16906	8.3	27
150	Transferable, Polarizable Force Field for Ionic Liquids. *Journal of Chemical Theory and Computation*, **2019**, 15, 5858-5871	6.4	59
149	Strong Microheterogeneity in Novel Deep Eutectic Solvents. *ChemPhysChem*, **2019**, 20, 1786-1792	3.2	26
148	Dispersion and Stabilization of Exfoliated Graphene in Ionic Liquids. *Frontiers in Chemistry*, **2019**, 7, 223	5	26
147	Using hydrogenated and perfluorinated gases to probe the interactions and structure of fluorinated ionic liquids. *Physical Chemistry Chemical Physics*, **2019**, 21, 8865-8873	3.6	12
146	Self-assembled nanostructures in ionic liquids facilitate charge storage at electrified interfaces. *Nature Materials*, **2019**, 18, 1350-1357	27	90
145	On the Regular Behavior of a Binary Mixture of Ionic Liquids. *Journal of Physical Chemistry B*, **2019**, 123, 6579-6587	3.4	7
144	Influence of Ionic Liquids on the Morphology of Corn Flour/Polyester Mixtures. *Starch/Staerke*, **2018**, 70, 1700233	2.3	2
143	Thermal Conductivity of Ionic Liquids and IoNanofluids and Their Feasibility as Heat Transfer Fluids. *Industrial & Engineering Chemistry Research*, **2018**, 57, 6516-6529	3.9	39
142	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	6	7
141	Ionic liquids at the surface of graphite: Wettability and structure. *Journal of Chemical Physics*, **2018**, 148, 193840	3.9	25
140	Porous Ionic Liquids or Liquid Metal-Organic Frameworks?. *Angewandte Chemie - International Edition*, **2018**, 57, 11909-11912	16.4	66
139	Porous Ionic Liquids or Liquid Metal□Organic Frameworks?. *Angewandte Chemie*, **2018**, 130, 12085-12088	3.6	22
138	Investigation of Li Cation Coordination and Transportation, by Molecular Modeling and NMR Studies, in a LiNTf-Doped Ionic Liquid-Vinylene Carbonate Mixture. *Journal of Physical Chemistry B*, **2018**, 122, 8560-8569	3.4	18
137	New solvent-stabilized few-layer black phosphorus for antibacterial applications. *Nanoscale*, **2018**, 10, 12543-12553	7.7	56
136	Structure and dynamics of ionic liquids: general discussion. *Faraday Discussions*, **2018**, 206, 291-337	3.6	6
135	Ionic liquids at interfaces: general discussion. *Faraday Discussions*, **2018**, 206, 549-586	3.6	
134	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	7

133	Can the tricyanomethanide anion improve CO absorption by acetate-based ionic liquids?. *Physical Chemistry Chemical Physics*, **2017**, 19, 12431-12440	3.6	23
132	Molecular interactions and thermal transport in ionic liquids with carbon nanomaterials. *Physical Chemistry Chemical Physics*, **2017**, 19, 17075-17087	3.6	27
131	Ab initio molecular dynamics simulations of SO2 solvation in choline chloride/glycerol deep eutectic solvent. *Fluid Phase Equilibria*, **2017**, 448, 59-68	2.5	43
130	Quantitative Modeling of MoS2Solvent Interfaces: Predicting Contact Angles and Exfoliation Performance using Molecular Dynamics. *Journal of Physical Chemistry C*, **2017**, 121, 9022-9031	3.8	58
129	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	3.4	32
128	Polycyclic aromatic hydrocarbons as model solutes for carbon nanomaterials in ionic liquids. *Physical Chemistry Chemical Physics*, **2017**, 19, 27694-27703	3.6	8
127	Experimental Study of the Interactions of Fullerene with Ionic Liquids. *ACS Symposium Series*, **2017**, 273-281	2.1	1
126	Exfoliation of graphene and fluorographene in molecular and ionic liquids. *Faraday Discussions*, **2017**, 206, 61-75	3.6	18
125	Structural effects on dynamic and energetic properties of mixtures of ionic liquids and water. *Journal of Molecular Liquids*, **2017**, 242, 204-212	6	17
124	Resolving dispersion and induction components for polarisable molecular simulations of ionic liquids. *Journal of Chemical Physics*, **2017**, 146, 204501	3.9	29
123	Phase behaviour and thermodynamics: general discussion. *Faraday Discussions*, **2017**, 206, 113-139	3.6	4
