

# Aglio A H Pdua

## List of Publications by Citations

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111  
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190  
ext. papers

14,100  
ext. citations

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6.77  
L-index

#	Paper	IF	Citations
168	Nanostructural organization in ionic liquids. <i>Journal of Physical Chemistry B</i> , <b>2006</b> , 110, 3330-5	3.4	1563
167	Modeling Ionic Liquids Using a Systematic All-Atom Force Field. <i>Journal of Physical Chemistry B</i> , <b>2004</b> , 108, 2038-2047	3.4	1029
166	Molecular Force Field for Ionic Liquids Composed of Triflate or Bistriflylimide Anions. <i>Journal of Physical Chemistry B</i> , <b>2004</b> , 108, 16893-16898	3.4	752
165	Density and viscosity of several pure and water-saturated ionic liquids. <i>Green Chemistry</i> , <b>2006</b> , 8, 172-180	1.0	676
164	Molecular force field for ionic liquids III: imidazolium, pyridinium, and phosphonium cations; chloride, bromide, and dicyanamide anions. <i>Journal of Physical Chemistry B</i> , <b>2006</b> , 110, 19586-92	3.4	436
163	Nonpolar, polar, and associating solutes in ionic liquids. <i>Journal of Physical Chemistry B</i> , <b>2006</b> , 110, 16816-24	3.4	416
162	Molecular solutes in ionic liquids: a structural perspective. <i>Accounts of Chemical Research</i> , <b>2007</b> , 40, 1087-96	1.6	415
161	Molecular force field for ionic liquids IV: trialkylimidazolium and alkoxy-carbonyl-imidazolium cations; alkylsulfonate and alkylsulfate anions. <i>Journal of Physical Chemistry B</i> , <b>2008</b> , 112, 5039-46	3.4	242
160	CL&P: A generic and systematic force field for ionic liquids modeling. <i>Theoretical Chemistry Accounts</i> , <b>2012</b> , 131, 1	1.9	224
159	Prediction of Ionic Liquid Properties. I. Volumetric Properties as a Function of Temperature at 0.1 MPa. <i>Journal of Chemical &amp; Engineering Data</i> , <b>2008</b> , 53, 716-726	2.8	218
158	Liquid structure of the ionic liquid 1,3-dimethylimidazolium bis[(trifluoromethyl)sulfonyl]amide. <i>Journal of Physical Chemistry B</i> , <b>2006</b> , 110, 12055-61	3.4	199
157	Enhancing effect of dimethylamine in sulfuric acid nucleation in the presence of water [a] computational study. <i>Atmospheric Chemistry and Physics</i> , <b>2010</b> , 10, 4961-4974	6.8	198
156	Improvement of Quality in Publication of Experimental Thermophysical Property Data: Challenges, Assessment Tools, Global Implementation, and Online Support. <i>Journal of Chemical &amp; Engineering Data</i> , <b>2013</b> , 58, 2699-2716	2.8	187
155	Understanding the role of co-solvents in the dissolution of cellulose in ionic liquids. <i>Green Chemistry</i> , <b>2014</b> , 16, 2528	1.0	181
154	Three commentaries on the nano-segregated structure of ionic liquids. <i>Computational and Theoretical Chemistry</i> , <b>2010</b> , 946, 70-76		146
153	Polarity, viscosity, and ionic conductivity of liquid mixtures containing [C4C1im][Ntf2] and a molecular component. <i>Journal of Physical Chemistry B</i> , <b>2011</b> , 115, 6088-99	3.4	141
152	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. <i>Journal of Physical Chemistry B</i> , <b>2010</b> , 114, 3608-17	3.4	138

