Claudio J Margulis

List of Publications by Year
in descending order

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83	6,019	125106	78623
papers	citations	35	77
		h-index	g-index

86	86	86	4938
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Ether tails make a large difference for the structural dynamics of imidazolium-based ionic liquids. Journal of Ionic Liquids, 2022, 2, 100012.	1.0	5
2	X-ray scattering reveals ion clustering of dilute chromium species in molten chloride medium. Chemical Science, 2021, 12, 8026-8035.	3.7	13
3	A Brief Guide to the Structure of High-Temperature Molten Salts and Key Aspects Making Them Different from Their Low-Temperature Relatives, the Ionic Liquids. Journal of Physical Chemistry B, 2021, 125, 6359-6372.	1.2	26
4	Unraveling Local Structure of Molten Salts via X-ray Scattering, Raman Spectroscopy, and Ab Initio Molecular Dynamics. Journal of Physical Chemistry B, 2021, 125, 5971-5982.	1.2	23
5	Relationship between the Relaxation of Ionic Liquid Structural Motifs and That of the Shear Viscosity. Journal of Physical Chemistry B, 2021, 125, 6264-6271.	1.2	11
6	SEM-Drude Model for the Accurate and Efficient Simulation of MgCl2â€“KCl Mixtures in the Condensed Phase. Journal of Physical Chemistry A, 2020, 124, 7832-7842.	1.1	12
7	Structure and dynamics of the molten alkali-chloride salts from an X-ray, simulation, and rate theory perspective. Physical Chemistry Chemical Physics, 2020, 22, 22900-22917.	1.3	22
8	Comparison of fixed charge and polarizable models for predicting the structural, thermodynamic, and transport properties of molten alkali chlorides. Journal of Chemical Physics, 2020, 153, 214502.	1.2	19
9	Temperature Dependence of Short and Intermediate Range Order in Molten MgCl₂ and Its Mixture with KCl. Journal of Physical Chemistry B, 2020, 124, 2892-2899.	1.2	38
10	A Pictorial View of Viscosity in Ionic Liquids and the Link to Nanostructural Heterogeneity. Journal of Physical Chemistry Letters, 2020, 11, 2062-2066.	2.1	36
11	Structure and Dynamics of an Ionic Liquid Mixture Film Confined by Mica. Journal of Physical Chemistry C, 2019, 123, 20971-20979.	1.5	7
12	Structural analysis of ionic liquids with symmetric and asymmetric fluorinated anions. Journal of Chemical Physics, 2019, 151, 074504.	1.2	20
13	Ionic Liquid Mixture at the Vacuum Interface and the Peaks and Antipeaks Analysis of X-ray Reflectivity. Journal of Physical Chemistry C, 2019, 123, 4914-4925.	1.5	11
14	Elucidating Ionic Correlations Beyond Simple Charge Alternation in Molten MgCl₂â€“KCl Mixtures. Journal of Physical Chemistry Letters, 2019, 10, 7603-7610.	2.1	49
15	Dynamics of an excess hole in the 1-methyl-1-butyl-pyrrolidinium dicyanamide ionic-liquid. Journal of Chemical Physics, 2018, 148, 193831.	1.2	7
16	In an ionic liquid, high local friction is determined by the proximity to the charge network. Journal of Chemical Physics, 2018, 149, 144503.	1.2	20
17	Comparison of the Structural Response to Pressure of Ionic Liquids with Ether and Alkyl Functionalities. Journal of Physical Chemistry B, 2017, 121, 6890-6897.	1.2	19
18	Ionic Liquids with Symmetric Diether Tails: Bulk and Vacuum-Liquid Interfacial Structures. Journal of Physical Chemistry B, 2017, 121, 174-179.	1.2	15

