

# Karina Shimizu

## List of Publications by Year in descending order

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88  
papers

3,914  
citations

117453

34  
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123241

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docs citations

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times ranked

3572  
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#	ARTICLE	IF	CITATIONS
1	Molecular Force Field for Ionic Liquids IV: Trialkylimidazolium and Alkoxy carbonyl-Imidazolium Cations; Alkylsulfonate and Alkylsulfate Anions. <i>Journal of Physical Chemistry B</i> , 2008, 112, 5039-5046.	1.2	286
2	Structure and Aggregation in the 1-Alkyl-3-Methylimidazolium Bis(trifluoromethylsulfonyl)imide Ionic Liquid Homologous Series. <i>Journal of Physical Chemistry B</i> , 2014, 118, 567-576.	1.2	223
3	High-Accuracy Vapor Pressure Data of the Extended [C <sub>n</sub> Im][Ntf <sub>2</sub> ] Ionic Liquid Series: Trend Changes and Structural Shifts. <i>Journal of Physical Chemistry B</i> , 2011, 115, 10919-10926.	1.2	199
4	Three commentaries on the nano-segregated structure of ionic liquids. <i>Computational and Theoretical Chemistry</i> , 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. <i>Green Chemistry</i> , 2015, 17, 3948-3963.	4.6	156
6	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> , 2010, 114, 3592-3600.	1.2	146
7	A Tale of Two Ions: The Conformational Landscapes of Bis(trifluoromethanesulfonyl)amide and N-Dialkylpyrrolidinium. <i>Journal of Physical Chemistry B</i> , 2008, 112, 1465-1472.	1.2	128
8	Nano-segregation in ionic liquids: scorpions and vanishing chains. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 16256.	1.3	119
9	On the Formation of a Third, Nanostructured Domain in Ionic Liquids. <i>Journal of Physical Chemistry B</i> , 2013, 117, 10826-10833.	1.2	99
10	Assessing the Dispersive and Electrostatic Components of the Cohesive Energy of Ionic Liquids Using Molecular Dynamics Simulations and Molar Refraction Data. <i>Journal of Physical Chemistry B</i> , 2010, 114, 5831-5834.	1.2	89
11	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> , 2009, 113, 9894-9900.	1.2	86
12	Density, Thermal Expansion and Viscosity of Cholinium-Derived Ionic Liquids. <i>ChemPhysChem</i> , 2012, 13, 1902-1909.	1.0	83
13	Nanosegregation and Structuring in the Bulk and at the Surface of Ionic-Liquid Mixtures. <i>Journal of Physical Chemistry B</i> , 2017, 121, 6002-6020.	1.2	82
14	Potential Energy Landscape of Bis(fluorosulfonyl)amide. <i>Journal of Physical Chemistry B</i> , 2008, 112, 9449-9455.	1.2	81
15	Structural and aggregate analyses of (Li salt + glyme) mixtures: the complex nature of solvate ionic liquids. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 22321-22335.	1.3	78
16	Binary mixtures of ionic liquids with a common ion revisited: A molecular dynamics simulation study. <i>Journal of Molecular Liquids</i> , 2010, 153, 52-56.	2.3	75
17	Cation Alkyl Side Chain Length and Symmetry Effects on the Surface Tension of Ionic Liquids. <i>Langmuir</i> , 2014, 30, 6408-6418.	1.6	75
18	Mutual Solubility of Water and Structural/Positional Isomers of N-Alkylpyridinium-Based Ionic Liquids. <i>Journal of Physical Chemistry B</i> , 2010, 114, 15925-15934.	1.2	74

