Karina Shimizu

List of Publications by Year
in descending order

88 papers	3,914 citations	117453 34 h-index	123241 61 g-index
89 all docs	89 docs citations	89 times ranked	3572 citing authors

#	Article	IF	Citations
1	Cation-Anion and Cation-Cation Interactions in Mixtures of Hydroxy-functionalized and Aprotic Ionic Liquids. Journal of Ionic Liquids, 2022, 2, 100022.	1.0	1
2	Immobilization of His-tagged proteins on NiO foams for recyclable enzymatic reactors. Applied Surface Science, 2021, 537, 147848.	3.1	5
3	Tailoring amphotericin B as an ionic liquid: an upfront strategy to potentiate the biological activity of antifungal drugs. RSC Advances, 2021, 11, 14441-14452.	1.7	7
4	The Solubility of Gases in Ionic Liquids: A Chemoinformatic Predictive and Interpretable Approach. ChemPhysChem, 2021, 22, 2190-2200.	1.0	9
5	Ionic Liquids and Water: Hydrophobicity vs. Hydrophilicity. Molecules, 2021, 26, 7159.	1.7	19
6	Bio-inspired hydrophilic bistriflimide-based ionic liquids: Molecular dynamics modeling and simulations. Journal of Molecular Liquids, 2020, 301, 112402.	2.3	6
7	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.	1.3	22
8	Vapor Pressure Assessment of Sulfolane-Based Eutectic Solvents: Experimental, PC-SAFT, and Molecular Dynamics. Journal of Physical Chemistry B, 2020, 124, 10386-10397.	1.2	12
9	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.	1.2	3
10	Computational insights into substituent effects on the stability and reactivity of flavylium cation analogs of anthocyanins. Arkivoc, 2020, 2020, 146-162.	0.3	2
11	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.	1.0	3
12	Ionic Liquids in Wonderland: From Electrostatics to Coordination Chemistry. Journal of Physical Chemistry C, 2019, 123, 5804-5811.	1.5	5
13	Probing the Surface Tension of Ionic Liquids Using the Langmuir Principle. Langmuir, 2018, 34, 4408-4416.	1.6	31
14	Enhanced dissolution of ibuprofen using ionic liquids as catanionic hydrotropes. Physical Chemistry Chemical Physics, 2018, 20, 2094-2103.	1.3	68
15	Structure and dynamics of mica-confined films of [C10C1Pyrr][NTf2] ionic liquid. Journal of Chemical Physics, 2018, 148, 193808.	1.2	15
16	Design of task-specific fluorinated ionic liquids: nanosegregation versus hydrogen-bonding ability in aqueous solutions. Chemical Communications, 2018, 54, 3524-3527.	2.2	17
17	ILs through the looking glass: electrostatics and structure probed using charge-inverted ionic liquid pairs. Faraday Discussions, 2018, 206, 203-218.	1.6	4
18	Structure and dynamics of ionic liquids: general discussion. Faraday Discussions, 2018, 206, 291-337.	1.6	8

