Vitaly V Chaban

List of Publications by Year
in descending order

81	2,582	172457	206112
papers	citations	29 h-index	48 g-index

81	81	81	2679
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	A new force field model for the simulation of transport properties of imidazolium-based ionic liquids. Physical Chemistry Chemical Physics, 2011, 13, 7910.	2.8	168
2	Polarizability versus mobility: atomistic force field for ionic liquids. Physical Chemistry Chemical Physics, 2011, 13, 16055.	2.8	149
3	Acetonitrile Boosts Conductivity of Imidazolium Ionic Liquids. Journal of Physical Chemistry B, 2012, 116, 7719-7727.	2.6	136
4	Water Boiling Inside Carbon Nanotubes: Toward Efficient Drug Release. ACS Nano, 2011, 5, 5647-5655.	14.6	108
5	Ionic and Molecular Liquids: Working Together for Robust Engineering. Journal of Physical Chemistry Letters, 2013, 4, 1423-1431.	4.6	103
6	Covalent Linking Greatly Enhances Photoinduced Electron Transfer in Fullerene-Quantum Dot Nanocomposites: Time-Domain Ab Initio Study. Journal of Physical Chemistry Letters, 2013, 4, 1-6.	4.6	90
7	Conductometric study of binary systems based on ionic liquids and acetonitrile in a wide concentration range. Electrochimica Acta, 2013, 105, 188-199.	5.2	77
8	Heat-Driven Release of a Drug Molecule from Carbon Nanotubes: A Molecular Dynamics Study. Journal of Physical Chemistry B, 2010, 114, 13481-13486.	2.6	70
9	Nanoscale Carbon Greatly Enhances Mobility of a Highly Viscous Ionic Liquid. ACS Nano, 2014, 8, 8190-8197.	14.6	65
10	Confinement by Carbon Nanotubes Drastically Alters the Boiling and Critical Behavior of Water Droplets. ACS Nano, 2012, 6, 2766-2773.	14.6	59
11	A new force field model of 1-butyl-3-methylimidazolium tetrafluoroborate ionic liquid and acetonitrile mixtures. Physical Chemistry Chemical Physics, 2011, 13, 19345.	2.8	57
12	Systematic Refinement of Canongia Lopesâ€“PÃ¡dua Force Field for Pyrrolidinium-Based Ionic Liquids. Journal of Physical Chemistry B, 2015, 119, 6242-6249.	2.6	55
13	Cellulose based poly(ionic liquids): Tuning cation-anion interaction to improve carbon dioxide sorption. Fuel, 2018, 211, 76-86.	6.4	54
14	Rationalizing the role of the anion in CO₂ capture and conversion using imidazolium-based ionic liquid modified mesoporous silica. RSC Advances, 2015, 5, 64220-64227.	3.6	53
15	A Highly Viscous Imidazolium Ionic Liquid inside Carbon Nanotubes. Journal of Physical Chemistry B, 2014, 118, 6234-6240.	2.6	50
16	Atomistic Force Field for Pyridinium-Based Ionic Liquids: Reliable Transport Properties. Journal of Physical Chemistry B, 2014, 118, 10716-10724.	2.6	50
17	Nitrogenâ€“Nitrogen Bonds Undermine Stability of N-Doped Graphene. Journal of the American Chemical Society, 2015, 137, 11688-11694.	13.7	49
18	How Toxic Are Ionic Liquid/Acetonitrile Mixtures?. Journal of Physical Chemistry Letters, 2011, 2, 2499-2503.	4.6	45

