Alexey V Onufriev

List of Publications by Year
in descending order

96	18,794	101384 36	62479 80
papers	citations	h-index	g-index

107	107	107	18788
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	The Amber biomolecular simulation programs. Journal of Computational Chemistry, 2005, 26, 1668-1688.	1.5	7,742
2	Exploring protein native states and large-scale conformational changes with a modified generalized born model. Proteins: Structure, Function and Bioinformatics, 2004, 55, 383-394.	1.5	2,068
3	H++ 3.0: automating pK prediction and the preparation of biomolecular structures for atomistic molecular modeling and simulations. Nucleic Acids Research, 2012, 40, W537-W541.	6.5	1,314
4	H++: a server for estimating pKas and adding missing hydrogens to macromolecules. Nucleic Acids Research, 2005, 33, W368-W371.	6.5	1,295
5	Modification of the Generalized Born Model Suitable for Macromolecules. Journal of Physical Chemistry B, 2000, 104, 3712-3720.	1.2	973
6	Building Water Models: A Different Approach. Journal of Physical Chemistry Letters, 2014, 5, 3863-3871.	2.1	640
7	Performance comparison of generalized born and Poisson methods in the calculation of electrostatic solvation energies for protein structures. Journal of Computational Chemistry, 2004, 25, 265-284.	1.5	523
8	Effective Born radii in the generalized Born approximation: The importance of being perfect. Journal of Computational Chemistry, 2002, 23, 1297-1304.	1.5	412
9	Generalized Born Model with a Simple, Robust Molecular Volume Correction. Journal of Chemical Theory and Computation, 2007, 3, 156-169.	2.3	334
10	A simple clustering algorithm can be accurate enough for use in calculations of pKs in macromolecules. Proteins: Structure, Function and Bioinformatics, 2006, 63, 928-938.	1.5	270
11	Accuracy limit of rigid 3-point water models. Journal of Chemical Physics, 2016, 145, 074501.	1.2	195
12	A Novel View of pH Titration in Biomoleculesâ€. Biochemistry, 2001, 40, 3413-3419.	1.2	183
13	Speed of Conformational Change: Comparing Explicit and Implicit Solvent Molecular Dynamics Simulations. Biophysical Journal, 2015, 108, 1153-1164.	0.2	158
14	Generalized Born Implicit Solvent Models for Biomolecules. Annual Review of Biophysics, 2019, 48, 275-296.	4.5	155
15	Protonation and pK changes in proteinâ€“ligand binding. Quarterly Reviews of Biophysics, 2013, 46, 181-209.	2.4	151
16	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, 9204-9209.	3.3	140
17	Water models for biomolecular simulations. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2018, 8, e1347.	6.2	140
18	Analytical electrostatics for biomolecules: Beyond the generalizedâ€‡ Born approximation. Journal of Chemical Physics, 2006, 124, 124902.	1.2	113

#	Article	IF	Citations
19	General Purpose Water Model Can Improve Atomistic Simulations of Intrinsically Disordered Proteins. Journal of Chemical Theory and Computation, 2019, 15, 2620-2634.	2.3	85
20	Incorporating variable dielectric environments into the generalized Born model. Journal of Chemical Physics, 2005, 122, 094511.	1.2	82
21	Implicit Solvent Models in Molecular Dynamics Simulations: A Brief Overview. Annual Reports in Computational Chemistry, 2008, 4, 125-137.	0.9	82
22	Modulation of nucleosomal DNA accessibility via charge-altering post-translational modifications in histone core. Epigenetics and Chromatin, 2018, 11, 11.	1.8	73
23	A Computational Study of Nucleosomal DNA Flexibility. Biophysical Journal, 2006, 91, 4121-4132.	0.2	72
24	Charge Hydration Asymmetry: The Basic Principle and How to Use It to Test and Improve Water Models. Journal of Physical Chemistry B, 2012, 116, 9776-9783.	1.2	72
25	Why double-stranded RNA resists condensation. Nucleic Acids Research, 2014, 42, 10823-10831.	6.5	67
26	Charge State of the Globular Histone Core Controls Stability of the Nucleosome. Biophysical Journal, 2010, 99, 1577-1585.	0.2	65
27	Proton Affinity Changes Driving Unidirectional Proton Transport in the Bacteriorhodopsin Photocycle. Journal of Molecular Biology, 2003, 332, 1183-1193.	2.0	63
28	Analysis of integral expressions for effective Born radii. Journal of Chemical Physics, 2007, 127, 185101.	1.2	54
29	Structural Details, Pathways, and Energetics of Unfolding Apomyoglobin. Journal of Molecular Biology, 2003, 325, 555-567.	2.0	52
30	The nucleosome: from structure to function through physics. Current Opinion in Structural Biology, 2019, 56, 119-130.	2.6	52
31	Partially Assembled Nucleosome Structures atÂAtomic Detail. Biophysical Journal, 2017, 112, 460-472.	0.2	50
32	Reducing the Secondary Structure Bias in the Generalized Born Model via R6 Effective Radii. Journal of Chemical Theory and Computation, 2010, 6, 3613-3630.	2.3	49
33	Spermine Condenses DNA, but Not RNA Duplexes. Biophysical Journal, 2017, 112, 22-30.	0.2	48
34	Opposing Effects of Multivalent Ions on the Flexibility of DNA and RNA. Physical Review Letters, 2016, 117, 028101.	2.9	47
35	Statistics and Physical Origins of pK and Ionization State Changes upon Protein-Ligand Binding. Biophysical Journal, 2010, 98, 872-880.	0.2	46
36	Binding of regulatory proteins to nucleosomes is modulated by dynamic histone tails. Nature Communications, 2021, 12, 5280.	5.8	43