151	Liquid-Phase Exfoliation of Phosphorene: Design Rules from Molecular Dynamics Simulations. <i>ACS Nano</i> , <b>2015</b> , 9, 8255-68	16.7	137
150	Prediction of Ionic Liquid Properties. II. Volumetric Properties as a Function of Temperature and Pressure. <i>Journal of Chemical &amp; Engineering Data</i> , <b>2008</b> , 53, 2133-2143	2.8	124
149	Molecular force field for ionic liquids v: hydroxyethylimidazolium, dimethoxy-2- methylimidazolium, and fluoroalkylimidazolium cations and bis(fluorosulfonyl)amide, perfluoroalkanesulfonylamide, and fluoroalkylfluorophosphate anions. <i>Journal of Physical Chemistry B</i> , <b>2010</b> , 114, 3592-600	3.4	121
148	Organized 3D-alkyl imidazolium ionic liquids could be used to control the size of in situ generated ruthenium nanoparticles?. <i>Journal of Materials Chemistry</i> , <b>2009</b> , 19, 3624		121
147	Solvation and stabilization of metallic nanoparticles in ionic liquids. <i>Angewandte Chemie - International Edition</i> , <b>2011</b> , 50, 8683-7	16.4	118
146	A tale of two ions: the conformational landscapes of bis(trifluoromethanesulfonyl)amide and N,N-dialkylpyrrolidinium. <i>Journal of Physical Chemistry B</i> , <b>2008</b> , 112, 1465-72	3.4	116
145	Effect of water on the carbon dioxide absorption by 1-alkyl-3-methylimidazolium acetate ionic liquids. <i>Journal of Physical Chemistry B</i> , <b>2012</b> , 116, 14416-25	3.4	98
144	Molecular simulation study of interactions of carbon dioxide and water with ionic liquids. <i>ChemPhysChem</i> , <b>2004</b> , 5, 1049-52	3.2	92
143	Multiresolution calculation of ionic liquids. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , <b>2015</b> , 5, 202-214	7.9	91
142	Self-assembled nanostructures in ionic liquids facilitate charge storage at electrified interfaces. <i>Nature Materials</i> , <b>2019</b> , 18, 1350-1357	27	90
141	Density and Viscosity Measurements of 2,2,4-Trimethylpentane (Isooctane) from 198 K to 348 K and up to 100 MPa. <i>Journal of Chemical &amp; Engineering Data</i> , <b>1996</b> , 41, 1488-1494	2.8	90
140	Interaction between the pi-system of toluene and the imidazolium ring of ionic liquids: a combined NMR and molecular simulation study. <i>Journal of Physical Chemistry B</i> , <b>2009</b> , 113, 170-7	3.4	87
139	Using spectroscopic data on imidazolium cation conformations to test a molecular force field for ionic liquids. <i>Journal of Physical Chemistry B</i> , <b>2006</b> , 110, 7485-9	3.4	87
138	Density scaling of the transport properties of molecular and ionic liquids. <i>Journal of Chemical Physics</i> , <b>2011</b> , 134, 144507	3.9	85
137	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). <i>Journal of Physical Chemistry B</i> , <b>2012</b> , 116, 7728-38	3.4	81
136	On the role of the dipole and quadrupole moments of aromatic compounds in the solvation by ionic liquids. <i>Journal of Physical Chemistry B</i> , <b>2009</b> , 113, 9894-900	3.4	81
135	Relationship between viscosity coefficients and volumetric properties using a scaling concept for molecular and ionic liquids. <i>Journal of Physical Chemistry B</i> , <b>2008</b> , 112, 5563-74	3.4	79
134	Effect of alkyl chain length and hydroxyl group functionalization on the surface properties of imidazolium ionic liquids. <i>Physical Chemistry Chemical Physics</i> , <b>2011</b> , 13, 13518-26	3.6	77