122	Dominance of Dispersion Interactions and Entropy over Electrostatics in Determining the Wettability and Friction of Two-Dimensional MoS Surfaces. *ACS Nano*, **2016**, 10, 9145-9155	16.7	50
121	Thermodynamic Properties of Selected Homologous Series of Ionic Liquids Calculated Using Molecular Dynamics. *Journal of Physical Chemistry B*, **2016**, 120, 2362-71	3.4	33
120	Thermalized Drude Oscillators with the LAMMPS Molecular Dynamics Simulator. *Journal of Chemical Information and Modeling*, **2016**, 56, 260-8	6.1	45
119	Mixing Enthalpy for Binary Mixtures Containing Ionic Liquids. *Chemical Reviews*, **2016**, 116, 6075-106	68.1	71
118	Solvation of C60 Fullerene and C60F48 Fluorinated Fullerene in Molecular and Ionic Liquids. *Journal of Physical Chemistry C*, **2016**, 120, 19396-19408	3.8	8
117	Tailoring the properties of acetate-based ionic liquids using the tricyanomethanide anion. *Physical Chemistry Chemical Physics*, **2016**, 18, 23285-95	3.6	25
116	Liquid-Phase Exfoliation of Phosphorene: Design Rules from Molecular Dynamics Simulations. *ACS Nano*, **2015**, 9, 8255-68	16.7	137

115	Molecular Modelling of Ionic Liquids **2015**, 83-106		
114	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	2.9	7
113	Multiresolution calculation of ionic liquids. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2015**, 5, 202-214	7.9	91
112	Thermodynamics of cellulose dissolution in an imidazolium acetate ionic liquid. *Chemical Communications*, **2015**, 51, 4485-7	5.8	43
111	Self-Organization in Ionic Liquids: From Bulk to Interfaces and Films. *Journal of the Brazilian Chemical Society*, **2015**,	1.5	10
110	Interactions and structure of ionic liquids on graphene and carbon nanotubes surfaces. *RSC Advances*, **2014**, 4, 18017-18024	3.7	61
109	Understanding the role of co-solvents in the dissolution of cellulose in ionic liquids. *Green Chemistry* , **2014**, 16, 2528	10	181
108	Interactions of Alkanolamines with Water: Excess Enthalpies and Hydrogen Bonding. *Journal of Chemical Theory and Computation*, **2014**, 10, 2471-8	6.4	4
107	Bulk and liquid-vapor interface of pyrrolidinium-based ionic liquids: a molecular simulation study. *Journal of Physical Chemistry B*, **2014**, 118, 731-42	3.4	47
106	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	3.9	22
105	Thermophysical properties of ionic liquid dicyanamide (DCA) nanosystems. *Journal of Chemical Thermodynamics*, **2014**, 79, 248-257	2.9	48
104	Solvation of a Cellulose Microfibril in Imidazolium Acetate Ionic Liquids: Effect of a Cosolvent. *Journal of Physical Chemistry B*, **2014**, 118, 14860-9	3.4	34
103	Glass transition of ionic liquids under high pressure. *Journal of Chemical Physics*, **2014**, 140, 244514	3.9	30
102	Equations of states for an ionic liquid under high pressure: A molecular dynamics simulation study. *Journal of Chemical Thermodynamics*, **2014**, 74, 39-42	2.9	10
101	Absorption of carbon dioxide by ionic liquids with carboxylate anions. *International Journal of Greenhouse Gas Control*, **2013**, 17, 78-88	4.2	47
100	Selectivity enhancement in the aqueous acid-catalyzed conversion of glucose to 5-hydroxymethylfurfural induced by choline chloride. *Green Chemistry*, **2013**, 15, 3205	10	56
99	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	2.8	187
98	Novel ionic lubricants for amorphous carbon surfaces: molecular modeling of the structure and friction. *Soft Matter*, **2013**, 9, 10606	3.6	16

97	Preparation of microfibers from wood/ionic liquid solutions. *Carbohydrate Polymers*, **2013**, 92, 214-7	10.3	18
96	Nonequilibrium Molecular Simulations of New Ionic Lubricants at Metallic Surfaces: Prediction of the Friction. *Journal of Chemical Theory and Computation*, **2013**, 9, 1600-10	6.4	60
95	Effect of unsaturation on the absorption of ethane and ethylene in imidazolium-based ionic liquids. *Journal of Physical Chemistry B*, **2013**, 117, 7416-25	3.4	30
94	Interaction Energies of Ionic Liquids with Metallic Nanoparticles: Solvation and Stabilization Effects. *Journal of Physical Chemistry C*, **2013**, 117, 3537-3547	3.8	48