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19	The scaled-charge additive force field for amino acid based ionic liquids. Chemical Physics Letters, 2014, 616-617, 205-211.	2.6	41
20	Does the Like Dissolves Like Rule Hold for Fullerene and Ionic Liquids?. Journal of Solution Chemistry, 2014, 43, 1019-1031.	1.2	40
21	New cellulose based ionic compounds as low-cost sorbents for CO2 capture. Fuel Processing Technology, 2016, 149, 131-138.	7.2	39
22	Imidazolium Ionic Liquid Helps to Disperse Fullerenes in Water. Journal of Physical Chemistry Letters, 2014, 5, 1795-1800.	4.6	38
23	CO2 capture: Tuning cation-anion interaction in urethane based poly(ionic liquids). Polymer, 2016, 102, 199-208.	3.8	38
24	Enhanced stability of the model miniâ€protein in amino acid ionic liquids and their aqueous solutions. Journal of Computational Chemistry, 2015, 36, 2044-2051.	3.3	35
25	Anticorrosion Protection by Amineâ€“Ionic Liquid Mixtures: Experiments and Simulations. Journal of Chemical & Engineering Data, 2016, 61, 1803-1810.	1.9	35
26	Ionic Vapor: What Does It Consist Of?. Journal of Physical Chemistry Letters, 2012, 3, 1657-1662.	4.6	32
27	Competitive solvation of the imidazolium cation by water and methanol. Chemical Physics Letters, 2015, 623, 76-81.	2.6	31
28	Boron doping of grapheneâ€“pushing the limit. Nanoscale, 2016, 8, 15521-15528.	5.6	31
29	Exfoliation of Graphene in Ionic Liquids: Pyridinium versus Pyrrolidinium. Journal of Physical Chemistry C, 2017, 121, 911-917.	3.1	30
30	Ionic liquids composed of linear amphiphilic anions: Synthesis, physicochemical characterization, hydrophilicity and interaction with carbon dioxide. Journal of Molecular Liquids, 2017, 241, 64-73.	4.9	29
31	Solvation of the fluorine containing anions and their lithium salts in propylene carbonate and dimethoxyethane. Journal of Molecular Modeling, 2015, 21, 172.	1.8	28
32	The thiocyanate anion is a primary driver of carbon dioxide capture by ionic liquids. Chemical Physics Letters, 2015, 618, 89-93.	2.6	28
33	Competitive solvation of (bis)(trifluoromethanesulfonyl)imide anion by acetonitrile and water. Chemical Physics Letters, 2014, 613, 90-94.	2.6	27
34	Selective chemical binding enhances cesium tolerance in plants through inhibition of cesium uptake. Scientific Reports, 2015, 5, 8842.	3.3	27
35	Graphene exfoliation in ionic liquids: unified methodology. RSC Advances, 2015, 5, 81229-81234.	3.6	26
36	Graphene/ionic liquid ultracapacitors: does ionic size correlate with energy storage performance?. New Journal of Chemistry, 2018, 42, 18409-18417.	2.8	26

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37	Distribution of Neutral Lipids in the Lipid Droplet Core. Journal of Physical Chemistry B, 2014, 118, 11145-11151.	2.6	24
38	Hydrogen fluoride capture by imidazolium acetate ionic liquid. Chemical Physics Letters, 2015, 625, 110-115.	2.6	24
39	The tricyanomethanide anion favors low viscosity of the pure ionic liquid and its aqueous mixtures. Physical Chemistry Chemical Physics, 2015, 17, 31839-31849.	2.8	24
40	Ionic Clusters vs Shear Viscosity in Aqueous Amino Acid Ionic Liquids. Journal of Physical Chemistry B, 2015, 119, 3824-3828.	2.6	23
41	Synergistic Amination of Graphene: Molecular Dynamics and Thermodynamics. Journal of Physical Chemistry Letters, 2015, 6, 4397-4403.	4.6	23
42	Lipid Structure in Triolein Lipid Droplets. Journal of Physical Chemistry B, 2014, 118, 10335-10340.	2.6	22
43	Global minimum search via annealing: Nanoscale gold clusters. Chemical Physics Letters, 2015, 622, 75-79.	2.6	21
44	Energy Storage in Cubane Derivatives and Their Real-Time Decomposition: Computational Molecular Dynamics and Thermodynamics. ACS Energy Letters, 2016, 1, 189-194.	17.4	21
45	Binary mixtures of novel sulfoxides and water: intermolecular structure, dynamic properties, thermodynamics, and cluster analysis. Physical Chemistry Chemical Physics, 2018, 20, 23754-23761.	2.8	20
46	Force field development and simulations of senior dialkyl sulfoxides. Physical Chemistry Chemical Physics, 2016, 18, 10507-10515.	2.8	19
47	Annealing relaxation of ultrasmall gold nanostructures. Chemical Physics Letters, 2015, 618, 46-50.	2.6	17
48	Computationally Efficient Prediction of Ionic Liquid Properties. Journal of Physical Chemistry Letters, 2014, 5, 1973-1977.	4.6	16
49	Electronic and thermodynamic properties of the amino- and carboxamido-functionalized C-60-based fullerenes: Towards non-volatile carbon dioxide scavengers. Journal of Chemical Thermodynamics, 2018, 116, 1-6.	2.0	15
50	DEVELOPMENT OF INEXPENSIVE CELLULOSE-BASED SORBENTS FOR CARBON DIOXIDE. Brazilian Journal of Chemical Engineering, 2019, 36, 511-521.	1.3	15
51	Protein remains stable at unusually high temperatures when solvated in aqueous mixtures of amino acid based ionic liquids. Journal of Molecular Modeling, 2016, 22, 258.	1.8	14
52	Performance of supported metal catalysts in the dimethyl carbonate production by direct synthesis using CO2 and methanol. Journal of CO2 Utilization, 2021, 53, 101721.	6.8	14
53	Novel Ultrathin Membranes Composed of Organic Ions. Journal of Physical Chemistry Letters, 2013, 4, 1216-1220.	4.6	13
54	Polarization versus Temperature in Pyridinium Ionic Liquids. Journal of Physical Chemistry B, 2014, 118, 13940-13945.	2.6	13