133	Validation of an accurate vibrating-wire densimeter: Density and viscosity of liquids over wide ranges of temperature and pressure. <i>International Journal of Thermophysics</i> , <b>1996</b> , 17, 781-802	2.1	73
132	Solubility of oxygen in n-hexane and in n-perfluorohexane. Experimental determination and prediction by molecular simulation. <i>Physical Chemistry Chemical Physics</i> , <b>2003</b> , 5, 543-549	3.6	72
131	Mixing Enthalpy for Binary Mixtures Containing Ionic Liquids. <i>Chemical Reviews</i> , <b>2016</b> , 116, 6075-106	68.1	71
130	Potential energy landscape of bis(fluorosulfonyl)amide. <i>Journal of Physical Chemistry B</i> , <b>2008</b> , 112, 9449-55	3.4	70
129	Simultaneous measurement of the solubility of nitrogen and carbon dioxide in polystyrene and of the associated polymer swelling. <i>Journal of Polymer Science, Part B: Polymer Physics</i> , <b>2001</b> , 39, 2063-2070	2.6	70
128	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. <i>Physical Chemistry Chemical Physics</i> , <b>2009</b> , 11, 8939-48	3.6	67
127	Viscosity and density of mixtures of methane and n-decane from 298 to 393 K and up to 75 MPa. <i>Fluid Phase Equilibria</i> , <b>2004</b> , 216, 235-244	2.5	67
126	Porous Ionic Liquids or Liquid Metal-Organic Frameworks?. <i>Angewandte Chemie - International Edition</i> , <b>2018</b> , 57, 11909-11912	16.4	66
125	A novel stabilisation model for ruthenium nanoparticles in imidazolium ionic liquids: in situ spectroscopic and labelling evidence. <i>Physical Chemistry Chemical Physics</i> , <b>2010</b> , 12, 4217-23	3.6	65
124	Interactions of Carbon Dioxide with Liquid Fluorocarbons. <i>Journal of Physical Chemistry B</i> , <b>2003</b> , 107, 14020-14024	3.4	65
123	Molecular dynamics simulations of the liquid surface of the ionic liquid 1-hexyl-3-methylimidazolium bis(trifluoromethanesulfonyl)amide: structure and surface tension. <i>Journal of Physical Chemistry B</i> , <b>2009</b> , 113, 14708-18	3.4	62
122	Interactions and structure of ionic liquids on graphene and carbon nanotubes surfaces. <i>RSC Advances</i> , <b>2014</b> , 4, 18017-18024	3.7	61
121	Dependence of the conformational isomerism in 1-n-butyl-3-methylimidazolium ionic liquids on the nature of the halide anion. <i>Journal of Physical Chemistry B</i> , <b>2010</b> , 114, 11715-24	3.4	61
120	Nonequilibrium Molecular Simulations of New Ionic Lubricants at Metallic Surfaces: Prediction of the Friction. <i>Journal of Chemical Theory and Computation</i> , <b>2013</b> , 9, 1600-10	6.4	60
119	Interactions and Ordering of Ionic Liquids at a Metal Surface. <i>Journal of Chemical Theory and Computation</i> , <b>2012</b> , 8, 3348-55	6.4	60
118	Transferable, Polarizable Force Field for Ionic Liquids. <i>Journal of Chemical Theory and Computation</i> , <b>2019</b> , 15, 5858-5871	6.4	59
117	Quantitative Modeling of MoS2/Solvent Interfaces: Predicting Contact Angles and Exfoliation Performance using Molecular Dynamics. <i>Journal of Physical Chemistry C</i> , <b>2017</b> , 121, 9022-9031	3.8	58
116	Thermophysical properties, low pressure solubilities and thermodynamics of solvation of carbon dioxide and hydrogen in two ionic liquids based on the alkylsulfate anion. <i>Green Chemistry</i> , <b>2008</b> , 10, 944	10	57

