Alexey V Onufriev

List of Publications by Citations

80 papers	14,537 citations	35 h-index	107 g-index
107 ext. papers	16,767 ext. citations	4.5 avg, IF	6.52 L-index

#	Paper	IF	Citations
80	The Amber biomolecular simulation programs. *Journal of Computational Chemistry*, **2005**, 26, 1668-88	3.5	6155
79	Exploring protein native states and large-scale conformational changes with a modified generalized born model. *Proteins: Structure, Function and Bioinformatics*, **2004**, 55, 383-94	4.2	1728
78	H++: a server for estimating pKas and adding missing hydrogens to macromolecules. *Nucleic Acids Research*, **2005**, 33, W368-71	20.1	967
77	H++ 3.0: automating pK prediction and the preparation of biomolecular structures for atomistic molecular modeling and simulations. *Nucleic Acids Research*, **2012**, 40, W537-41	20.1	876
76	Modification of the Generalized Born Model Suitable for Macromolecules. *Journal of Physical Chemistry B*, **2000**, 104, 3712-3720	3.4	830
75	Performance comparison of generalized born and Poisson methods in the calculation of electrostatic solvation energies for protein structures. *Journal of Computational Chemistry*, **2004**, 25, 265-84	3.5	465
74	Effective Born radii in the generalized Born approximation: the importance of being perfect. *Journal of Computational Chemistry*, **2002**, 23, 1297-304	3.5	364
73	Building Water Models: A Different Approach. *Journal of Physical Chemistry Letters*, **2014**, 5, 3863-3871	6.4	321
72	Generalized Born model with a simple, robust molecular volume correction. *Journal of Chemical Theory and Computation*, **2007**, 3, 156-169	6.4	267
71	A simple clustering algorithm can be accurate enough for use in calculations of pKs in macromolecules. *Proteins: Structure, Function and Bioinformatics*, **2006**, 63, 928-38	4.2	204
70	A novel view of pH titration in biomolecules. *Biochemistry*, **2001**, 40, 3413-9	3.2	169
69	Atomic level computational identification of ligand migration pathways between solvent and binding site in myoglobin. *Proceedings of the National Academy of Sciences of the United States of America*, **2008**, 105, 9204-9	11.5	132
68	Speed of conformational change: comparing explicit and implicit solvent molecular dynamics simulations. *Biophysical Journal*, **2015**, 108, 1153-64	2.9	109
67	Protonation and pK changes in protein-ligand binding. *Quarterly Reviews of Biophysics*, **2013**, 46, 181-209	7	109
66	Accuracy limit of rigid 3-point water models. *Journal of Chemical Physics*, **2016**, 145, 074501	3.9	106
65	Analytical electrostatics for biomolecules: beyond the generalized Born approximation. *Journal of Chemical Physics*, **2006**, 124, 124902	3.9	90
64	Water models for biomolecular simulations. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2018**, 8, e1347	7.9	84

63	Incorporating variable dielectric environments into the generalized Born model. *Journal of Chemical Physics*, **2005**, 122, 094511	3.9	69
62	Generalized Born Implicit Solvent Models for Biomolecules. *Annual Review of Biophysics*, **2019**, 48, 275-296	26.1	68
61	Charge hydration asymmetry: the basic principle and how to use it to test and improve water models. *Journal of Physical Chemistry B*, **2012**, 116, 9776-83	3.4	68
60	A computational study of nucleosomal DNA flexibility. *Biophysical Journal*, **2006**, 91, 4121-32	2.9	65
59	Implicit Solvent Models in Molecular Dynamics Simulations: A Brief Overview. *Annual Reports in Computational Chemistry*, **2008**, 4, 125-137	1.8	63
58	Proton affinity changes driving unidirectional proton transport in the bacteriorhodopsin photocycle. *Journal of Molecular Biology*, **2003**, 332, 1183-93	6.5	59
57	Charge state of the globular histone core controls stability of the nucleosome. *Biophysical Journal*, **2010**, 99, 1577-85	2.9	54
56	General Purpose Water Model Can Improve Atomistic Simulations of Intrinsically Disordered Proteins. *Journal of Chemical Theory and Computation*, **2019**, 15, 2620-2634	6.4	52
55	Why double-stranded RNA resists condensation. *Nucleic Acids Research*, **2014**, 42, 10823-31	20.1	50
54	Structural details, pathways, and energetics of unfolding apomyoglobin. *Journal of Molecular Biology*, **2003**, 325, 555-67	6.5	50
53	Modulation of nucleosomal DNA accessibility via charge-altering post-translational modifications in histone core. *Epigenetics and Chromatin*, **2018**, 11, 11	5.8	48
52	Analysis of integral expressions for effective Born radii. *Journal of Chemical Physics*, **2007**, 127, 185101	3.9	48
51	Reducing the Secondary Structure Bias in the Generalized Born Model via R6 Effective Radii. *Journal of Chemical Theory and Computation*, **2010**, 6, 3613-3630	6.4	44
50	Spermine Condenses DNA, but Not RNA Duplexes. *Biophysical Journal*, **2017**, 112, 22-30	2.9	38
49	Statistics and physical origins of pK and ionization state changes upon protein-ligand binding. *Biophysical Journal*, **2010**, 98, 872-80	2.9	38
48	Analysis of basic clustering algorithms for numerical estimation of statistical averages in biomolecules. *Journal of Computational Biology*, **2008**, 15, 165-84	1.7	38
47	Opposing Effects of Multivalent Ions on the Flexibility of DNA and RNA. *Physical Review Letters*, **2016**, 117, 028101	7.4	37
46	Heat conductivity of DNA double helix. *Physical Review B*, **2011**, 83,	3.3	37