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19	Excess Electron and Hole in 1-Benzylpyridinium-Based Ionic Liquids. Journal of Physical Chemistry B, 2017, 121, 8809-8816.	1.2	8
20	Communication: Stiff and soft nano-environments and the â€œOctopus Effectâ€•are the crux of ionic liquid structural and dynamical heterogeneity. Journal of Chemical Physics, 2017, 147, 061102.	1.2	28
21	Structure of cyano-anion ionic liquids: X-ray scattering and simulations. Journal of Chemical Physics, 2016, 145, 024503.	1.2	54
22	Communication: Nanoscale structure of tetradecyltrihexylphosphonium based ionic liquids. Journal of Chemical Physics, 2016, 144, 121102.	1.2	44
23	A link between structure, diffusion and rotations of hydrogen bonding tracers in ionic liquids. Journal of Chemical Physics, 2016, 144, 204504.	1.2	36
24	Structures of Ionic Liquids Having Both Anionic and Cationic Octyl Tails: Lamellar Vacuum Interface vs Sponge-Like Bulk Order. Journal of Physical Chemistry Letters, 2016, 7, 3785-3790.	2.1	46
25	Rotational Dynamics in Ionic Liquids from NMR Relaxation Experiments and Simulations: Benzene and 1-Ethyl-3-Methylimidazolium. Journal of Physical Chemistry B, 2016, 120, 9450-9467.	1.2	31
26	Ionic liquidsâ€”Conventional solvent mixtures, structurally different but dynamically similar. Journal of Chemical Physics, 2015, 143, 134505.	1.2	33
27	A Rigid Hinge Region Is Necessary for High-Affinity Binding of Dimannose to Cyanovirin and Associated Constructs. Biochemistry, 2015, 54, 6951-6960.	1.2	15
28	Solvation of an Excess Electron in Pyrrolidinium Dicyanamide Based Ionic Liquids. Journal of Physical Chemistry B, 2015, 119, 532-542.	1.2	19
29	Modern Room Temperature Ionic Liquids, a Simple Guide to Understanding Their Structure and How It May Relate to Dynamics. Journal of Physical Chemistry B, 2015, 119, 12727-12740.	1.2	266
30	How Is Diffusion of Neutral and Charged Tracers Related to the Structure and Dynamics of a Room-Temperature Ionic Liquid? Large Deviations from Stokesâ€“Einstein Behavior Explained. Journal of Physical Chemistry B, 2015, 119, 7015-7029.	1.2	158
31	Communication: Anomalous temperature dependence of the intermediate range order in phosphonium ionic liquids. Journal of Chemical Physics, 2014, 140, 111102.	1.2	49
32	Bicontinuity and Multiple Length Scale Ordering in Triphilic Hydrogen-Bonding Ionic Liquids. Journal of Physical Chemistry B, 2014, 118, 12706-12716.	1.2	69
33	The Role of Glu41 in the Binding of Dimannose to P51G-m4-CVN. Biochemistry, 2014, 53, 1477-1484.	1.2	3
34	Structure of 1-Alkyl-1-methylpyrrolidinium Bis(trifluoromethylsulfonyl)amide Ionic Liquids with Linear, Branched, and Cyclic Alkyl Groups. Journal of Physical Chemistry B, 2013, 117, 15328-15337.	1.2	121
35	Dynamics of Excess Electronic Charge in Aliphatic Ionic Liquids Containing the Bis(trifluoromethylsulfonyl)amide Anion. Journal of the American Chemical Society, 2013, 135, 17528-17536.	6.6	28
36	Anions, the Reporters of Structure in Ionic Liquids. Journal of Physical Chemistry Letters, 2013, 4, 105-110.	2.1	116