115	New solvent-stabilized few-layer black phosphorus for antibacterial applications. <i>Nanoscale</i> , <b>2018</b> , 10, 12543-12553	7.7	56
114	Selectivity enhancement in the aqueous acid-catalyzed conversion of glucose to 5-hydroxymethylfurfural induced by choline chloride. <i>Green Chemistry</i> , <b>2013</b> , 15, 3205	10	56
113	Raman spectroscopic study, DFT calculations and MD simulations on the conformational isomerism of N-alkyl-N-methylpyrrolidinium bis-(trifluoromethanesulfonyl) amide ionic liquids. <i>Journal of Physical Chemistry B</i> , <b>2009</b> , 113, 4338-46	3.4	53
112	2D or not 2D: structural and charge ordering at the solid-liquid interface of the 1-(2-hydroxyethyl)-3-methylimidazolium tetrafluoroborate ionic liquid. <i>Faraday Discussions</i> , <b>2012</b> , 154, 155-69; discussion 189-220, 465-71	3.6	52
111	Simultaneous measurement of density and viscosity of n-pentane from 298 to 383 K and up to 100 MPa using a vibrating-wire instrument. <i>Fluid Phase Equilibria</i> , <b>2001</b> , 181, 147-161	2.5	51
110	Torsion Energy Profiles and Force Fields Derived from Ab Initio Calculations for Simulations of Hydrocarbon/Fluorocarbon Diblocks and Perfluoroalkylbromides. <i>Journal of Physical Chemistry A</i> , <b>2002</b> , 106, 10116-10123	2.8	51
109	Dominance of Dispersion Interactions and Entropy over Electrostatics in Determining the Wettability and Friction of Two-Dimensional MoS Surfaces. <i>ACS Nano</i> , <b>2016</b> , 10, 9145-9155	16.7	50
108	Thermodynamics and micro heterogeneity of ionic liquids. <i>Topics in Current Chemistry</i> , <b>2010</b> , 290, 161-83		50
107	What far-infrared spectra can contribute to the development of force fields for ionic liquids used in molecular dynamics simulations. <i>ChemPhysChem</i> , <b>2009</b> , 10, 1181-6	3.2	49
106	Thermophysical properties of ionic liquid dicyanamide (DCA) nanosystems. <i>Journal of Chemical Thermodynamics</i> , <b>2014</b> , 79, 248-257	2.9	48
105	Interaction Energies of Ionic Liquids with Metallic Nanoparticles: Solvation and Stabilization Effects. <i>Journal of Physical Chemistry C</i> , <b>2013</b> , 117, 3537-3547	3.8	48
104	Bulk and liquid-vapor interface of pyrrolidinium-based ionic liquids: a molecular simulation study. <i>Journal of Physical Chemistry B</i> , <b>2014</b> , 118, 731-42	3.4	47
103	Absorption of carbon dioxide by ionic liquids with carboxylate anions. <i>International Journal of Greenhouse Gas Control</i> , <b>2013</b> , 17, 78-88	4.2	47
102	Electromechanical model for vibrating-wire instruments. <i>Review of Scientific Instruments</i> , <b>1998</b> , 69, 2392-2399		47
101	Thermalized Drude Oscillators with the LAMMPS Molecular Dynamics Simulator. <i>Journal of Chemical Information and Modeling</i> , <b>2016</b> , 56, 260-8	6.1	45
100	Nanostructure of trialkylmethylammonium bistriflamide ionic liquids studied by molecular dynamics. <i>Journal of Physical Chemistry B</i> , <b>2010</b> , 114, 15635-41	3.4	45
99	Are There Magic Compositions in Deep Eutectic Solvents? Effects of Composition and Water Content in Choline Chloride/Ethylene Glycol from Ab Initio Molecular Dynamics. <i>Journal of Physical Chemistry B</i> , <b>2020</b> , 124, 7433-7443	3.4	45
98	Interactions of fluorinated gases with ionic liquids: solubility of CF <sub>4</sub> , C <sub>2</sub> F <sub>6</sub> , and C <sub>3</sub> F <sub>8</sub> in trihexyltetradecylphosphonium bis(trifluoromethylsulfonyl)amide. <i>Journal of Physical Chemistry B</i> , <b>2008</b> , 112, 12394-400	3.4	44

