

# Marina V Fedotova

## List of Publications by Year in descending order

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33  
papers

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citations

430874

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552781

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docs citations

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times ranked

551  
citing authors

#	ARTICLE	IF	CITATIONS
1	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
2	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
3	Hydration and dynamics of $\text{Ca}^{2+}$ -glutamate ion in aqueous solution. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 1590-1600.	2.8	14
4	Renormalized site density functional theory. <i>Journal of Statistical Mechanics: Theory and Experiment</i> , 2021, 2021, 033205.	2.3	7
5	Renormalized site density functional theory for models of ion hydration. <i>Journal of Chemical Physics</i> , 2021, 155, 064501.	3.0	6
6	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
7	Hydration and counterion binding of aqueous acetylcholine chloride and carbamoylcholine chloride. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 25086-25096.	2.8	2
8	Molecular insight on ion hydration and association in aqueous choline chloride solutions. <i>Journal of Molecular Liquids</i> , 2020, 313, 113563.	4.9	8
9	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
10	Hydration features of the neurotransmitter acetylcholine. <i>Journal of Molecular Liquids</i> , 2020, 304, 112757.	4.9	17
11	Compatible osmolytes - bioprotectants: Is there a common link between their hydration and their protective action under abiotic stresses?. <i>Journal of Molecular Liquids</i> , 2019, 292, 111339.	4.9	32
12	Hydration and ion association of aqueous choline chloride and chlorocholine chloride. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 10970-10980.	2.8	24
13	Features of local ordering of biocompatible ionic liquids: The case of choline-based amino acid ionic liquids. <i>Journal of Molecular Liquids</i> , 2019, 296, 112081.	4.9	20
14	Hydration structure of osmolyte TMAO: concentration/pressure-induced response. <i>New Journal of Chemistry</i> , 2017, 41, 1219-1228.	2.8	28
15	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
16	Hydration and ion-binding of glycine betaine: How they may be involved into protection of proteins under abiotic stresses. <i>Journal of Molecular Liquids</i> , 2017, 244, 489-498.	4.9	26
17	Evidence for cooperative $\text{Na}^{+}$ and $\text{Cl}^{-}$ binding by strongly hydrated $\text{Ca}^{2+}$ -proline. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 20474-20483.	2.8	23
18	Proline hydration at low temperatures: its role in the protection of cell from freeze-induced stress. <i>Amino Acids</i> , 2016, 48, 1685-1694.	2.7	25

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19	Mobility and association of ions in aqueous solutions: the case of imidazolium based ionic liquids. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 28594-28605.	2.8	47
20	Hydration and Ion Binding of the Osmolyte Ectoine. <i>Journal of Physical Chemistry B</i> , 2015, 119, 15203-15211.	2.6	64
21	Ion-selective interactions of biologically relevant inorganic ions with alanine zwitterion: a 3D-RISM study. <i>Amino Acids</i> , 2015, 47, 1015-1023.	2.7	24
22	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
23	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
24	Ion-binding of glycine zwitterion with inorganic ions in biologically relevant aqueous electrolyte solutions. <i>Biophysical Chemistry</i> , 2014, 190-191, 25-31.	2.8	38
25	The hydration of aniline and benzoic acid: Analysis of radial and spatial distribution functions. <i>Journal of Molecular Liquids</i> , 2013, 179, 27-33.	4.9	20
26	Electron-electron attraction caused by dispersion forces in metal-ammonia solutions. <i>Chemical Physics Letters</i> , 2013, 556, 138-141.	2.6	1
27	Hydration of para-aminobenzoic acid (PABA) and its anion-The view from statistical mechanics. <i>Journal of Molecular Liquids</i> , 2013, 186, 90-97.	4.9	23
28	Integral Equation Theory of Molecular Solvation Coupled with Quantum Mechanical/Molecular Mechanics Method in NWChem Package. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 1246-1254.	5.3	31
29	1D-RISM study of glycine zwitterion hydration and ion-molecular complex formation in aqueous NaCl solutions. <i>Journal of Molecular Liquids</i> , 2012, 169, 1-7.	4.9	28
30	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
31	Hydration of acetic acid and acetate ion in water studied by 1D-RISM theory. <i>Journal of Molecular Liquids</i> , 2011, 164, 201-206.	4.9	52
32	Effect of temperature and pressure on structural self-organization of aqueous sodium chloride solutions. <i>Journal of Molecular Liquids</i> , 2010, 153, 9-14.	4.9	26
33	Structural features of concentrated aqueous NaCl solution in the sub- and supercritical state at different densities. <i>Journal of Molecular Liquids</i> , 2008, 143, 35-41.	4.9	20