93	Surface composition/organization of ionic liquids with Au nanoparticles revealed by high-sensitivity low-energy ion scattering. *Langmuir*, **2013**, 29, 14301-6	4	30
92	Pressure effect on vibrational frequency and dephasing of 1-alkyl-3-methylimidazolium hexafluorophosphate ionic liquids. *Journal of Chemical Physics*, **2013**, 139, 054510	3.9	15
91	Molecular simulations of primary alkanolamines using an extendable force field. *ChemPhysChem*, **2012**, 13, 3866-74	3.2	17
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; discussion 81-96, 465-71	3.6	34
89	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, 155-69; discussion 189-220, 465-71	3.6	52
88	Effect of water on the carbon dioxide absorption by 1-alkyl-3-methylimidazolium acetate ionic liquids. *Journal of Physical Chemistry B*, **2012**, 116, 14416-25	3.4	98
87	Using molecular simulation to understand the structure of [C2C1im]+-alkylsulfate ionic liquids: bulk and liquid-vapor interfaces. *Journal of Physical Chemistry B*, **2012**, 116, 14159-70	3.4	27
86	Ligand effect on the catalytic activity of ruthenium nanoparticles in ionic liquids. *Dalton Transactions*, **2012**, 41, 13919-26	4.3	18
85	Interactions and Ordering of Ionic Liquids at a Metal Surface. *Journal of Chemical Theory and Computation*, **2012**, 8, 3348-55	6.4	60
84	Absorption of carbon dioxide, nitrous oxide, ethane and nitrogen by 1-alkyl-3-methylimidazolium (C(n)mim, n = 2,4,6) tris(pentafluoroethyl)trifluorophosphate ionic liquids (eFAP). *Journal of Physical Chemistry B*, **2012**, 116, 7728-38	3.4	81
83	Glycine in 1-butyl-3-methylimidazolium acetate and trifluoroacetate ionic liquids: effect of fluorination and hydrogen bonding. *ChemPhysChem*, **2012**, 13, 1753-63	3.2	17
82	CL&P: A generic and systematic force field for ionic liquids modeling. *Theoretical Chemistry Accounts*, **2012**, 131, 1	1.9	224
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	1.4	9
80	Polarity, viscosity, and ionic conductivity of liquid mixtures containing [C4C1im][Ntf2] and a molecular component. *Journal of Physical Chemistry B*, **2011**, 115, 6088-99	3.4	141

79	Density scaling of the transport properties of molecular and ionic liquids. *Journal of Chemical Physics*, **2011**, 134, 144507	3.9	85
78	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, 3942-8	3.4	29
77	Effect of alkyl chain length and hydroxyl group functionalization on the surface properties of imidazolium ionic liquids. *Physical Chemistry Chemical Physics*, **2011**, 13, 13518-26	3.6	77
76	Quantum chemical studies on peroxodisulfuric acid□sulfuric acid□water clusters. *Computational and Theoretical Chemistry*, **2011**, 967, 219-225	2	1
75	Solvation and Stabilization of Metallic Nanoparticles in Ionic Liquids. *Angewandte Chemie*, **2011**, 123, 8842-8846	3.6	19
74	Solvation and stabilization of metallic nanoparticles in ionic liquids. *Angewandte Chemie - International Edition*, **2011**, 50, 8683-7	16.4	118
73	Ruthenium nanoparticles in ionic liquids: structural and stability effects of polar solutes. *Physical Chemistry Chemical Physics*, **2011**, 13, 13527-36	3.6	38
72	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, 12150-9	3.4	17
71	Characteristics of aggregation in aqueous solutions of dialkylpyrrolidinium bromides. *Journal of Colloid and Interface Science*, **2011**, 360, 606-16	9.3	31
70	Enhancing effect of dimethylamine in sulfuric acid nucleation in the presence of water□a computational study. *Atmospheric Chemistry and Physics*, **2010**, 10, 4961-4974	6.8	198
69	Nanostructure of trialkylmethylammonium bistriflamide ionic liquids studied by molecular dynamics. *Journal of Physical Chemistry B*, **2010**, 114, 15635-41	3.4	45
68	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	2.8	41
67	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, 3608-17	3.4	138
