Karina Shimizu

List of Publications by Year
in descending order

88 papers	3,914 citations	117625 34 h-index	123424 61 g-index
89 all docs	89 docs citations	89 times ranked	3572 citing authors

#	Article	IF	Citations
1	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
2	Structure and Aggregation in the 1-Alkyl-3-Methylimidazolium Bis(trifluoromethylsulfonyl)imide Ionic Liquid Homologous Series. Journal of Physical Chemistry B, 2014, 118, 567-576.	2.6	223
3	High-Accuracy Vapor Pressure Data of the Extended [C_nC₁im][Ntf₂] Ionic Liquid Series: Trend Changes and Structural Shifts. Journal of Physical Chemistry B, 2011, 115, 10919-10926.	2.6	199
4	Three commentaries on the nano-segregated structure of ionic liquids. Computational and Theoretical Chemistry, 2010, 946, 70-76.	1.5	156
5	The magic of aqueous solutions of ionic liquids: ionic liquids as a powerful class of catanionic hydrotropes. Green Chemistry, 2015, 17, 3948-3963.	9.0	156
6	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
7	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
8	Nano-segregation in ionic liquids: scorpions and vanishing chains. Physical Chemistry Chemical Physics, 2013, 15, 16256.	2.8	119
9	On the Formation of a Third, Nanostructured Domain in Ionic Liquids. Journal of Physical Chemistry B, 2013, 117, 10826-10833.	2.6	99
10	Assessing the Dispersive and Electrostatic Components of the Cohesive Energy of Ionic Liquids Using Molecular Dynamics Simulations and Molar Refraction Data. Journal of Physical Chemistry B, 2010, 114, 5831-5834.	2.6	89
11	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
12	Density, Thermal Expansion and Viscosity of Cholinium–Derived Ionic Liquids. ChemPhysChem, 2012, 13, 1902-1909.	2.1	83
13	Nanosegregation and Structuring in the Bulk and at the Surface of Ionic-Liquid Mixtures. Journal of Physical Chemistry B, 2017, 121, 6002-6020.	2.6	82
14	Potential Energy Landscape of Bis(fluorosulfonyl)amide. Journal of Physical Chemistry B, 2008, 112, 9449-9455.	2.6	81
15	Structural and aggregate analyses of (Li salt + glyme) mixtures: the complex nature of solvate ionic liquids. Physical Chemistry Chemical Physics, 2015, 17, 22321-22335.	2.8	78
16	Binary mixtures of ionic liquids with a common ion revisited: A molecular dynamics simulation study. Journal of Molecular Liquids, 2010, 153, 52-56.	4.9	75
17	Cation Alkyl Side Chain Length and Symmetry Effects on the Surface Tension of Ionic Liquids. Langmuir, 2014, 30, 6408-6418.	3.5	75
18	Mutual Solubility of Water and Structural/Positional Isomers of N-Alkylpyridinium-Based Ionic Liquids. Journal of Physical Chemistry B, 2010, 114, 15925-15934.	2.6	74