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19	Enhanced dissolution of ibuprofen using ionic liquids as cationic hydrotropes. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 2094-2103.	1.3	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. <i>Journal of Physical Chemistry B</i> , 2014, 118, 6885-6895.	1.2	65
21	The effect of the cation alkyl chain branching on mutual solubilities with water and toxicities. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 19952.	1.3	64
22	Charge-Transfer Complexation as a General Phenomenon in the Copigmentation of Anthocyanins. <i>Journal of Physical Chemistry A</i> , 2005, 109, 7329-7338.	1.1	63
23	A thermophysical and structural characterization of ionic liquids with alkyl and perfluoroalkyl side chains. <i>RSC Advances</i> , 2015, 5, 65337-65350.	1.7	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. <i>Faraday Discussions</i> , 2012, 154, 155-169.	1.6	56
25	Nanostructure of Trialkylmethylammonium Bistriflamide Ionic Liquids Studied by Molecular Dynamics. <i>Journal of Physical Chemistry B</i> , 2010, 114, 15635-15641.	1.2	50
26	Imidazolium-Based Lipid Analogues and Their Interaction with Phosphatidylcholine Membranes. <i>Langmuir</i> , 2016, 32, 12579-12592.	1.6	50
27	Bulk nanostructure of the prototypical "good" and "poor" solvate ionic liquids [Li(G4)][TFSI] and [Li(G4)][NO <sub>3</sub> ]. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 17224-17236.	1.3	49
28	Complex Structure of Ionic Liquids. Molecular Dynamics Studies with Different Cation/Anion Combinations. <i>Journal of Chemical &amp; Engineering Data</i> , 2014, 59, 3120-3129.	1.0	47
29	Influence of Nanosegregation on the Phase Behavior of Fluorinated Ionic Liquids. <i>Journal of Physical Chemistry C</i> , 2017, 121, 5415-5427.	1.5	46
30	Exploring the bulk-phase structure of ionic liquid mixtures using small-angle neutron scattering. <i>Faraday Discussions</i> , 2018, 206, 265-289.	1.6	42
31	A computational study of substituted flavylum salts and their quinonoidal conjugate-bases: S0 & S1 electronic transition, absolute pKa and reduction potential calculations by DFT and semiempirical methods. <i>Journal of the Brazilian Chemical Society</i> , 2007, 18, 1537-1546.	0.6	38
32	Influence of Nanosegregation on the Surface Tension of Fluorinated Ionic Liquids. <i>Langmuir</i> , 2016, 32, 6130-6139.	1.6	38
33	Plasma membrane permeabilisation by ionic liquids: a matter of charge. <i>Green Chemistry</i> , 2015, 17, 4587-4598.	4.6	37
34	Additive polarizabilities in ionic liquids. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 1665-1670.	1.3	37
35	Liquid-Crystalline Ionic Liquids as Ordered Reaction Media for the Diels-Alder Reaction. <i>Chemistry - A European Journal</i> , 2016, 22, 16113-16123.	1.7	35
36	Liquid-Liquid Equilibrium of Cholinium-Derived Bistriflimide Ionic Liquids with Water and Octanol. <i>Journal of Physical Chemistry B</i> , 2012, 116, 9186-9195.	1.2	34