97	Viscosity and density measurements for carbon dioxide + pentaerythritol ester lubricant mixtures at low lubricant concentration. <i>Journal of Supercritical Fluids</i> , <b>2008</b> , 44, 172-185	4.2	44
96	Ab initio molecular dynamics simulations of SO <sub>2</sub> solvation in choline chloride/glycerol deep eutectic solvent. <i>Fluid Phase Equilibria</i> , <b>2017</b> , 448, 59-68	2.5	43
95	Thermodynamics of cellulose dissolution in an imidazolium acetate ionic liquid. <i>Chemical Communications</i> , <b>2015</b> , 51, 4485-7	5.8	43
94	Diffusion Coefficients of 1-Alkyl-3-methylimidazolium Ionic Liquids in Water, Methanol, and Acetonitrile at Infinite Dilution <i>Journal of Chemical &amp; Engineering Data</i> , <b>2009</b> , 54, 2389-2394	2.8	43
93	Density and Viscosity Measurements of 1,1,1,2-Tetrafluoroethane (HFC-134a) from 199 K to 298 K and up to 100 MPa. <i>Journal of Chemical &amp; Engineering Data</i> , <b>1996</b> , 41, 731-735	2.8	42
92	Calorimetric and Volumetric Study on Binary Mixtures 2,2,2-Trifluoroethanol + (1-Butyl-3-methylimidazolium Tetrafluoroborate or 1-Ethyl-3-methylimidazolium Tetrafluoroborate) <i>Journal of Chemical &amp; Engineering Data</i> , <b>2010</b> , 55, 5504-5512	2.8	41
91	Thermal Conductivity of Ionic Liquids and IoNanofluids and Their Feasibility as Heat Transfer Fluids. <i>Industrial &amp; Engineering Chemistry Research</i> , <b>2018</b> , 57, 6516-6529	3.9	39
90	Ruthenium nanoparticles in ionic liquids: structural and stability effects of polar solutes. <i>Physical Chemistry Chemical Physics</i> , <b>2011</b> , 13, 13527-36	3.6	38
89	Predicting the solubility of xenon in n-hexane and n-perfluorohexane: a simulation and theoretical study. <i>Molecular Physics</i> , <b>2002</b> , 100, 2547-2553	1.7	38
88	Gas-liquid interactions in solution. <i>Pure and Applied Chemistry</i> , <b>2005</b> , 77, 653-665	2.1	37
87	Solvation of a Cellulose Microfibril in Imidazolium Acetate Ionic Liquids: Effect of a Cosolvent. <i>Journal of Physical Chemistry B</i> , <b>2014</b> , 118, 14860-9	3.4	34
86	Using ethane and butane as probes to the molecular structure of 1-alkyl-3-methylimidazolium bis[(trifluoromethyl)sulfonyl] imide ionic liquids. <i>Faraday Discussions</i> , <b>2012</b> , 154, 41-52; discussion 81-96, 465-71	3.6	34
85	Thermodynamic Properties of Selected Homologous Series of Ionic Liquids Calculated Using Molecular Dynamics. <i>Journal of Physical Chemistry B</i> , <b>2016</b> , 120, 2362-71	3.4	33
84	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. <i>Journal of Physical Chemistry B</i> , <b>2017</b> , 121, 426-436	3.4	32
83	How do physical-chemical parameters influence the catalytic hydrogenation of 1,3-cyclohexadiene in ionic liquids?. <i>Journal of Physical Chemistry B</i> , <b>2010</b> , 114, 8156-65	3.4	31
82	Phase equilibria in ionic liquid-aromatic compound mixtures, including benzene fluorination effects. <i>Journal of Physical Chemistry B</i> , <b>2009</b> , 113, 7631-6	3.4	31
81	Characteristics of aggregation in aqueous solutions of dialkylpyrrolidinium bromides. <i>Journal of Colloid and Interface Science</i> , <b>2011</b> , 360, 606-16	9.3	31
80	Glass transition of ionic liquids under high pressure. <i>Journal of Chemical Physics</i> , <b>2014</b> , 140, 244514	3.9	30

