

# Karina Shimizu

## List of Publications by Year in descending order

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88  
papers

3,914  
citations

117625

34  
h-index

123424

61  
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89  
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89  
docs citations

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times ranked

3572  
citing authors

#	ARTICLE	IF	CITATIONS
1	Cation-Anion and Cation-Cation Interactions in Mixtures of Hydroxy-functionalized and Aprotic Ionic Liquids. <i>Journal of Ionic Liquids</i> , 2022, 2, 100022.	2.7	1
2	Immobilization of His-tagged proteins on NiO foams for recyclable enzymatic reactors. <i>Applied Surface Science</i> , 2021, 537, 147848.	6.1	5
3	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.	3.6	7
4	The Solubility of Gases in Ionic Liquids: A Chemoinformatic Predictive and Interpretable Approach. <i>ChemPhysChem</i> , 2021, 22, 2190-2200.	2.1	9
5	Ionic Liquids and Water: Hydrophobicity vs. Hydrophilicity. <i>Molecules</i> , 2021, 26, 7159.	3.8	19
6	Bio-inspired hydrophilic bistriflimide-based ionic liquids: Molecular dynamics modeling and simulations. <i>Journal of Molecular Liquids</i> , 2020, 301, 112402.	4.9	6
7	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.	2.8	22
8	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.	2.6	12
9	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.	2.6	3
10	Computational insights into substituent effects on the stability and reactivity of flavylum cation analogs of anthocyanins. <i>Arkivoc</i> , 2020, 2020, 146-162.	0.5	2
11	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.	1.9	3
12	Ionic Liquids in Wonderland: From Electrostatics to Coordination Chemistry. <i>Journal of Physical Chemistry C</i> , 2019, 123, 5804-5811.	3.1	5
13	Probing the Surface Tension of Ionic Liquids Using the Langmuir Principle. <i>Langmuir</i> , 2018, 34, 4408-4416.	3.5	31
14	Enhanced dissolution of ibuprofen using ionic liquids as catanionic hydrotropes. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 2094-2103.	2.8	68
15	Structure and dynamics of mica-confined films of [C10C1Pyr][NTf2] ionic liquid. <i>Journal of Chemical Physics</i> , 2018, 148, 193808.	3.0	15
16	Design of task-specific fluorinated ionic liquids: nanosegregation versus hydrogen-bonding ability in aqueous solutions. <i>Chemical Communications</i> , 2018, 54, 3524-3527.	4.1	17
17	ILs through the looking glass: electrostatics and structure probed using charge-inverted ionic liquid pairs. <i>Faraday Discussions</i> , 2018, 206, 203-218.	3.2	4
18	Structure and dynamics of ionic liquids: general discussion. <i>Faraday Discussions</i> , 2018, 206, 291-337.	3.2	8

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19	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.	2.0	9
20	Exploring the bulk-phase structure of ionic liquid mixtures using small-angle neutron scattering. <i>Faraday Discussions</i> , 2018, 206, 265-289.	3.2	42
21	Halogen and Hydrogen Bonding Interplay in the Crystal Packing of Halometallocenes. <i>Molecules</i> , 2018, 23, 2959.	3.8	16
22	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.	2.8	19
23	Designing the ammonium cation to achieve a higher hydrophilicity of bistriflimide-based ionic liquids. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 19307-19313.	2.8	17
24	Influence of Nanosegregation on the Phase Behavior of Fluorinated Ionic Liquids. <i>Journal of Physical Chemistry C</i> , 2017, 121, 5415-5427.	3.1	46
25	The role of halogen interactions in the crystal structure of bicyclopentadienyl dihalides. <i>CrystEngComm</i> , 2017, 19, 2802-2812.	2.6	9
26	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.	2.6	82
27	Structural characterization of the [C <sub>n</sub> C1im][C <sub>4</sub> F <sub>9</sub> SO <sub>3</sub> ] ionic liquid series: Alkyl versus perfluoroalkyl side chains. <i>Journal of Molecular Liquids</i> , 2017, 226, 28-34.	4.9	30
28	Crystalline-like structures and multilayering in Langmuir films of ionic liquids at the air/water interface. <i>Chemical Communications</i> , 2016, 52, 5585-5588.	4.1	10
29	Liquid-Crystalline Ionic Liquids as Ordered Reaction Media for the Diels-Alder Reaction. <i>Chemistry - A European Journal</i> , 2016, 22, 16113-16123.	3.3	35
30	Imidazolium-Based Lipid Analogues and Their Interaction with Phosphatidylcholine Membranes. <i>Langmuir</i> , 2016, 32, 12579-12592.	3.5	50
31	Influence of Nanosegregation on the Surface Tension of Fluorinated Ionic Liquids. <i>Langmuir</i> , 2016, 32, 6130-6139.	3.5	38
32	Comparing the structure of different ionic liquid series: Bistriflamide v. hexafluorophosphate; pure v. equimolar mixtures. <i>Fluid Phase Equilibria</i> , 2016, 418, 181-191.	2.5	16
33	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.	2.8	49
34	Additive polarizabilities in ionic liquids. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 1665-1670.	2.8	37
35	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.	0.1	0
36	Effect of substituents in the molecular and supramolecular architectures of 1-ferrocenyl-2-(aryl)thioethanones. <i>CrystEngComm</i> , 2015, 17, 3089-3102.	2.6	3