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37	The alternation effect in ionic liquid homologous series. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 4033-4038.	1.3	34
38	Phase Equilibria in Ionic Liquid-Aromatic Compound Mixtures, Including Benzene Fluorination Effects. <i>Journal of Physical Chemistry B</i> , 2009, 113, 7631-7636.	1.2	33
39	Parameterization of the electronegativity equalization method based on the charge model 1. <i>Physical Chemistry Chemical Physics</i> , 2002, 4, 5933-5936.	1.3	31
40	Probing the Surface Tension of Ionic Liquids Using the Langmuir Principle. <i>Langmuir</i> , 2018, 34, 4408-4416.	1.6	31
41	The impact of ionic liquid fluorinated moieties on their thermophysical properties and aqueous phase behaviour. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 21340-21348.	1.3	30
42	Structural characterization of the [CnClim][C4F9SO3] ionic liquid series: Alkyl versus perfluoroalkyl side chains. <i>Journal of Molecular Liquids</i> , 2017, 226, 28-34.	2.3	30
43	Probing the structural features of the 1-alkyl-3-methylimidazolium hexafluorophosphate ionic liquid series using Molecular Dynamics simulations. <i>Journal of Molecular Liquids</i> , 2015, 210, 257-263.	2.3	28
44	Ultrafast Internal Conversion in a Model Anthocyanin-Polyphenol Complex: Implications for the Biological Role of Anthocyanins in Vegetative Tissues of Plants. <i>Chemistry - A European Journal</i> , 2009, 15, 1397-1402.	1.7	27
45	Using <sup>129</sup> Xe NMR to Probe the Structure of Ionic Liquids. <i>Journal of Physical Chemistry Letters</i> , 2013, 4, 2758-2762.	2.1	26
46	Phase Equilibria of Haloalkanes Dissolved in Ethylsulfate- or Ethylsulfonate-Based Ionic Liquids. <i>Journal of Physical Chemistry B</i> , 2010, 114, 7329-7337.	1.2	24
47	Liquid- or Solid-Like Behavior of [omim][BF <sub>4</sub> ] at a Solid Interface?. <i>Journal of Physical Chemistry Letters</i> , 2011, 2, 1551-1555.	2.1	24
48	Unusual LCST-type behaviour found in binary mixtures of choline-based ionic liquids with ethers. <i>RSC Advances</i> , 2013, 3, 10262.	1.7	24
49	Vaporisation of a Dicationic Ionic Liquid Revisited. <i>ChemPhysChem</i> , 2010, 11, 3673-3677.	1.0	23
50	Calculation of the Dipole Moment for Polypeptides Using the Generalized Born-Electronegativity Equalization Method: Results in Vacuum and Continuum-Dielectric Solvent. <i>Journal of Physical Chemistry B</i> , 2004, 108, 4171-4177.	1.2	22
51	Solvate ionic liquids based on lithium bis(trifluoromethanesulfonyl)imide-glyme systems: coordination in MD simulations with scaled charges. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 525-535.	1.3	22
52	Charge Templates in Aromatic Plus Ionic Liquid Systems Revisited: NMR Experiments and Molecular Dynamics Simulations. <i>Journal of Physical Chemistry B</i> , 2014, 118, 5772-5780.	1.2	21
53	Viscosity minima in binary mixtures of ionic liquids + molecular solvents. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 13480-13494.	1.3	21
54	Molecular dynamics studies on the structure and interactions of ionic liquids containing amino-acid anions. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 23864-23872.	1.3	19

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55	Ionic Liquids and Water: Hydrophobicity vs. Hydrophilicity. <i>Molecules</i> , 2021, 26, 7159.	1.7	19
56	Design of task-specific fluorinated ionic liquids: nanosegregation <i>versus</i> hydrogen-bonding ability in aqueous solutions. <i>Chemical Communications</i> , 2018, 54, 3524-3527.	2.2	17
57	Designing the ammonium cation to achieve a higher hydrophilicity of bistriflimide-based ionic liquids. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 19307-19313.	1.3	17
58	Wetting Films of Two Ionic Liquids: [C <sub>8</sub> mim][BF <sub>4</sub> ] and [C <sub>2</sub> OHmim][BF <sub>4</sub> ]. <i>Journal of Physical Chemistry C</i> , 2011, 115, 16116-16123.	1.5	16
59	Comparing the structure of different ionic liquid series: Bistriflamide v. hexafluorophosphate; pure v. equimolar mixtures. <i>Fluid Phase Equilibria</i> , 2016, 418, 181-191.	1.4	16
60	Halogen and Hydrogen Bonding Interplay in the Crystal Packing of Halometallocenes. <i>Molecules</i> , 2018, 23, 2959.	1.7	16
61	The complex structure of ionic liquids at an atomistic level: from <i>red-and-greens</i> to charge templates. <i>Pure and Applied Chemistry</i> , 2014, 86, 119-133.	0.9	15
62	Structure and dynamics of mica-confined films of [C <sub>10</sub> C <sub>1</sub> Pyrr][NTf <sub>2</sub> ] ionic liquid. <i>Journal of Chemical Physics</i> , 2018, 148, 193808.	1.2	15
63	Novel Ground- and Excited-State Prototropic Reactivity of a Hydroxycarboxyflavylium Salt. <i>Journal of Physical Chemistry A</i> , 2006, 110, 2089-2096.	1.1	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. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 30328-30342.	1.3	14
65	Mixtures of Pyridine and Nicotine with Pyridinium-Based Ionic Liquids. <i>Journal of Chemical &amp; Engineering Data</i> , 2011, 56, 4356-4363.	1.0	13
66	Ionic Liquid Films at the Water-Air Interface: Langmuir Isotherms of Tetra-alkylphosphonium-Based Ionic Liquids. <i>Langmuir</i> , 2015, 31, 8371-8378.	1.6	12
67	Solvent effects on the polar network of ionic liquid solutions. <i>Journal of Physics Condensed Matter</i> , 2015, 27, 194116.	0.7	12
68	Vapor Pressure Assessment of Sulfolane-Based Eutectic Solvents: Experimental, PC-SAFT, and Molecular Dynamics. <i>Journal of Physical Chemistry B</i> , 2020, 124, 10386-10397.	1.2	12
69	Self-Organization in Ionic Liquids: From Bulk to Interfaces and Films. <i>Journal of the Brazilian Chemical Society</i> , 2015, , .	0.6	12
70	Crystalline-like structures and multilayering in Langmuir films of ionic liquids at the air-water interface. <i>Chemical Communications</i> , 2016, 52, 5585-5588.	2.2	10
71	Predicting Hydration Free Energies of Neutral Compounds by a Parametrization of the Polarizable Continuum Model. <i>Journal of Physical Chemistry A</i> , 2005, 109, 11322-11327.	1.1	9
72	The role of halogen interactions in the crystal structure of bicyclopentadienyl dihalides. <i>CrystEngComm</i> , 2017, 19, 2802-2812.	1.3	9