79	Effect of unsaturation on the absorption of ethane and ethylene in imidazolium-based ionic liquids. <i>Journal of Physical Chemistry B</i> , <b>2013</b> , 117, 7416-25	3.4	30
78	Surface composition/organization of ionic liquids with Au nanoparticles revealed by high-sensitivity low-energy ion scattering. <i>Langmuir</i> , <b>2013</b> , 29, 14301-6	4	30
77	Solubility isotope effects in aqueous solutions of methane. <i>Journal of Chemical Physics</i> , <b>2002</b> , 116, 10816-10824	3.9	30
76	Resolving dispersion and induction components for polarisable molecular simulations of ionic liquids. <i>Journal of Chemical Physics</i> , <b>2017</b> , 146, 204501	3.9	29
75	Influence of ester functional groups on the liquid-phase structure and solvation properties of imidazolium-based ionic liquids. <i>Journal of Physical Chemistry B</i> , <b>2011</b> , 115, 3942-8	3.4	29
74	Solubility of oxygen, carbon dioxide and water in semifluorinated alkanes and in perfluorooctylbromide by molecular simulation. <i>Journal of Fluorine Chemistry</i> , <b>2004</b> , 125, 409-413	2.1	28
73	Molecular interactions and thermal transport in ionic liquids with carbon nanomaterials. <i>Physical Chemistry Chemical Physics</i> , <b>2017</b> , 19, 17075-17087	3.6	27
72	Ionic Liquids Can Enable the Recycling of Fluorinated Greenhouse Gases. <i>ACS Sustainable Chemistry and Engineering</i> , <b>2019</b> , 7, 16900-16906	8.3	27
71	Using molecular simulation to understand the structure of [C2C1im] <sup>+</sup> -alkylsulfate ionic liquids: bulk and liquid-vapor interfaces. <i>Journal of Physical Chemistry B</i> , <b>2012</b> , 116, 14159-70	3.4	27
70	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. <i>International Journal of Thermophysics</i> , <b>1994</b> , 15, 229-243	2.1	27
69	Strong Microheterogeneity in Novel Deep Eutectic Solvents. <i>ChemPhysChem</i> , <b>2019</b> , 20, 1786-1792	3.2	26
68	Dispersion and Stabilization of Exfoliated Graphene in Ionic Liquids. <i>Frontiers in Chemistry</i> , <b>2019</b> , 7, 223	5	26
67	The viscosity of liquid carbon dioxide. <i>International Journal of Thermophysics</i> , <b>1994</b> , 15, 767-777	2.1	26
66	Ionic liquids at the surface of graphite: Wettability and structure. <i>Journal of Chemical Physics</i> , <b>2018</b> , 148, 193840	3.9	25
65	Perfluoroalkanes in Water: Experimental Henry's Law Coefficients for Hexafluoroethane and Computer Simulations for Tetrafluoromethane and Hexafluoroethane. <i>Journal of Physical Chemistry B</i> , <b>2001</b> , 105, 8403-8409	3.4	25
64	Tailoring the properties of acetate-based ionic liquids using the tricyanomethanide anion. <i>Physical Chemistry Chemical Physics</i> , <b>2016</b> , 18, 23285-95	3.6	25
63	Can the tricyanomethanide anion improve CO absorption by acetate-based ionic liquids?. <i>Physical Chemistry Chemical Physics</i> , <b>2017</b> , 19, 12431-12440	3.6	23
62	Low pressure solubility and thermodynamics of solvation of oxygen, carbon dioxide, and carbon monoxide in fluorinated liquids. <i>Journal of Chemical Thermodynamics</i> , <b>2007</b> , 39, 847-854	2.9	23