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19	Comparative structural analyses in four ionic liquid systems: the two low-q peaks of IL structure factor functions. Molecular Simulation, 2018, 44, 478-484.	0.9	9
20	Exploring the bulk-phase structure of ionic liquid mixtures using small-angle neutron scattering. Faraday Discussions, 2018, 206, 265-289.	1.6	42
21	Halogen and Hydrogen Bonding Interplay in the Crystal Packing of Halometallocenes. Molecules, 2018, 23, 2959.	1.7	16
22	Molecular dynamics studies on the structure and interactions of ionic liquids containing amino-acid anions. Physical Chemistry Chemical Physics, 2018, 20, 23864-23872.	1.3	19
23	Designing the ammonium cation to achieve a higher hydrophilicity of bistriflimide-based ionic liquids. Physical Chemistry Chemical Physics, 2018, 20, 19307-19313.	1.3	17
24	Influence of Nanosegregation on the Phase Behavior of Fluorinated Ionic Liquids. Journal of Physical Chemistry C, 2017, 121, 5415-5427.	1.5	46
25	The role of halogen interactions in the crystal structure of biscyclopentadienyl dihalides. CrystEngComm, 2017, 19, 2802-2812.	1.3	9
26	Nanosegregation and Structuring in the Bulk and at the Surface of Ionic-Liquid Mixtures. Journal of Physical Chemistry B, 2017, 121, 6002-6020.	1.2	82
27	Structural characterization of the [CnC1im][C4F9SO3] ionic liquid series: Alkyl versus perfluoroalkyl side chains. Journal of Molecular Liquids, 2017, 226, 28-34.	2.3	30
28	Crystalline-like structures and multilayering in Langmuir films of ionic liquids at the airâ€“water interface. Chemical Communications, 2016, 52, 5585-5588.	2.2	10
29	Liquidâ€Crystalline Ionic Liquids as Ordered Reaction Media for the Dielsâ€“Alder Reaction. Chemistry - A European Journal, 2016, 22, 16113-16123.	1.7	35
30	Imidazolium-Based Lipid Analogues and Their Interaction with Phosphatidylcholine Membranes. Langmuir, 2016, 32, 12579-12592.	1.6	50
31	Influence of Nanosegregation on the Surface Tension of Fluorinated Ionic Liquids. Langmuir, 2016, 32, 6130-6139.	1.6	38
32	Comparing the structure of different ionic liquid series: Bistriflamide v. hexafluorophosphate; pure v. equimolar mixtures. Fluid Phase Equilibria, 2016, 418, 181-191.	1.4	16
33	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.	1.3	49
34	Additive polarizabilities in ionic liquids. Physical Chemistry Chemical Physics, 2016, 18, 1665-1670.	1.3	37
35	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.	0.0	0
36	Effect of substituents in the molecular and supramolecular architectures of 1-ferrocenyl-2-(aryl)thioethanones. CrystEngComm, 2015, 17, 3089-3102.	1.3	3

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37	The magic of aqueous solutions of ionic liquids: ionic liquids as a powerful class of catanionic hydrotropes. Green Chemistry, 2015, 17, 3948-3963.	4.6	156
38	Structural and aggregate analyses of (Li salt + glyme) mixtures: the complex nature of solvate ionic liquids. Physical Chemistry Chemical Physics, 2015, 17, 22321-22335.	1.3	78
39	Plasma membrane permeabilisation by ionic liquids: a matter of charge. Green Chemistry, 2015, 17, 4587-4598.	4.6	37
40	A thermophysical and structural characterization of ionic liquids with alkyl and perfluoroalkyl side chains. RSC Advances, 2015, 5, 65337-65350.	1.7	63
41	Ionic Liquid Films at the Waterâ€“Air Interface: Langmuir Isotherms of Tetra-alkylphosphonium-Based Ionic Liquids. Langmuir, 2015, 31, 8371-8378.	1.6	12
42	Viscosity minima in binary mixtures of ionic liquids + molecular solvents. Physical Chemistry Chemical Physics, 2015, 17, 13480-13494.	1.3	21
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.	2.3	28
44	Solvent effects on the polar network of ionic liquid solutions. Journal of Physics Condensed Matter, 2015, 27, 194116.	0.7	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. Physical Chemistry Chemical Physics, 2015, 17, 30328-30342.	1.3	14
46	Self-Organization in Ionic Liquids: From Bulk to Interfaces and Films. Journal of the Brazilian Chemical Society, 2015, , .	0.6	12
47	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.	0.9	15
48	Cation Alkyl Side Chain Length and Symmetry Effects on the Surface Tension of Ionic Liquids. Langmuir, 2014, 30, 6408-6418.	1.6	75
49	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.	1.2	223
50	The impact of ionic liquid fluorinated moieties on their thermophysical properties and aqueous phase behaviour. Physical Chemistry Chemical Physics, 2014, 16, 21340-21348.	1.3	30
51	The alternation effect in ionic liquid homologous series. Physical Chemistry Chemical Physics, 2014, 16, 4033-4038.	1.3	34
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.	1.2	21
53	The effect of the cation alkyl chain branching on mutual solubilities with water and toxicities. Physical Chemistry Chemical Physics, 2014, 16, 19952.	1.3	64
54	Complex Structure of Ionic Liquids. Molecular Dynamics Studies with Different Cationâ€“Anion Combinations. Journal of Chemical & Engineering Data, 2014, 59, 3120-3129.	1.0	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. Journal of Physical Chemistry B, 2014, 118, 6885-6895.	1.2	65
56	Using ¹²⁹Xe NMR to Probe the Structure of Ionic Liquids. Journal of Physical Chemistry Letters, 2013, 4, 2758-2762.	2.1	26
57	Nano-segregation in ionic liquids: scorpions and vanishing chains. Physical Chemistry Chemical Physics, 2013, 15, 16256.	1.3	119
58	On the Formation of a Third, Nanostructured Domain in Ionic Liquids. Journal of Physical Chemistry B, 2013, 117, 10826-10833.	1.2	99
59	Unusual LCST-type behaviour found in binary mixtures of choline-based ionic liquids with ethers. RSC Advances, 2013, 3, 10262.	1.7	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. Faraday Discussions, 2012, 154, 155-169.	1.6	56
61	Liquidâ€"Liquid Equilibrium of Cholinium-Derived Bistriflimide Ionic Liquids with Water and Octanol. Journal of Physical Chemistry B, 2012, 116, 9186-9195.	1.2	34
62	Density, Thermal Expansion and Viscosity of Choliniumâ€Derived Ionic Liquids. ChemPhysChem, 2012, 13, 1902-1909.	1.0	83
63	Wetting Films of Two Ionic Liquids: [C₈mim][BF4] and [C₂OHmim][BF₄]. Journal of Physical Chemistry C, 2011, 115, 16116-16123.	1.5	16
64	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.	1.2	199
65	Mixtures of Pyridine and Nicotine with Pyridinium-Based Ionic Liquids. Journal of Chemical & Engineering Data, 2011, 56, 4356-4363.	1.0	13
66	Liquid- or Solid-Like Behavior of [omim][BF₄] at a Solid Interface?. Journal of Physical Chemistry Letters, 2011, 2, 1551-1555.	2.1	24
67	Three commentaries on the nano-segregated structure of ionic liquids. Computational and Theoretical Chemistry, 2010, 946, 70-76.	1.5	156
68	Vaporisation of a Dicationic Ionic Liquid Revisited. ChemPhysChem, 2010, 11, 3673-3677.	1.0	23
69	Binary mixtures of ionic liquids with a common ion revisited: A molecular dynamics simulation study. Journal of Molecular Liquids, 2010, 153, 52-56.	2.3	75
70	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.	1.2	89
71	Nanostructure of Trialkylmethylammonium Bistriflamide Ionic Liquids Studied by Molecular Dynamics. Journal of Physical Chemistry B, 2010, 114, 15635-15641.	1.2	50
72	Phase Equilibria of Haloalkanes Dissolved in Ethylsulfate- or Ethylsulfonate-Based Ionic Liquids. Journal of Physical Chemistry B, 2010, 114, 7329-7337.	1.2	24