45	Partially Assembled Nucleosome Structures at Atomic Detail. *Biophysical Journal*, **2017**, 112, 460-472	2.9	34
44	Modeling of flap endonuclease interactions with DNA substrate. *Journal of Molecular Biology*, **2003**, 328, 537-54	6.5	34
43	Introducing Charge Hydration Asymmetry into the Generalized Born Model. *Journal of Chemical Theory and Computation*, **2014**, 10, 1788-1794	6.4	27
42	Efficient Computation of the Total Solvation Energy of Small Molecules via the R6 Generalized Born Model. *Journal of Chemical Theory and Computation*, **2012**, 8, 2404-11	6.4	27
41	Continuum Electrostatics Solvent Modeling with the Generalized Born Model127-165		25
40	Protein-Ligand Electrostatic Binding Free Energies from Explicit and Implicit Solvation. *Journal of Chemical Theory and Computation*, **2015**, 11, 4450-9	6.4	24
39	The Role of Correlation and Solvation in Ion Interactions with B-DNA. *Biophysical Journal*, **2016**, 110, 315-326	2.9	24
38	Decomposing Complex Cooperative Ligand Binding into Simple Components: Connections between Microscopic and Macroscopic Models. *Journal of Physical Chemistry B*, **2004**, 108, 11157-11169	3.4	24
37	Two-phase stretching of molecular chains. *Proceedings of the National Academy of Sciences of the United States of America*, **2013**, 110, 2816-21	11.5	23
36	An analytical approach to computing biomolecular electrostatic potential. I. Derivation and analysis. *Journal of Chemical Physics*, **2008**, 129, 075101	3.9	23
35	Point charges optimally placed to represent the multipole expansion of charge distributions. *PLoS ONE*, **2013**, 8, e67715	3.7	23
34	The nucleosome: from structure to function through physics. *Current Opinion in Structural Biology*, **2019**, 56, 119-130	8.1	22
33	Why Computed Protein Folding Landscapes Are Sensitive to the Water Model. *Journal of Chemical Theory and Computation*, **2019**, 15, 625-636	6.4	22
32	An analytical approach to computing biomolecular electrostatic potential. II. Validation and applications. *Journal of Chemical Physics*, **2008**, 129, 075102	3.9	21
31	Implicit Solvent Model for Million-Atom Atomistic Simulations: Insights into the Organization of 30-nm Chromatin Fiber. *Journal of Chemical Theory and Computation*, **2016**, 12, 5946-5959	6.4	20
30	Accuracy of continuum electrostatic calculations based on three common dielectric boundary definitions. *Journal of Theoretical and Computational Chemistry*, **2014**, 13,	1.8	19
29	A strategy for reducing gross errors in the generalized Born models of implicit solvation. *Journal of Chemical Physics*, **2011**, 134, 164104	3.9	19
28	Accelerating electrostatic surface potential calculation with multi-scale approximation on graphics processing units. *Journal of Molecular Graphics and Modelling*, **2010**, 28, 904-10	2.8	18