66	How do physical-chemical parameters influence the catalytic hydrogenation of 1,3-cyclohexadiene in ionic liquids?. *Journal of Physical Chemistry B*, **2010**, 114, 8156-65	3.4	31
65	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, 11715-24	3.4	61
64	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, 3592-600	3.4	121
63	A novel stabilisation model for ruthenium nanoparticles in imidazolium ionic liquids: in situ spectroscopic and labelling evidence. *Physical Chemistry Chemical Physics*, **2010**, 12, 4217-23	3.6	65
62	Thermodynamics and micro heterogeneity of ionic liquids. *Topics in Current Chemistry*, **2010**, 290, 161-83		50

61	Three commentaries on the nano-segregated structure of ionic liquids. *Computational and Theoretical Chemistry*, **2010**, 946, 70-76		146
60	What far-infrared spectra can contribute to the development of force fields for ionic liquids used in molecular dynamics simulations. *ChemPhysChem*, **2009**, 10, 1181-6	3.2	49
59	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, 9894-900	3.4	81
58	Phase equilibria in ionic liquid-aromatic compound mixtures, including benzene fluorination effects. *Journal of Physical Chemistry B*, **2009**, 113, 7631-6	3.4	31
57	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, 4338-46	3.4	53
56	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	2.8	43
55	1-Alkyl-3-methylimidazolium alkanesulfonate ionic liquids, [C(n)H(2)(n)(+1)mim][C(k)H(2)(k)(+1)SO(3)]: synthesis and physicochemical properties. *Physical Chemistry Chemical Physics*, **2009**, 11, 8939-48	3.6	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, 14708-18	3.4	62
53	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		121
52	Interaction between the pi-system of toluene and the imidazolium ring of ionic liquids: a combined NMR and molecular simulation study. *Journal of Physical Chemistry B*, **2009**, 113, 170-7	3.4	87
51	Prediction of Ionic Liquid Properties. II. Volumetric Properties as a Function of Temperature and Pressure. *Journal of Chemical & Engineering Data*, **2008**, 53, 2133-2143	2.8	124
50	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	2.8	218
49	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	10	57
48	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, 12394-400	3.4	44
47	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, 6653-64	3.4	13
46	A tale of two ions: the conformational landscapes of bis(trifluoromethanesulfonyl)amide and N,N-dialkylpyrrolidinium. *Journal of Physical Chemistry B*, **2008**, 112, 1465-72	3.4	116
45	Relationship between viscosity coefficients and volumetric properties using a scaling concept for molecular and ionic liquids. *Journal of Physical Chemistry B*, **2008**, 112, 5563-74	3.4	79
44	Molecular force field for ionic liquids IV: trialkylimidazolium and alkoxycarbonyl-imidazolium cations; alkylsulfonate and alkylsulfate anions. *Journal of Physical Chemistry B*, **2008**, 112, 5039-46	3.4	242

43	Potential energy landscape of bis(fluorosulfonyl)amide. *Journal of Physical Chemistry B*, **2008**, 112, 9449-55	3.4	70
42	High-pressure viscosity and density of carbon dioxide + pentaerythritol ester mixtures: Measurements and modeling. *AICHE Journal*, **2008**, 54, 1625-1636	3.6	16
41	Viscosity and density measurements for carbon dioxide + pentaerythritol ester lubricant mixtures at low lubricant concentration. *Journal of Supercritical Fluids*, **2008**, 44, 172-185	4.2	44
40	Effect of bromine substitution on the solubility of gases in hydrocarbons and fluorocarbons. *Fluid Phase Equilibria*, **2007**, 251, 128-136	2.5	6
39	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	2.9	23
38	Molecular solutes in ionic liquids: a structural perspective. *Accounts of Chemical Research*, **2007**, 40, 1087-96	24.3	415
37	Intra- and Intermodular Structure of Ionic Liquids: From Conformers to Nanostructures. *ACS Symposium Series*, **2007**, 86-101	0.4	6
36	Chapter 10:Solubility and Molecular Modelling **2007**, 153-170		3
