Maxim V Fedorov

List of Publications by Year
in descending order

81	4,846	126907 33	95266 68
papers	citations	h-index	g-index

91	91	91	4799
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Image2SMILES: Transformerâ€Based Molecular Optical Recognition Engine**. Chemistry Methods, 2022, 2, .	3.8	15
2	Transformer-based artificial neural networks for the conversion between chemical notations. Scientific Reports, 2021, 11, 14798.	3.3	8
3	How risky is it to visit a supermarket during the pandemic?. PLoS ONE, 2021, 16, e0253835.	2.5	6
4	Exploring Chemical Reaction Space with Reaction Difference Fingerprints and Parametric t-SNE. ACS Omega, 2021, 6, 30743-30751.	3.5	12
5	Enabling Precision Agriculture Through Embedded Sensing With Artificial Intelligence. IEEE Transactions on Instrumentation and Measurement, 2020, 69, 4103-4113.	4.7	69
6	Baseline Model for Predicting Proteinâ€“Ligand Unbinding Kinetics through Machine Learning. Journal of Chemical Information and Modeling, 2020, 60, 5946-5956.	5.4	15
7	Machine learning to predict retention time of small molecules in nano-HPLC. Analytical and Bioanalytical Chemistry, 2020, 412, 7767-7776.	3.7	26
8	Optical Mapping-Validated Machine Learning Improves Atrial Fibrillation Driver Detection by Multi-Electrode Mapping. Circulation: Arrhythmia and Electrophysiology, 2020, 13, e008249.	4.8	21
9	Grapheneâ€“Ionic Liquid Interfacial Potential Drop from Density Functional Theory-Based Molecular Dynamics Simulations. Journal of Physical Chemistry C, 2020, 124, 19548-19555.	3.1	24
10	Recommender Systems in Antiviral Drug Discovery. ACS Omega, 2020, 5, 15039-15051.	3.5	14
11	Artificial intelligence models to predict acute phytotoxicity in petroleum contaminated soils. Ecotoxicology and Environmental Safety, 2020, 194, 110410.	6.0	17
12	graphDelta: MPNN Scoring Function for the Affinity Prediction of Proteinâ€“Ligand Complexes. ACS Omega, 2020, 5, 5150-5159.	3.5	58
13	Multisolvent Models for Solvation Free Energy Predictions Using 3D-RISM Hydration Thermodynamic Descriptors. Journal of Chemical Information and Modeling, 2020, 60, 2977-2988.	5.4	9
14	Deep Learning for Non-invasive Cortical Potential Imaging. Lecture Notes in Computer Science, 2020, , 45-55.	1.3	7
15	FEM-based Scalp-to-Cortex EEG data mapping via the solution of the Cauchy problem. Journal of Inverse and Ill-Posed Problems, 2020, 28, 517-532.	1.0	6
16	Mechanisms of Surface Charge Modification of Carbonates in Aqueous Electrolyte Solutions. Colloids and Interfaces, 2019, 3, 62.	2.1	57
17	â€œZhoresâ€•â€” Petaflops supercomputer for data-driven modeling, machine learning and artificial intelligence installed in Skolkovo Institute of Science and Technology. Open Engineering, 2019, 9, 512-520.	1.6	148
18	Chemical space exploration guided by deep neural networks. RSC Advances, 2019, 9, 5151-5157.	3.6	33