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19	Enhanced dissolution of ibuprofen using ionic liquids as catanionic hydrotropes. Physical Chemistry Chemical Physics, 2018, 20, 2094-2103.	2.8	68
20	Structure and Aggregation in the 1,3-Dialkyl-imidazolium Bis(trifluoromethylsulfonyl)imide Ionic Liquid Family: 2. From Single to Double Long Alkyl Side Chains. Journal of Physical Chemistry B, 2014, 118, 6885-6895.	2.6	65
21	The effect of the cation alkyl chain branching on mutual solubilities with water and toxicities. Physical Chemistry Chemical Physics, 2014, 16, 19952.	2.8	64
22	Charge-Transfer Complexation as a General Phenomenon in the Copigmentation of Anthocyanins. Journal of Physical Chemistry A, 2005, 109, 7329-7338.	2.5	63
23	A thermophysical and structural characterization of ionic liquids with alkyl and perfluoroalkyl side chains. RSC Advances, 2015, 5, 65337-65350.	3.6	63
24	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
25	Nanostructure of Trialkylmethylammonium Bistriflamide Ionic Liquids Studied by Molecular Dynamics. Journal of Physical Chemistry B, 2010, 114, 15635-15641.	2.6	50
26	Imidazolium-Based Lipid Analogues and Their Interaction with Phosphatidylcholine Membranes. Langmuir, 2016, 32, 12579-12592.	3.5	50
27	Bulk nanostructure of the prototypical â€˜goodâ€™ and â€˜poorâ€™ solvate ionic liquids [Li(G4)][TFSI] and [Li(G4)][NO₃]. Physical Chemistry Chemical Physics, 2016, 18, 17224-17236.	2.8	49
28	Complex Structure of Ionic Liquids. Molecular Dynamics Studies with Different Cationâ€“Anion Combinations. Journal of Chemical & Engineering Data, 2014, 59, 3120-3129.	1.9	47
29	Influence of Nanosegregation on the Phase Behavior of Fluorinated Ionic Liquids. Journal of Physical Chemistry C, 2017, 121, 5415-5427.	3.1	46
30	Exploring the bulk-phase structure of ionic liquid mixtures using small-angle neutron scattering. Faraday Discussions, 2018, 206, 265-289.	3.2	42
31	A computational study of substituted flavylium salts and their quinonoidal conjugate-bases: S0 -> S1 electronic transition, absolute pKa and reduction potential calculations by DFT and semiempirical methods. Journal of the Brazilian Chemical Society, 2007, 18, 1537-1546.	0.6	38
32	Influence of Nanosegregation on the Surface Tension of Fluorinated Ionic Liquids. Langmuir, 2016, 32, 6130-6139.	3.5	38
33	Plasma membrane permeabilisation by ionic liquids: a matter of charge. Green Chemistry, 2015, 17, 4587-4598.	9.0	37
34	Additive polarizabilities in ionic liquids. Physical Chemistry Chemical Physics, 2016, 18, 1665-1670.	2.8	37
35	Liquidâ€Crystalline Ionic Liquids as Ordered Reaction Media for the Dielsâ€“Alder Reaction. Chemistry - A European Journal, 2016, 22, 16113-16123.	3.3	35
36	Liquidâ€“Liquid Equilibrium of Cholinium-Derived Bistriflimide Ionic Liquids with Water and Octanol. Journal of Physical Chemistry B, 2012, 116, 9186-9195.	2.6	34