35	Using spectroscopic data on imidazolium cation conformations to test a molecular force field for ionic liquids. *Journal of Physical Chemistry B*, **2006**, 110, 7485-9	3.4	87
34	Interactions of nitrous oxide with fluorinated liquids. *Journal of Physical Chemistry B*, **2006**, 110, 18566-73	3.4	8
33	Liquid structure of the ionic liquid 1,3-dimethylimidazolium bis[(trifluoromethyl)sulfonyl]amide. *Journal of Physical Chemistry B*, **2006**, 110, 12055-61	3.4	199
32	Molecular force field for ionic liquids III: imidazolium, pyridinium, and phosphonium cations; chloride, bromide, and dicyanamide anions. *Journal of Physical Chemistry B*, **2006**, 110, 19586-92	3.4	436
31	Nonpolar, polar, and associating solutes in ionic liquids. *Journal of Physical Chemistry B*, **2006**, 110, 16816-8	3.4	416
30	Density and viscosity of several pure and water-saturated ionic liquids. *Green Chemistry*, **2006**, 8, 172-180	10	676
29	Nanostructural organization in ionic liquids. *Journal of Physical Chemistry B*, **2006**, 110, 3330-5	3.4	1563
28	Modeling Ionic Liquids of the 1-Alkyl-3-methylimidazolium Family Using an All-Atom Force Field. *ACS Symposium Series*, **2005**, 134-149	0.4	15
27	Interactions of Gases with Ionic Liquids: Molecular Simulation. *ACS Symposium Series*, **2005**, 150-158	0.4	14
26	Gas–liquid interactions in solution. *Pure and Applied Chemistry*, **2005**, 77, 653-665	2.1	37

25	Molecular Force Field for Ionic Liquids Composed of Triflate or Bistriflylimide Anions. *Journal of Physical Chemistry B*, **2004**, 108, 16893-16898	3.4	752
24	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	67
23	Molecular simulation study of interactions of carbon dioxide and water with ionic liquids. *ChemPhysChem*, **2004**, 5, 1049-52	3.2	92
22	Solubility of oxygen, carbon dioxide and water in semifluorinated alkanes and in perfluorooctylbromide by molecular simulation. *Journal of Fluorine Chemistry*, **2004**, 125, 409-413	2.1	28
21	Modeling Ionic Liquids Using a Systematic All-Atom Force Field. *Journal of Physical Chemistry B*, **2004**, 108, 2038-2047	3.4	1029
20	Interactions of Carbon Dioxide with Liquid Fluorocarbons. *Journal of Physical Chemistry B*, **2003**, 107, 14020-14024	3.4	65
19	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	3.6	72
18	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	3.9	17
17	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	22
16	Solubility isotope effects in aqueous solutions of methane. *Journal of Chemical Physics*, **2002**, 116, 10816-10824	3.9	30
15	Predicting the solubility of xenon in n-hexane and n-perfluorohexane: a simulation and theoretical study. *Molecular Physics*, **2002**, 100, 2547-2553	1.7	38
14	Torsion Energy Profiles and Force Fields Derived from Ab Initio Calculations for Simulations of Hydrocarbon−Fluorocarbon Diblocks and Perfluoroalkylbromides. *Journal of Physical Chemistry A*, **2002**, 106, 10116-10123	2.8	51
13	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	2.5	51
12	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	2.6	70
11	Perfluoroalkanes in Water: Experimental Henry's Law Coefficients for Hexafluoroethane and Computer Simulations for Tetrafluoromethane and Hexafluoroethane. *Journal of Physical Chemistry B*, **2001**, 105, 8403-8409	3.4	25
10	Nonadditive intermolecular potential and thermodynamic properties of ethane. *Journal of Chemical Physics*, **2000**, 113, 312-319	3.9	4
9	Electromechanical model for vibrating-wire instruments. *Review of Scientific Instruments*, **1998**, 69, 2392-2399	1.7	47
8	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	2.8	42

7	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	2.8	90
6	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	2.1	73
5	Application of integral equation theories to the nitrogen molecule. *Journal of Chemical Physics*, **1996**, 105, 5956-5967	3.9	2
4	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	2.1	27
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