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19	Comparative Study of Multitask Toxicity Modeling on a Broad Chemical Space. Journal of Chemical Information and Modeling, 2019, 59, 1062-1072.	5.4	63
20	A Survey of Multiâ€task Learning Methods in Chemoinformatics. Molecular Informatics, 2019, 38, e1800108.	2.5	57
21	Interfacial structure and structural forces in mixtures of ionic liquid with a polar solvent. Faraday Discussions, 2018, 206, 427-442.	3.2	40
22	NaRIBaSâ€"A Scripting Framework for Computational Modeling of Nanomaterials and Room Temperature Ionic Liquids in Bulk and Slab. Computation, 2018, 6, 57.	2.0	7
23	3D matters! 3D-RISM and 3D convolutional neural network for accurate bioaccumulation prediction. Journal of Physics Condensed Matter, 2018, 30, 32LT03.	1.8	16
24	The nanostructure of a lithium glyme solvate ionic liquid at electrified interfaces. Physical Chemistry Chemical Physics, 2017, 19, 11004-11010.	2.8	27
25	Molecular dynamics simulation of the structure and interfacial free energy barriers of mixtures of ionic liquids and divalent salts near a graphene wall. Physical Chemistry Chemical Physics, 2017, 19, 846-853.	2.8	33
26	Salting-out effects by pressure-corrected 3D-RISM. Journal of Chemical Physics, 2016, 145, 194501.	3.0	14
27	Biopolymer-based hydrogels for encapsulation of photocatalytic TiO 2 nanoparticles prepared by the freezing/thawing method. Journal of Molecular Liquids, 2016, 223, 16-20.	4.9	25
28	Quantifying mineral surface energy by scanning force microscopy. Journal of Colloid and Interface Science, 2016, 472, 237-246.	9.4	21
29	Predicting Solvation Free Energies Using Parameter-Free Solvent Models. Journal of Physical Chemistry B, 2016, 120, 5724-5731.	2.6	30
30	Hydration Free Energies of Molecular Ions from Theory and Simulation. Journal of Physical Chemistry B, 2016, 120, 975-983.	2.6	63
31	Self-interaction error in DFT-based modelling of ionic liquids. Physical Chemistry Chemical Physics, 2016, 18, 2175-2182.	2.8	20
32	Molecular origin of high free energy barriers for alkali metal ion transfer through ionic liquidâ€"graphene electrode interfaces. Physical Chemistry Chemical Physics, 2016, 18, 1302-1310.	2.8	39
33	Molecular dynamics simulations of the structure and single-particle dynamics of mixtures of divalent salts and ionic liquids. Journal of Chemical Physics, 2015, 143, 124507.	3.0	17
34	Solvation Thermodynamics of Organic Molecules by the Molecular Integral Equation Theory: Approaching Chemical Accuracy. Chemical Reviews, 2015, 115, 6312-6356.	47.7	166
35	Communication: Accurate hydration free energies at a wide range of temperatures from 3D-RISM. Journal of Chemical Physics, 2015, 142, 091105.	3.0	60
36	Fast and General Method To Predict the Physicochemical Properties of Druglike Molecules Using the Integral Equation Theory of Molecular Liquids. Molecular Pharmaceutics, 2015, 12, 3420-3432.	4.6	22

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37	Ionic Liquids at Electrified Interfaces. Chemical Reviews, 2014, 114, 2978-3036.	47.7	1,101
38	Dynamic and Static Characteristics of Drug Dissolution in Supercritical CO₂ by Infrared Spectroscopy: Measurements of Acetaminophen Solubility in a Wide Range of State Parameters. Journal of Chemical & Engineering Data, 2014, 59, 3517-3523.	1.9	28
39	Influence of the Drude charge value on the performance of polarisable water model: A test for microscopic and macroscopic parameters. Journal of Molecular Liquids, 2013, 188, 245-251.	4.9	2
40	Î±-Cyclodextrin/aminobenzoic acid binding in salt solutions at different pH: Dependence on guest structure. International Journal of Biological Macromolecules, 2013, 57, 255-258.	7.5	7
41	Solvent Binding Analysis and Computational Alanine Scanning of the Bovine Chymosinâ€“Bovine Îº-Casein Complex Using Molecular Integral Equation Theory. Journal of Chemical Theory and Computation, 2013, 9, 5706-5717.	5.3	11
42	3DRISM Multigrid Algorithm for Fast Solvation Free Energy Calculations. Journal of Chemical Theory and Computation, 2012, 8, 2062-2070.	5.3	25
43	Molecular mechanisms of salt effects on carbon nanotube dispersions in an organic solvent (N-methyl-2-pyrrolidone). Chemical Science, 2012, 3, 541-548.	7.4	28
44	Molecular-scale insights into the mechanisms of ionic liquids interactions with carbon nanotubes. Faraday Discussions, 2012, 154, 235-247.	3.2	70
45	First-Principles Calculation of the Intrinsic Aqueous Solubility of Crystalline Druglike Molecules. Journal of Chemical Theory and Computation, 2012, 8, 3322-3337.	5.3	84
46	Probing the neutral grapheneâ€“ionic liquid interface: insights from molecular dynamics simulations. Physical Chemistry Chemical Physics, 2012, 14, 2552.	2.8	112
47	Molecular Sinkers: X-ray Photoemission and Atomistic Simulations of Benzoic Acid and Benzoate at the Aqueous Solution/Vapor Interface. Journal of Physical Chemistry B, 2012, 116, 13017-13023.	2.6	19
48	Influence of the structure of carbon onions on their electrochemical performance in supercapacitor electrodes. Carbon, 2012, 50, 3298-3309.	10.3	218
49	Self-assembly of trehalose molecules on a lysozyme surface: the broken glass hypothesis. Physical Chemistry Chemical Physics, 2011, 13, 2294-2299.	2.8	49
50	Salting out in organic solvents: a new route to carbon nanotube bundle engineering. Physical Chemistry Chemical Physics, 2011, 13, 12399.	2.8	13
51	Hydration Thermodynamics Using the Reference Interaction Site Model: Speed or Accuracy?. Journal of Physical Chemistry B, 2011, 115, 6011-6022.	2.6	57
52	Toward a Universal Model To Calculate the Solvation Thermodynamics of Druglike Molecules: The Importance of New Experimental Databases. Molecular Pharmaceutics, 2011, 8, 1423-1429.	4.6	38
53	On a relationship between molecular polarizability and partial molar volume in water. Journal of Chemical Physics, 2011, 135, 244109.	3.0	14
54	In Silico Screening of Bioactive and Biomimetic Solutes Using Molecular Integral Equation Theory. Current Pharmaceutical Design, 2011, 17, 1695-1708.	1.9	20