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73	Comparative structural analyses in four ionic liquid systems: the two low- $q$ peaks of IL structure factor functions. <i>Molecular Simulation</i> , 2018, 44, 478-484.	0.9	9
74	The Solubility of Gases in Ionic Liquids: A Chemoinformatic Predictive and Interpretable Approach. <i>ChemPhysChem</i> , 2021, 22, 2190-2200.	1.0	9
75	Does the Photochemical Conversion of Colchicine into Lumicolchicines Involve Triplet Transients? A Solvent Dependence Study. <i>Photochemistry and Photobiology</i> , 2001, 73, 213.	1.3	9
76	Structure and dynamics of ionic liquids: general discussion. <i>Faraday Discussions</i> , 2018, 206, 291-337.	1.6	8
77	Tailoring amphotericin B as an ionic liquid: an upfront strategy to potentiate the biological activity of antifungal drugs. <i>RSC Advances</i> , 2021, 11, 14441-14452.	1.7	7
78	Bio-inspired hydrophilic bistriflimide-based ionic liquids: Molecular dynamics modeling and simulations. <i>Journal of Molecular Liquids</i> , 2020, 301, 112402.	2.3	6
79	Ionic Liquids in Wonderland: From Electrostatics to Coordination Chemistry. <i>Journal of Physical Chemistry C</i> , 2019, 123, 5804-5811.	1.5	5
80	Immobilization of His-tagged proteins on NiO foams for recyclable enzymatic reactors. <i>Applied Surface Science</i> , 2021, 537, 147848.	3.1	5
81	A simple method for the fast calculation of charge redistribution of solutes in an implicit solvent model. <i>Chemical Physics</i> , 2002, 282, 237-243.	0.9	4
82	ILs through the looking glass: electrostatics and structure probed using charge-inverted ionic liquid pairs. <i>Faraday Discussions</i> , 2018, 206, 203-218.	1.6	4
83	Effect of substituents in the molecular and supramolecular architectures of 1-ferrocenyl-2-(aryl)thioethanones. <i>CrystEngComm</i> , 2015, 17, 3089-3102.	1.3	3
84	Evidences for a Null Molar Volume Contribution by Hydroxyl Groups in Ammonium Bistriflimide-Based Ionic Liquids. <i>Journal of Chemical &amp; Engineering Data</i> , 2019, 64, 4932-4945.	1.0	3
85	Photon Upconversion in TTA-Inducing Ionic Liquids: Pinpointing the Role of IL Nanostructured Media Using MD Simulations. <i>Journal of Physical Chemistry B</i> , 2020, 124, 3137-3144.	1.2	3
86	Computational insights into substituent effects on the stability and reactivity of flavylum cation analogs of anthocyanins. <i>Arkivoc</i> , 2020, 2020, 146-162.	0.3	2
87	Cation-Anion and Cation-Cation Interactions in Mixtures of Hydroxy-functionalized and Aprotic Ionic Liquids. <i>Journal of Ionic Liquids</i> , 2022, 2, 100022.	1.0	1
88	Back to the Future: applying 2000's interactions to explain supramolecular arrangements in 1950's compounds. <i>Acta Crystallographica Section A: Foundations and Advances</i> , 2015, 71, s452-s453.	0.0	0