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37	How Does the Ionic Liquid Organizational Landscape Change when Nonpolar Cationic Alkyl Groups Are Replaced by Polar Isoelectronic Diethers?. Journal of Physical Chemistry B, 2013, 117, 1130-1135.	1.2	134
38	SAXS anti-peaks reveal the length-scales of dual positiveâ€“negative and polarâ€“apolar ordering in room-temperature ionic liquids. Chemical Communications, 2012, 48, 5103.	2.2	223
39	Temperature-dependent structure of ionic liquids: X-ray scattering and simulations. Faraday Discussions, 2012, 154, 133-143.	1.6	171
40	Dry Excess Electrons in Room-Temperature Ionic Liquids. Journal of the American Chemical Society, 2011, 133, 20186-20193.	6.6	40
41	How Is Charge Transport Different in Ionic Liquids and Electrolyte Solutions?. Journal of Physical Chemistry B, 2011, 115, 13212-13221.	1.2	190
42	Searching and Optimizing Structure Ensembles for Complex Flexible Sugars. Journal of the American Chemical Society, 2011, 133, 15252-15255.	6.6	18
43	Ionic Liquids: Structure and Photochemical Reactions. Annual Review of Physical Chemistry, 2011, 62, 85-105.	4.8	310
44	Measuring the magnitude of internal motion in a complex hexasaccharide. Biopolymers, 2011, 95, 39-50.	1.2	11
45	Temperature-dependent structure of methyltributylammonium bis(trifluoromethylsulfonyl)amide: X ray scattering and simulations. Journal of Chemical Physics, 2011, 134, 064501.	1.2	139
46	In Silico Prediction of the 3D Structure of Trimeric Asialoglycoprotein Receptor Bound to Triantennary Oligosaccharide. Journal of the American Chemical Society, 2010, 132, 9087-9095.	6.6	16
47	What is the Origin of the Prepeak in the X-ray Scattering of Imidazolium-Based Room-Temperature Ionic Liquids?. Journal of Physical Chemistry B, 2010, 114, 16838-16846.	1.2	350
48	Controlling the Outcome of Electron Transfer Reactions in Ionic Liquids. Journal of Physical Chemistry B, 2009, 113, 12005-12012.	1.2	37
49	Computational Study of the Conformational Structures of Saccharides in Solution Based on J Couplings and the â€œFast Sugar Structure Prediction Softwareâ€• Biomacromolecules, 2009, 10, 3081-3088.	2.6	9
50	When Sugars Get Wet. A Comprehensive Study of the Behavior of Water on the Surface of Oligosaccharides. Journal of Physical Chemistry B, 2009, 113, 11003-11015.	1.2	27
51	A tool for the prediction of structures of complex sugars. Journal of Biomolecular NMR, 2008, 42, 241-256.	1.6	23
52	Dynamics of Water Adsorption onto a Calcite Surface as a Function of Relative Humidity. Journal of Physical Chemistry C, 2008, 112, 2109-2115.	1.5	83
53	Molecular Dynamics Study of the Temperature-Dependent Optical Kerr Effect Spectra and Intermolecular Dynamics of Room Temperature Ionic Liquid 1-Methoxyethylpyridinium Dicyanoamide. Journal of Physical Chemistry B, 2008, 112, 7837-7849.	1.2	82
54	Rationalization of the Difference in Lifetime of Two Covalent Sialosylâ^'Enzyme Intermediates of Trypanosoma rangeli Sialidase. Journal of Physical Chemistry B, 2008, 112, 14093-14095.	1.2	0