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55	The force field for imidazolium-based ionic liquids: Novel anions with polar residues. Chemical Physics Letters, 2015, 633, 132-138.	2.6	13
56	Amino-functionalized ionic liquids as carbon dioxide scavengers. Ab initio thermodynamics for chemisorption. Journal of Chemical Thermodynamics, 2016, 103, 1-6.	2.0	13
57	Structure and Supersaturation of Highly Concentrated Solutions of Buckyball in 1-Butyl-3-Methylimidazolium Tetrafluoroborate. Journal of Physical Chemistry B, 2014, 118, 7376-7382.	2.6	12
58	Water Phase Diagram Is Significantly Altered by Imidazolium Ionic Liquid. Journal of Physical Chemistry Letters, 2014, 5, 1623-1627.	4.6	11
59	Electrostatic charge confinement using bulky tetraoctylammonium cation and four anions. Chemical Physics Letters, 2016, 649, 44-47.	2.6	11
60	Amination of Five Families of Room-Temperature Ionic Liquids: Computational Thermodynamics and Vibrational Spectroscopy. Journal of Chemical & Engineering Data, 2016, 61, 1917-1923.	1.9	11
61	Peculiar Aqueous Solubility Trend in Cucurbiturils Unraveled by Atomistic Simulations. Journal of Physical Chemistry B, 2016, 120, 7511-7516.	2.6	11
62	Ammonium-, phosphonium- and sulfonium-based 2-cyanopyrrolidine ionic liquids for carbon dioxide fixation. Physical Chemistry Chemical Physics, 2022, 24, 9659-9672.	2.8	11
63	Carbon Dioxide Chemisorption by Ammonium and Phosphonium Ionic Liquids: Quantum Chemistry Calculations. Journal of Physical Chemistry B, 2022, 126, 5497-5506.	2.6	10
64	Are Fluorination and Chlorination of Morpholinium-Based Ionic Liquids Favorable?. Journal of Physical Chemistry B, 2015, 119, 9920-9924.	2.6	9
65	Understanding weakly coordinating anions: tetrakis(pentafluorophenyl)borate paired with inorganic and organic cations. Journal of Molecular Modeling, 2017, 23, 86.	1.8	9
66	Structure, thermodynamic and electronic properties of carbon-nitrogen cubanes and protonated polynitrogen cations. Journal of Molecular Structure, 2017, 1149, 828-834.	3.6	9
67	A Weakly Coordinating Anion Substantially Enhances Carbon Dioxide Fixation by Calcium and Barium Salts. Energy & Fuels, 2017, 31, 9668-9674.	5.1	9
68	Mutual miscibility of diethyl sulfoxide and acetonitrile: Fundamental origin. Journal of Molecular Liquids, 2022, 349, 118110.	4.9	9
69	A new model of chemical bonding in ionic melts. Journal of Chemical Physics, 2012, 136, 164112.	3.0	8
70	Sodium-ion electrolytes based on ionic liquids: a role of cation-anion hydrogen bonding. Journal of Molecular Modeling, 2016, 22, 172.	1.8	8
71	Epoxy resinâ€cement paste composite for wellbores: Evaluation of chemical degradation fostered carbon dioxide. , 2017, 7, 1065-1079.		8
72	The Phenomenological Account for Electronic Polarization in Ionic Liquid. ECS Transactions, 2010, 33, 43-55.	0.5	7

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73	Triethylsulfonium-based ionic liquids enforce lithium salt electrolytes. Physical Chemistry Chemical Physics, 2022, 24, 9418-9431.	2.8	7
74	Diethyl sulfoxide as a novel neutral ligand in the platinum complex compound. Computational and Theoretical Chemistry, 2022, 1211, 113683.	2.5	7
75	Vapor-liquid interface properties of diethyl sulfoxide-water and ethyl methyl sulfoxide-water mixtures: Molecular dynamics simulations and quantum-chemical calculations. Fluid Phase Equilibria, 2016, 427, 180-186.	2.5	6
76	Transport Properties and Ion Aggregation in Mixtures of Room Temperature Ionic Liquids with Aprotic Dipolar Solvents. Springer Proceedings in Physics, 2018, , 67-109.	0.2	6
77	Mixtures of Diethyl Sulfoxide and Methanol: Structure and Thermodynamics. Journal of Solution Chemistry, 2022, 51, 788-801.	1.2	6
78	Vaporâ€“liquid equilibria in the binary mixtures of N-butylpyridinium hexafluorophophate and bis(trifluoromethanesulfonyl)imide ionic liquids with acetone: Molecular dynamics simulations. Fluid Phase Equilibria, 2016, 419, 75-83.	2.5	4
79	Solvation of the morpholinium cation in acetonitrile. Effect of an anion. Journal of Molecular Modeling, 2016, 22, 26.	1.8	4
80	Ionization of cucurbiturils as a pathway to more stable hostâ€“guest complexes. Computational and Theoretical Chemistry, 2016, 1083, 7-11.	2.5	4
81	Halogenation of imidazolium-based ionic liquids: Thermodynamic perspective. Journal of Chemical Thermodynamics, 2016, 98, 81-85.	2.0	2