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73	Mutual Solubility of Water and Structural/Positional Isomers of N-Alkylpyridinium-Based Ionic Liquids. Journal of Physical Chemistry B, 2010, 114, 15925-15934.	1.2	74
74	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.	1.2	146
75	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.	1.7	27
76	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.	1.2	86
77	Phase Equilibria in Ionic Liquidâ^'Aromatic Compound Mixtures, Including Benzene Fluorination Effects. Journal of Physical Chemistry B, 2009, 113, 7631-7636.	1.2	33
78	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.	1.2	128
79	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.	1.2	286
80	Potential Energy Landscape of Bis(fluorosulfonyl)amide. Journal of Physical Chemistry B, 2008, 112, 9449-9455.	1.2	81
81	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
82	Novel Ground- and Excited-State Prototropic Reactivity of a Hydroxycarboxyflavylium Salt. Journal of Physical Chemistry A, 2006, 110, 2089-2096.	1.1	14
83	Predicting Hydration Free Energies of Neutral Compounds by a Parametrization of the Polarizable Continuum Model. Journal of Physical Chemistry A, 2005, 109, 11322-11327.	1.1	9
84	Charge-Transfer Complexation as a General Phenomenon in the Copigmentation of Anthocyanins. Journal of Physical Chemistry A, 2005, 109, 7329-7338.	1.1	63
85	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.	1.2	22
86	Parameterization of the electronegativity equalization method based on the charge model 1. Physical Chemistry Chemical Physics, 2002, 4, 5933-5936.	1.3	31
87	A simple method for the fast calculation of charge redistribution of solutes in an implicit solvent model. Chemical Physics, 2002, 282, 237-243.	0.9	4
88	Does the Photochemical Conversion of Colchicine into Lumicolchicines Involve Triplet Transients? A Solvent Dependence StudyÂ¶. Photochemistry and Photobiology, 2001, 73, 213.	1.3	9