

Marina V Fedotova

List of Publications by Year in descending order

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33
papers

691
citations

430874

18
h-index

552781

26
g-index

34
all docs

34
docs citations

34
times ranked

551
citing authors

#	ARTICLE	IF	CITATIONS
1	Hydration and Ion Binding of the Osmolyte Ectoine. Journal of Physical Chemistry B, 2015, 119, 15203-15211.	2.6	64
2	Hydration of acetic acid and acetate ion in water studied by 1D-RISM theory. Journal of Molecular Liquids, 2011, 164, 201-206.	4.9	52
3	Mobility and association of ions in aqueous solutions: the case of imidazolium based ionic liquids. Physical Chemistry Chemical Physics, 2016, 18, 28594-28605.	2.8	47
4	Ion-binding of glycine zwitterion with inorganic ions in biologically relevant aqueous electrolyte solutions. Biophysical Chemistry, 2014, 190-191, 25-31.	2.8	38
5	Compatible osmolytes - bioprotectants: Is there a common link between their hydration and their protective action under abiotic stresses?. Journal of Molecular Liquids, 2019, 292, 111339.	4.9	32
6	Integral Equation Theory of Molecular Solvation Coupled with Quantum Mechanical/Molecular Mechanics Method in NWChem Package. Journal of Chemical Theory and Computation, 2012, 8, 1246-1254.	5.3	31
7	1D-RISM study of glycine zwitterion hydration and ion-molecular complex formation in aqueous NaCl solutions. Journal of Molecular Liquids, 2012, 169, 1-7.	4.9	28
8	Hydration structure of osmolyte TMAO: concentration/pressure-induced response. New Journal of Chemistry, 2017, 41, 1219-1228.	2.8	28
9	Effect of temperature and pressure on structural self-organization of aqueous sodium chloride solutions. Journal of Molecular Liquids, 2010, 153, 9-14.	4.9	26
10	Hydration and ion-binding of glycine betaine: How they may be involved into protection of proteins under abiotic stresses. Journal of Molecular Liquids, 2017, 244, 489-498.	4.9	26
11	Proline hydration at low temperatures: its role in the protection of cell from freeze-induced stress. Amino Acids, 2016, 48, 1685-1694.	2.7	25
12	Ion-selective interactions of biologically relevant inorganic ions with alanine zwitterion: a 3D-RISM study. Amino Acids, 2015, 47, 1015-1023.	2.7	24
13	Hydration and ion association of aqueous choline chloride and chlorocholine chloride. Physical Chemistry Chemical Physics, 2019, 21, 10970-10980.	2.8	24
14	Hydration of para-aminobenzoic acid (PABA) and its anion—The view from statistical mechanics. Journal of Molecular Liquids, 2013, 186, 90-97.	4.9	23
15	Evidence for cooperative Na ⁺ and Cl ⁻ binding by strongly hydrated L-proline. Physical Chemistry Chemical Physics, 2017, 19, 20474-20483.	2.8	23
16	Structural features of concentrated aqueous NaCl solution in the sub- and supercritical state at different densities. Journal of Molecular Liquids, 2008, 143, 35-41.	4.9	20
17	The hydration of aniline and benzoic acid: Analysis of radial and spatial distribution functions. Journal of Molecular Liquids, 2013, 179, 27-33.	4.9	20
18	Features of local ordering of biocompatible ionic liquids: The case of choline-based amino acid ionic liquids. Journal of Molecular Liquids, 2019, 296, 112081.	4.9	20

#	ARTICLE	IF	CITATIONS
19	Local ion hydration structure in aqueous imidazolium-based ionic liquids: The effects of concentration and anion nature. <i>Journal of Molecular Liquids</i> , 2017, 247, 100-108.	4.9	19
20	Hydration features of the neurotransmitter acetylcholine. <i>Journal of Molecular Liquids</i> , 2020, 304, 112757.	4.9	17
21	Characterization of selective binding of biologically relevant inorganic ions with the proline zwitterion by 3D-RISM theory. <i>New Journal of Chemistry</i> , 2015, 39, 8594-8601.	2.8	16
22	Specific and nonspecific effects of biologically active inorganic salts on inclusion complex formation of cyclodextrins with aromatic carboxylic acids. <i>Chemical Engineering Science</i> , 2015, 122, 97-103.	3.8	14
23	Hydration and dynamics of L-glutamate ion in aqueous solution. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 1590-1600.	2.8	14
24	Chemical bond effects in classical site density functional theory of inhomogeneous molecular liquids. <i>Journal of Chemical Physics</i> , 2020, 152, 041101.	3.0	10
25	Ion Pairing of the Neurotransmitters Acetylcholine and Glutamate in Aqueous Solutions. <i>Journal of Physical Chemistry B</i> , 2021, 125, 11219-11231.	2.6	9
26	Molecular insight on ion hydration and association in aqueous choline chloride solutions. <i>Journal of Molecular Liquids</i> , 2020, 313, 113563.	4.9	8
27	Renormalized site density functional theory. <i>Journal of Statistical Mechanics: Theory and Experiment</i> , 2021, 2021, 033205.	2.3	7
28	Renormalized site density functional theory for models of ion hydration. <i>Journal of Chemical Physics</i> , 2021, 155, 064501.	3.0	6
29	CDFTPY: A python package for performing classical density functional theory calculations for molecular liquids. <i>Computer Physics Communications</i> , 2022, 276, 108338.	7.5	6
30	Site Density Functional Theory and Structural Bioinformatics Analysis of the SARS-CoV Spike Protein and hACE2 Complex. <i>Molecules</i> , 2022, 27, 799.	3.8	5
31	Temperature and density effects on structural features of a dilute aqueous lithium chloride solution at near- and supercritical conditions. <i>Journal of Molecular Liquids</i> , 2011, 164, 39-43.	4.9	4
32	Hydration and counterion binding of aqueous acetylcholine chloride and carbamoylcholine chloride. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 25086-25096.	2.8	2
33	Electron π electron attraction caused by dispersion forces in metal π ammonia solutions. <i>Chemical Physics Letters</i> , 2013, 556, 138-141.	2.6	1