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37	The alternation effect in ionic liquid homologous series. Physical Chemistry Chemical Physics, 2014, 16, 4033-4038.	2.8	34
38	Phase Equilibria in Ionic Liquidâ^'Aromatic Compound Mixtures, Including Benzene Fluorination Effects. Journal of Physical Chemistry B, 2009, 113, 7631-7636.	2.6	33
39	Parameterization of the electronegativity equalization method based on the charge model 1. Physical Chemistry Chemical Physics, 2002, 4, 5933-5936.	2.8	31
40	Probing the Surface Tension of Ionic Liquids Using the Langmuir Principle. Langmuir, 2018, 34, 4408-4416.	3.5	31
41	The impact of ionic liquid fluorinated moieties on their thermophysical properties and aqueous phase behaviour. Physical Chemistry Chemical Physics, 2014, 16, 21340-21348.	2.8	30
42	Structural characterization of the [CnC1im][C4F9SO3] ionic liquid series: Alkyl versus perfluoroalkyl side chains. Journal of Molecular Liquids, 2017, 226, 28-34.	4.9	30
43	Probing the structural features of the 1-alkyl-3-methylimidazolium hexafluorophosphate ionic liquid series using Molecular Dynamics simulations. Journal of Molecular Liquids, 2015, 210, 257-263.	4.9	28
44	Ultrafast Internal Conversion in a Model Anthocyaninâ€"Polyphenol Complex: Implications for the Biological Role of Anthocyanins in Vegetative Tissues of Plants. Chemistry - A European Journal, 2009, 15, 1397-1402.	3.3	27
45	Using ¹²⁹Xe NMR to Probe the Structure of Ionic Liquids. Journal of Physical Chemistry Letters, 2013, 4, 2758-2762.	4.6	26
46	Phase Equilibria of Haloalkanes Dissolved in Ethylsulfate- or Ethylsulfonate-Based Ionic Liquids. Journal of Physical Chemistry B, 2010, 114, 7329-7337.	2.6	24
47	Liquid- or Solid-Like Behavior of [omim][BF₄] at a Solid Interface?. Journal of Physical Chemistry Letters, 2011, 2, 1551-1555.	4.6	24
48	Unusual LCST-type behaviour found in binary mixtures of choline-based ionic liquids with ethers. RSC Advances, 2013, 3, 10262.	3.6	24
49	Vaporisation of a Dicationic Ionic Liquid Revisited. ChemPhysChem, 2010, 11, 3673-3677.	2.1	23
50	Calculation of the Dipole Moment for Polypeptides Using the Generalized Born-Electronegativity Equalization Method:â€‰ Results in Vacuum and Continuum-Dielectric Solvent. Journal of Physical Chemistry B, 2004, 108, 4171-4177.	2.6	22
51	Solvate ionic liquids based on lithium bis(trifluoromethanesulfonyl)imideâ€"glyme systems: coordination in MD simulations with scaled charges. Physical Chemistry Chemical Physics, 2020, 22, 525-535.	2.8	22
52	Charge Templates in Aromatic Plus Ionic Liquid Systems Revisited: NMR Experiments and Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2014, 118, 5772-5780.	2.6	21
53	Viscosity minima in binary mixtures of ionic liquids + molecular solvents. Physical Chemistry Chemical Physics, 2015, 17, 13480-13494.	2.8	21
54	Molecular dynamics studies on the structure and interactions of ionic liquids containing amino-acid anions. Physical Chemistry Chemical Physics, 2018, 20, 23864-23872.	2.8	19

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55	Ionic Liquids and Water: Hydrophobicity vs. Hydrophilicity. Molecules, 2021, 26, 7159.	3.8	19
56	Design of task-specific fluorinated ionic liquids: nanosegregation versus hydrogen-bonding ability in aqueous solutions. Chemical Communications, 2018, 54, 3524-3527.	4.1	17
57	Designing the ammonium cation to achieve a higher hydrophilicity of bistriflimide-based ionic liquids. Physical Chemistry Chemical Physics, 2018, 20, 19307-19313.	2.8	17
58	Wetting Films of Two Ionic Liquids: [C₈mim][BF4] and [C₂OHmim][BF₄]. Journal of Physical Chemistry C, 2011, 115, 16116-16123.	3.1	16
59	Comparing the structure of different ionic liquid series: Bistriflamide v. hexafluorophosphate; pure v. equimolar mixtures. Fluid Phase Equilibria, 2016, 418, 181-191.	2.5	16
60	Halogen and Hydrogen Bonding Interplay in the Crystal Packing of Halometallocenes. Molecules, 2018, 23, 2959.	3.8	16
61	The complex structure of ionic liquids at an atomistic level: from â€œred-and-greensâ€•to charge templates. Pure and Applied Chemistry, 2014, 86, 119-133.	1.9	15
62	Structure and dynamics of mica-confined films of [C10C1Pyrr][NTf2] ionic liquid. Journal of Chemical Physics, 2018, 148, 193808.	3.0	15
63	Novel Ground- and Excited-State Prototropic Reactivity of a Hydroxycarboxyflavylium Salt. Journal of Physical Chemistry A, 2006, 110, 2089-2096.	2.5	14
64	Solubility of n-butane and 2-methylpropane (isobutane) in 1-alkyl-3-methylimidazolium-based ionic liquids with linear and branched alkyl side-chains. Physical Chemistry Chemical Physics, 2015, 17, 30328-30342.	2.8	14
65	Mixtures of Pyridine and Nicotine with Pyridinium-Based Ionic Liquids. Journal of Chemical & Engineering Data, 2011, 56, 4356-4363.	1.9	13
66	Ionic Liquid Films at the Waterâ€“Air Interface: Langmuir Isotherms of Tetra-alkylphosphonium-Based Ionic Liquids. Langmuir, 2015, 31, 8371-8378.	3.5	12
67	Solvent effects on the polar network of ionic liquid solutions. Journal of Physics Condensed Matter, 2015, 27, 194116.	1.8	12
68	Vapor Pressure Assessment of Sulfolane-Based Eutectic Solvents: Experimental, PC-SAFT, and Molecular Dynamics. Journal of Physical Chemistry B, 2020, 124, 10386-10397.	2.6	12
69	Self-Organization in Ionic Liquids: From Bulk to Interfaces and Films. Journal of the Brazilian Chemical Society, 2015, , .	0.6	12
70	Crystalline-like structures and multilayering in Langmuir films of ionic liquids at the airâ€“water interface. Chemical Communications, 2016, 52, 5585-5588.	4.1	10
71	Predicting Hydration Free Energies of Neutral Compounds by a Parametrization of the Polarizable Continuum Model. Journal of Physical Chemistry A, 2005, 109, 11322-11327.	2.5	9
72	The role of halogen interactions in the crystal structure of biscyclopentadienyl dihalides. CrystEngComm, 2017, 19, 2802-2812.	2.6	9