27	Pathogenic peptide deviations support a model of adaptive evolution of chordate cardiac performance by troponin mutations. *Physiological Genomics*, **2010**, 42, 287-99	3.6	17
26	Chromosome-nuclear envelope attachments affect interphase chromosome territories and entanglement. *Epigenetics and Chromatin*, **2018**, 11, 3	5.8	16
25	Grid-Based Surface Generalized Born Model for Calculation of Electrostatic Binding Free Energies. *Journal of Chemical Information and Modeling*, **2017**, 57, 2505-2513	6.1	16
24	Investigation of the chromosome regions with significant affinity for the nuclear envelope in fruit fly--a model based approach. *PLoS ONE*, **2014**, 9, e91943	3.7	16
23	Accuracy Comparison of Generalized Born Models in the Calculation of Electrostatic Binding Free Energies. *Journal of Chemical Theory and Computation*, **2018**, 14, 1656-1670	6.4	13
22	Accurate evaluation of charge asymmetry in aqueous solvation. *Journal of Physical Chemistry B*, **2015**, 119, 6092-100	3.4	12
21	An n log n Generalized Born Approximation. *Journal of Chemical Theory and Computation*, **2011**, 7, 544-55	6.4	12
20	An N log N approximation based on the natural organization of biomolecules for speeding up the computation of long range interactions. *Journal of Computational Chemistry*, **2010**, 31, 691-706	3.5	11
19	Understanding nucleic acid structural changes by comparing wide-angle x-ray scattering (WAXS) experiments to molecular dynamics simulations. *Journal of Chemical Physics*, **2016**, 144, 205102	3.9	10
18	Three-dimensional Organization of Polytene Chromosomes in Somatic and Germline Tissues of Malaria Mosquitoes. *Cells*, **2020**, 9,	7.9	8
17	Multi-shell model of ion-induced nucleic acid condensation. *Journal of Chemical Physics*, **2016**, 144, 155101	3.9	8
16	Quantified effects of chromosome-nuclear envelope attachments on 3D organization of chromosomes. *Nucleus*, **2015**, 6, 212-24	3.9	6
15	High-temperature dynamic behavior in bulk liquid water: A molecular dynamics simulation study using the OPC and TIP4P-Ew potentials. *Frontiers of Physics*, **2018**, 13, 1	3.7	6
14	Linear relationship between peak and season-long abundances in insects. *PLoS ONE*, **2018**, 13, e0193110	3.7	5
13	Multidimensional Global Optimization and Robustness Analysis in the Context of Protein-Ligand Binding. *Journal of Chemical Theory and Computation*, **2020**, 16, 4669-4684	6.4	5
12	Strongly Bent Double-Stranded DNA: Reconciling Theory and Experiment. *Frontiers in Physics*, **2019**, 7,	3.9	5
11	Validation and estimation of parameters for a general probabilistic model of the PCR process. *Journal of Computational Biology*, **2007**, 14, 97-112	1.7	4
10	Similarities and Differences between Na and K Distributions around DNA Obtained with Three Popular Water Models. *Journal of Chemical Theory and Computation*, **2021**, 17, 7246-7259	6.4	4

9	MMGB/SA Consensus Estimate of the Binding Free Energy Between the Novel Coronavirus Spike Protein to the Human ACE2 Receptor **2020**,		4
8	Explicit ions/implicit water generalized Born model for nucleic acids. *Journal of Chemical Physics*, **2018**, 148, 195101	3.9	3
7	Binding of regulatory proteins to nucleosomes is modulated by dynamic histone tails		3
6	Binding of regulatory proteins to nucleosomes is modulated by dynamic histone tails. *Nature Communications*, **2021**, 12, 5280	17.4	3
5	Exploring optimization strategies for improving explicit water models: Rigid n-point model and polarizable model based on Drude oscillator. *PLoS ONE*, **2019**, 14, e0224991	3.7	2
4	Insights from All-Atom Molecular Dynamics Simulations of 40 Nucleosome Chromatin Fiber. *Biophysical Journal*, **2015**, 108, 319a	2.9	2
3	Melting Points of OPC and OPC3 Water Models. *ACS Omega*, **2020**, 5, 25087-25094	3.9	2
2	Bounds on Absolute Gypsy Moth () (Lepidoptera: Erebidae) Population Density as Derived from Counts in Single Milk Carton Traps. *Insects*, **2020**, 11,	2.8	1
1	Significant compaction of H4 histone tail upon charge neutralization by acetylation and its mimics, possible effects on chromatin structure. *Journal of Molecular Biology*, **2021**, 433, 166683	6.5	1