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55	Combination of RISM and Cheminformatics for Efficient Predictions of Hydration Free Energy of Polyfragment Molecules: Application to a Set of Organic Pollutants. Journal of Chemical Theory and Computation, 2011, 7, 1450-1457.	5.3	22
56	Multigrid solver for the reference interaction site model of molecular liquids theory. Journal of Computational Chemistry, 2011, 32, 1982-1992.	3.3	19
57	An Accurate Prediction of Hydration Free Energies by Combination of Molecular Integral Equations Theory with Structural Descriptors. Journal of Physical Chemistry B, 2010, 114, 12068-12079.	2.6	74
58	Ion Interactions with the Carbon Nanotube Surface in Aqueous Solutions: Understanding the Molecular Mechanisms. ChemPhysChem, 2010, 11, 2612-2616.	2.1	40
59	End-point calculation of solvation free energy of amino-acid analogs by molecular theories of solution. Chemical Physics Letters, 2010, 496, 351-355.	2.6	71
60	Accurate calculations of the hydration free energies of druglike molecules using the reference interaction site model. Journal of Chemical Physics, 2010, 133, 044104.	3.0	44
61	Global Energy Matching Method for Atomistic-to-Continuum Modeling of Self-Assembling Biopolymer Aggregates. Multiscale Modeling and Simulation, 2010, 8, 1958-1980.	1.6	4
62	Selective Na⁺/K⁺ Effects on the Formation of Î±-Cyclodextrin Complexes with Aromatic Carboxylic Acids: Competition for the Guest. Journal of Physical Chemistry B, 2010, 114, 12607-12613.	2.6	31
63	Towards a universal method for calculating hydration free energies: a 3D reference interaction site model with partial molar volume correction. Journal of Physics Condensed Matter, 2010, 22, 492101.	1.8	109
64	Conformational changes of trialanine in sodium halide solutions: An in silico study. Journal of Molecular Liquids, 2009, 147, 117-123.	4.9	11
65	Reference interaction site model study of self-aggregating cyanine dyes. Journal of Chemical Physics, 2009, 131, 074503.	3.0	29
66	The effect of sodium chloride on poly-l-glutamate conformation. Chemical Communications, 2009, , 896-898.	4.1	26
67	To Switch or Not To Switch: The Effects of Potassium and Sodium Ions on Î±-Poly-l-glutamate Conformations in Aqueous Solutions. Journal of the American Chemical Society, 2009, 131, 10854-10856.	13.7	51
68	Hydration of ionic species studied by the reference interaction site model with a repulsive bridge correction. Journal of Computational Chemistry, 2008, 29, 2406-2415.	3.3	38
69	Towards understanding the structure and capacitance of electrical double layer in ionic liquids. Electrochimica Acta, 2008, 53, 6835-6840.	5.2	378
70	Ionic Liquid Near a Charged Wall: Structure and Capacitance of Electrical Double Layer. Journal of Physical Chemistry B, 2008, 112, 11868-11872.	2.6	383
71	Structural transitions in model Î²-sheet tapes. Journal of Chemical Physics, 2008, 128, 195105.	3.0	12
72	Solvent effects and hydration of a tripeptide in sodium halide aqueous solutions: an in silico study. Physical Chemistry Chemical Physics, 2007, 9, 5423.	2.8	36

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73	Unravelling the solvent response to neutral and charged solutes. Molecular Physics, 2007, 105, 1-16.	1.7	98
74	Improved estimates for hydration free energy obtained by the reference interaction site model. Chemical Physics Letters, 2007, 448, 198-202.	2.6	94
75	Molecular dynamics study of structural properties of -sheet assemblies formed by synthetic de novo oligopeptides. Physica A: Statistical Mechanics and Its Applications, 2007, 373, 455-476.	2.6	12
76	Solvent Effects and Conformational Stability of a Tripeptide. Lecture Notes in Computer Science, 2006, , 141-149.	1.3	1
77	Density functional study of fluorocarbon emulsions with adsorbed polymer surfactant. Journal of Molecular Liquids, 2005, 120, 155-157.	4.9	9
78	Wavelet method for solving integral equations of simple liquids. Journal of Molecular Liquids, 2005, 120, 159-162.	4.9	13
79	Structure and stability of chiral Î²-tapes: A computational coarse-grained approach. Journal of Chemical Physics, 2005, 122, 134901.	3.0	13
80	Wavelet algorithm for solving integral equations of molecular liquids. A test for the reference interaction site model. Journal of Computational Chemistry, 2004, 25, 1369-1377.	3.3	45
81	Density functional study of polarons and bipolarons in polar liquids. Physical Review B, 2003, 67, .	3.2	13