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37	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.	9.0	156
38	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.	2.8	78
39	Plasma membrane permeabilisation by ionic liquids: a matter of charge. <i>Green Chemistry</i> , 2015, 17, 4587-4598.	9.0	37
40	A thermophysical and structural characterization of ionic liquids with alkyl and perfluoroalkyl side chains. <i>RSC Advances</i> , 2015, 5, 65337-65350.	3.6	63
41	Ionic Liquid Films at the Water-Air Interface: Langmuir Isotherms of Tetra-alkylphosphonium-Based Ionic Liquids. <i>Langmuir</i> , 2015, 31, 8371-8378.	3.5	12
42	Viscosity minima in binary mixtures of ionic liquids + molecular solvents. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 13480-13494.	2.8	21
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.	4.9	28
44	Solvent effects on the polar network of ionic liquid solutions. <i>Journal of Physics Condensed Matter</i> , 2015, 27, 194116.	1.8	12
45	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.	2.8	14
46	Self-Organization in Ionic Liquids: From Bulk to Interfaces and Films. <i>Journal of the Brazilian Chemical Society</i> , 2015, , .	0.6	12
47	The complex structure of ionic liquids at an atomistic level: from "ordered-and-greens" to charge templates. <i>Pure and Applied Chemistry</i> , 2014, 86, 119-133.	1.9	15
48	Cation Alkyl Side Chain Length and Symmetry Effects on the Surface Tension of Ionic Liquids. <i>Langmuir</i> , 2014, 30, 6408-6418.	3.5	75
49	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.	2.6	223
50	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.	2.8	30
51	The alternation effect in ionic liquid homologous series. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 4033-4038.	2.8	34
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.	2.6	21
53	The effect of the cation alkyl chain branching on mutual solubilities with water and toxicities. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 19952.	2.8	64
54	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.	1.9	47

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55	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.	2.6	65
56	Using <sup>129</sup> Xe NMR to Probe the Structure of Ionic Liquids. <i>Journal of Physical Chemistry Letters</i> , 2013, 4, 2758-2762.	4.6	26
57	Nano-segregation in ionic liquids: scorpions and vanishing chains. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 16256.	2.8	119
58	On the Formation of a Third, Nanostructured Domain in Ionic Liquids. <i>Journal of Physical Chemistry B</i> , 2013, 117, 10826-10833.	2.6	99
59	Unusual LCST-type behaviour found in binary mixtures of choline-based ionic liquids with ethers. <i>RSC Advances</i> , 2013, 3, 10262.	3.6	24
60	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.	3.2	56
61	Liquid-Liquid Equilibrium of Cholinium-Derived Bistriflimide Ionic Liquids with Water and Octanol. <i>Journal of Physical Chemistry B</i> , 2012, 116, 9186-9195.	2.6	34
62	Density, Thermal Expansion and Viscosity of Cholinium-Derived Ionic Liquids. <i>ChemPhysChem</i> , 2012, 13, 1902-1909.	2.1	83
63	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.	3.1	16
64	High-Accuracy Vapor Pressure Data of the Extended [C <sub>1</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.	2.6	199
65	Mixtures of Pyridine and Nicotine with Pyridinium-Based Ionic Liquids. <i>Journal of Chemical &amp; Engineering Data</i> , 2011, 56, 4356-4363.	1.9	13
66	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.	4.6	24
67	Three commentaries on the nano-segregated structure of ionic liquids. <i>Computational and Theoretical Chemistry</i> , 2010, 946, 70-76.	1.5	156
68	Vaporisation of a Dicationic Ionic Liquid Revisited. <i>ChemPhysChem</i> , 2010, 11, 3673-3677.	2.1	23
69	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.	4.9	75
70	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.	2.6	89
71	Nanostructure of Trialkylmethylammonium Bistriflamide Ionic Liquids Studied by Molecular Dynamics. <i>Journal of Physical Chemistry B</i> , 2010, 114, 15635-15641.	2.6	50
72	Phase Equilibria of Haloalkanes Dissolved in Ethylsulfate- or Ethylsulfonate-Based Ionic Liquids. <i>Journal of Physical Chemistry B</i> , 2010, 114, 7329-7337.	2.6	24

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73	Mutual Solubility of Water and Structural/Positional Isomers of <i>N</i> -Alkylpyridinium-Based Ionic Liquids. <i>Journal of Physical Chemistry B</i> , 2010, 114, 15925-15934.	2.6	74
74	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.	2.6	146
75	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.	3.3	27
76	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.	2.6	86
77	Phase Equilibria in Ionic Liquid-Aromatic Compound Mixtures, Including Benzene Fluorination Effects. <i>Journal of Physical Chemistry B</i> , 2009, 113, 7631-7636.	2.6	33
78	A Tale of Two Ions: The Conformational Landscapes of Bis(trifluoromethanesulfonyl)amide and <i>N,N</i> -Dialkylpyrrolidinium. <i>Journal of Physical Chemistry B</i> , 2008, 112, 1465-1472.	2.6	128
79	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.	2.6	286
80	Potential Energy Landscape of Bis(fluorosulfonyl)amide. <i>Journal of Physical Chemistry B</i> , 2008, 112, 9449-9455.	2.6	81
81	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
82	Novel Ground- and Excited-State Prototropic Reactivity of a Hydroxycarboxyflavylum Salt. <i>Journal of Physical Chemistry A</i> , 2006, 110, 2089-2096.	2.5	14
83	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.	2.5	9
84	Charge-Transfer Complexation as a General Phenomenon in the Copigmentation of Anthocyanins. <i>Journal of Physical Chemistry A</i> , 2005, 109, 7329-7338.	2.5	63
85	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.	2.6	22
86	Parameterization of the electronegativity equalization method based on the charge model 1. <i>Physical Chemistry Chemical Physics</i> , 2002, 4, 5933-5936.	2.8	31
87	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.	1.9	4
88	Does the Photochemical Conversion of Colchicine into Lumicolchicines Involve Triplet Transients? A Solvent Dependence Study. <i>Photochemistry and Photobiology</i> , 2001, 73, 213.	2.5	9