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73	Comparative structural analyses in four ionic liquid systems: the two low-q peaks of IL structure factor functions. Molecular Simulation, 2018, 44, 478-484.	2.0	9
74	The Solubility of Gases in Ionic Liquids: A Chemoinformatic Predictive and Interpretable Approach. ChemPhysChem, 2021, 22, 2190-2200.	2.1	9
75	Does the Photochemical Conversion of Colchicine into Lumicolchicines Involve Triplet Transients? A Solvent Dependence StudyÂ¶. Photochemistry and Photobiology, 2001, 73, 213.	2.5	9
76	Structure and dynamics of ionic liquids: general discussion. Faraday Discussions, 2018, 206, 291-337.	3.2	8
77	Tailoring amphotericin B as an ionic liquid: an upfront strategy to potentiate the biological activity of antifungal drugs. RSC Advances, 2021, 11, 14441-14452.	3.6	7
78	Bio-inspired hydrophilic bistriflimide-based ionic liquids: Molecular dynamics modeling and simulations. Journal of Molecular Liquids, 2020, 301, 112402.	4.9	6
79	Ionic Liquids in Wonderland: From Electrostatics to Coordination Chemistry. Journal of Physical Chemistry C, 2019, 123, 5804-5811.	3.1	5
80	Immobilization of His-tagged proteins on NiO foams for recyclable enzymatic reactors. Applied Surface Science, 2021, 537, 147848.	6.1	5
81	A simple method for the fast calculation of charge redistribution of solutes in an implicit solvent model. Chemical Physics, 2002, 282, 237-243.	1.9	4
82	ILs through the looking glass: electrostatics and structure probed using charge-inverted ionic liquid pairs. Faraday Discussions, 2018, 206, 203-218.	3.2	4
83	Effect of substituents in the molecular and supramolecular architectures of 1-ferrocenyl-2-(aryl)thioethanones. CrystEngComm, 2015, 17, 3089-3102.	2.6	3
84	Evidences for a Null Molar Volume Contribution by Hydroxyl Groups in Ammonium Bistriflimide-Based Ionic Liquids. Journal of Chemical & Engineering Data, 2019, 64, 4932-4945.	1.9	3
85	Photon Upconversion in TTA-Inducing Ionic Liquids: Pinpointing the Role of IL Nanostructured Media Using MD Simulations. Journal of Physical Chemistry B, 2020, 124, 3137-3144.	2.6	3
86	Computational insights into substituent effects on the stability and reactivity of flavylium cation analogs of anthocyanins. Arkivoc, 2020, 2020, 146-162.	0.5	2
87	Cation-Anion and Cation-Cation Interactions in Mixtures of Hydroxy-functionalized and Aprotic Ionic Liquids. Journal of Ionic Liquids, 2022, 2, 100022.	2.7	1
88	Back to the Future: applying 2000's interactions to explain supramolecular arrangements in 1950's compounds. Acta Crystallographica Section A: Foundations and Advances, 2015, 71, s452-s453.	0.1	0