61	Porous Ionic Liquids or Liquid Metal/Organic Frameworks?. <i>Angewandte Chemie</i> , <b>2018</b> , 130, 12085-12088	3.6	22
60	High-Pressure Densities of 2,2,2-Trifluoroethanol + Ionic Liquid Mixtures Useful for Possible Applications in Absorption Cycles. <i>Industrial &amp; Engineering Chemistry Research</i> , <b>2014</b> , 53, 10791-10802	3.9	22
59	Density and Viscosity of Mixtures of n-Hexane and 1-Hexanol from 303 to 423 K up to 50 MPa. <i>International Journal of Thermophysics</i> , <b>2002</b> , 23, 1537-1550	2.1	22
58	Extension of the CL&Pol Polarizable Force Field to Electrolytes, Protic Ionic Liquids, and Deep Eutectic Solvents. <i>Journal of Chemical Theory and Computation</i> , <b>2021</b> , 17, 1606-1617	6.4	20
57	Solvation and Stabilization of Metallic Nanoparticles in Ionic Liquids. <i>Angewandte Chemie</i> , <b>2011</b> , 123, 8842-8846	3.6	19
56	Connecting chloride solvation with hydration in deep eutectic systems. <i>Physical Chemistry Chemical Physics</i> , <b>2021</b> , 23, 107-111	3.6	19
55	Exfoliation of graphene and fluorographene in molecular and ionic liquids. <i>Faraday Discussions</i> , <b>2017</b> , 206, 61-75	3.6	18
54	Investigation of Li Cation Coordination and Transportation, by Molecular Modeling and NMR Studies, in a LiNTf-Doped Ionic Liquid-Vinylene Carbonate Mixture. <i>Journal of Physical Chemistry B</i> , <b>2018</b> , 122, 8560-8569	3.4	18
53	Preparation of microfibers from wood/ionic liquid solutions. <i>Carbohydrate Polymers</i> , <b>2013</b> , 92, 214-7	10.3	18
52	Ligand effect on the catalytic activity of ruthenium nanoparticles in ionic liquids. <i>Dalton Transactions</i> , <b>2012</b> , 41, 13919-26	4.3	18
51	Structural effects on dynamic and energetic properties of mixtures of ionic liquids and water. <i>Journal of Molecular Liquids</i> , <b>2017</b> , 242, 204-212	6	17
50	Molecular simulations of primary alkanolamines using an extendable force field. <i>ChemPhysChem</i> , <b>2012</b> , 13, 3866-74	3.2	17
49	Glycine in 1-butyl-3-methylimidazolium acetate and trifluoroacetate ionic liquids: effect of fluorination and hydrogen bonding. <i>ChemPhysChem</i> , <b>2012</b> , 13, 1753-63	3.2	17
48	Influence of ionic association, transport properties, and solvation on the catalytic hydrogenation of 1,3-cyclohexadiene in ionic liquids. <i>Journal of Physical Chemistry B</i> , <b>2011</b> , 115, 12150-9	3.4	17
47	Calculation of vapor pressure isotope effects in the rare gases and their mixtures using an integral equation theory. <i>Journal of Chemical Physics</i> , <b>2003</b> , 118, 5028-5037	3.9	17
46	High-Performance Porous Ionic Liquids for Low-Pressure CO Capture*. <i>Angewandte Chemie - International Edition</i> , <b>2021</b> , 60, 12876-12882	16.4	17
45	Novel ionic lubricants for amorphous carbon surfaces: molecular modeling of the structure and friction. <i>Soft Matter</i> , <b>2013</b> , 9, 10606	3.6	16
44	High-pressure viscosity and density of carbon dioxide + pentaerythritol ester mixtures: Measurements and modeling. <i>AIChE Journal</i> , <b>2008</b> , 54, 1625-1636	3.6	16



43	Pressure effect on vibrational frequency and dephasing of 1-alkyl-3-methylimidazolium hexafluorophosphate ionic liquids. <i>Journal of Chemical Physics</i> , <b>2013</b> , 139, 054510	3.9	15
42	Modeling Ionic Liquids of the 1-Alkyl-3-methylimidazolium Family Using an All-Atom Force Field. <i>ACS Symposium Series</i> , <b>2005</b> , 134-149	0.4	15
41	Interactions of Gases with Ionic Liquids: Molecular Simulation. <i>ACS Symposium Series</i> , <b>2005</b> , 150-158	0.4	14
40	Kinetic analysis of microwave-enhanced cellulose dissolution in ionic solvents. <i>Physical Chemistry Chemical Physics</i> , <b>2020</b> , 22, 1003-1010	3.6	14
39	Systematic Comparison of the Structural and Dynamic Properties of Commonly Used Water Models for Molecular Dynamics Simulations. <i>Journal of Chemical Information and Modeling</i> , <b>2021</b> , 61, 4521-4536	6.1	14
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