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55	How Does Water Affect the Dynamics of the Room-Temperature Ionic Liquid 1-Hexyl-3-methylimidazolium Hexafluorophosphate and the Fluorescence Spectroscopy of Coumarin-153 When Dissolved in It?. Journal of Physical Chemistry B, 2008, 112, 1770-1776.	1.2	73
56	Sugar Folding:â€‰ A Novel Structural Prediction Tool for Oligosaccharides and Polysaccharides 1. Journal of Chemical Theory and Computation, 2007, 3, 1620-1628.	2.3	17
57	Sugar Folding:â€‰ A Novel Structural Prediction Tool for Oligosaccharides and Polysaccharides 2. Journal of Chemical Theory and Computation, 2007, 3, 1629-1643.	2.3	30
58	Diffusion and Residence Time of Hydrogen Peroxide and Water in Crowded Protein Environments. Journal of Physical Chemistry B, 2007, 111, 13336-13344.	1.2	26
59	On the Response of an Ionic Liquid to External Perturbations and the Calculation of Shear Viscosityâ€. Journal of Physical Chemistry B, 2007, 111, 4705-4714.	1.2	43
60	Room-Temperature Ionic Liquids: Slow Dynamics, Viscosity, and the Red Edge Effect. Accounts of Chemical Research, 2007, 40, 1097-1105.	7.6	198
61	Heterogeneity in a room-temperature ionic liquid: Persistent local environments and the red-edge effect. Proceedings of the National Academy of Sciences of the United States of America, 2006, 103, 831-836.	3.3	377
62	A Study of the Time-Resolved Fluorescence Spectrum and Red Edge Effect of ANF in a Room-Temperature Ionic Liquid. Journal of Physical Chemistry B, 2006, 110, 11025-11028.	1.2	48
63	Why Is the Partial Molar Volume of CO2 So Small When Dissolved in a Room Temperature Ionic Liquid? Structure and Dynamics of CO2 Dissolved in [Bmim+] [PF6-]. Journal of the American Chemical Society, 2005, 127, 17842-17851.	6.6	335
64	Conformational Dynamics of Sialyl Lewis^xin Aqueous Solution and Its Interaction with SelectinE. A Study by Molecular Dynamics. Journal of Biomolecular Structure and Dynamics, 2005, 23, 101-111.	2.0	31
65	Computational Study of the Dynamics of Mannose Disaccharides Free in Solution and Bound to the Potent Anti-HIV Virucidal Protein Cyanovirin. Journal of Physical Chemistry B, 2005, 109, 3639-3647.	1.2	22
66	Ultrafast nonadiabatic dynamics: Quasiclassical calculation of the transient photoelectron spectrum of I2â^'â‹…(CO2)8. Journal of Chemical Physics, 2004, 120, 3657-3664.	1.2	5
67	Hydrophobic Collapse in Multidomain Protein Folding. Science, 2004, 305, 1605-1609.	6.0	482
68	Reply to the Comment on â€œDo Molecules as Small as Neopentane Induce a Hydrophobic Response Similar to that of Large Hydrophobic Surfaces?. Journal of Physical Chemistry B, 2004, 108, 9373-9374.	1.2	0
69	Computational study of imidazolium-based ionic solvents with alkyl substituents of different lengths. Molecular Physics, 2004, 102, 829-838.	0.8	164
70	Do Molecules as Small as Neopentane Induce a Hydrophobic Response Similar to That of Large Hydrophobic Surfaces?. Journal of Physical Chemistry B, 2003, 107, 11742-11748.	1.2	66
71	Dewetting-induced collapse of hydrophobic particles. Proceedings of the National Academy of Sciences of the United States of America, 2003, 100, 11953-11958.	3.3	264
72	A New Semiempirical Approach to Study Ground and Excited States of Metal Complexes in Biological Systemsâ€. Journal of Physical Chemistry B, 2002, 106, 8038-8046.	1.2	13

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73	Computer Simulation of a â€œGreen Chemistryâ€•Room-Temperature Ionic Solvent. Journal of Physical Chemistry B, 2002, 106, 12017-12021.	1.2	268
74	Helix Unfolding and Intramolecular Hydrogen Bond Dynamics in Small Î±-Helices in Explicit Solvent. Journal of Physical Chemistry B, 2002, 106, 10748-10752.	1.2	33
75	Solvation effects on equilibria: Triazoles and N-methyl piperidinol. Physical Chemistry Chemical Physics, 2002, 4, 5281-5288.	1.3	9
76	A Monte Carlo study of symmetry breaking of I[sub 3][sup â^’] in aqueous solution using a multistate diabatic Hamiltonian. Journal of Chemical Physics, 2001, 114, 367.	1.2	33
77	Influence of Solvation Environment on Excited State Avoided Crossings and Photodissociation Dynamicsâ€. Journal of Physical Chemistry B, 2001, 105, 6728-6737.	1.2	26
78	Symmetry breaking of the triiodide ion in acetonitrile solution. Chemical Physics Letters, 2001, 341, 557-560.	1.2	41
79	Modeling solvation of excited electronic states of flexible polyatomic molecules: Diatomics-in-molecules for I3 in argon clusters. Journal of Chemical Physics, 2001, 114, 6744-6749.	1.2	7
80	Nonadiabatic molecular dynamics simulations of the photofragmentation and geminate recombination dynamics in size-selected I2â^’â‹…(CO2)n cluster ions. Journal of Chemical Physics, 1999, 110, 5677-5690.	1.2	37
81	Vibrational Dynamics of the I3Radical:Â A Semiempirical Potential Surface, and Semiclassical Calculation of the Anion Photoelectron Spectrum. Journal of Physical Chemistry A, 1999, 103, 9552-9563.	1.1	12
82	Ionic aggregates in steam. Part 1.â€”Equilibrium configurations. Journal of the Chemical Society, Faraday Transactions, 1996, 92, 2703-2708.	1.7	5
83	Structure of Molten Alkali Chlorides at Charged Interfaces and the Prediction and Interpretation of Their X-ray Reflectivity. Journal of Physical Chemistry C, 0, , .	1.5	2