#	Article	IF	Citations
37	Heat conductivity of the DNA double helix. Physical Review B, 2011, 83, .	1.1	41
38	Analysis of Basic Clustering Algorithms for Numerical Estimation of Statistical Averages in Biomolecules. Journal of Computational Biology, 2008, 15, 165-184.	0.8	39
39	Modeling of Flap Endonuclease Interactions with DNA Substrate. Journal of Molecular Biology, 2003, 328, 537-554.	2.0	36
40	The Role of Correlation and Solvation in Ion Interactions with B-DNA. Biophysical Journal, 2016, 110, 315-326.	0.2	33
41	Proteinâ€“Ligand Electrostatic Binding Free Energies from Explicit and Implicit Solvation. Journal of Chemical Theory and Computation, 2015, 11, 4450-4459.	2.3	32
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, 2404-2411.	2.3	31
43	Why Computed Protein Folding Landscapes Are Sensitive to the Water Model. Journal of Chemical Theory and Computation, 2019, 15, 625-636.	2.3	31
44	Introducing Charge Hydration Asymmetry into the Generalized Born Model. Journal of Chemical Theory and Computation, 2014, 10, 1788-1794.	2.3	30
45	Two-phase stretching of molecular chains. Proceedings of the National Academy of Sciences of the United States of America, 2013, 110, 2816-2821.	3.3	29
46	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.	2.3	29
47	An analytical approach to computing biomolecular electrostatic potential. I. Derivation and analysis. Journal of Chemical Physics, 2008, 129, 075101.	1.2	27
48	An analytical approach to computing biomolecular electrostatic potential. II. Validation and applications. Journal of Chemical Physics, 2008, 129, 075102.	1.2	27
49	Grid-Based Surface Generalized Born Model for Calculation of Electrostatic Binding Free Energies. Journal of Chemical Information and Modeling, 2017, 57, 2505-2513.	2.5	27
50	Decomposing Complex Cooperative Ligand Binding into Simple Components:Â Connections between Microscopic and Macroscopic Models. Journal of Physical Chemistry B, 2004, 108, 11157-11169.	1.2	25
51	Ten simple rules on how to create open access and reproducible molecular simulations of biological systems. PLoS Computational Biology, 2019, 15, e1006649.	1.5	25
52	Point Charges Optimally Placed to Represent the Multipole Expansion of Charge Distributions. PLoS ONE, 2013, 8, e67715.	1.1	25
53	A strategy for reducing gross errors in the generalized Born models of implicit solvation. Journal of Chemical Physics, 2011, 134, 164104.	1.2	23
54	Accuracy Comparison of Generalized Born Models in the Calculation of Electrostatic Binding Free Energies. Journal of Chemical Theory and Computation, 2018, 14, 1656-1670.	2.3	23

#	Article	IF	Citations
55	Chromosomeâ€“nuclear envelope attachments affect interphase chromosome territories and entanglement. Epigenetics and Chromatin, 2018, 11, 3.	1.8	23
56	Accelerating electrostatic surface potential calculation with multi-scale approximation on graphics processing units. Journal of Molecular Graphics and Modelling, 2010, 28, 904-910.	1.3	22
57	Accuracy of continuum electrostatic calculations based on three common dielectric boundary definitions. Journal of Theoretical and Computational Chemistry, 2014, 13, 1440006.	1.8	22
58	Pathogenic peptide deviations support a model of adaptive evolution of chordate cardiac performance by troponin mutations. Physiological Genomics, 2010, 42, 287-299.	1.0	20
59	Investigation of the Chromosome Regions with Significant Affinity for the Nuclear Envelope in Fruit Fly â€“ A Model Based Approach. PLoS ONE, 2014, 9, e91943.	1.1	19
60	AnnlognGeneralized Born Approximation. Journal of Chemical Theory and Computation, 2011, 7, 544-559.	2.3	18
61	Accurate Evaluation of Charge Asymmetry in Aqueous Solvation. Journal of Physical Chemistry B, 2015, 119, 6092-6100.	1.2	16
62	Explicit ions/implicit water generalized Born model for nucleic acids. Journal of Chemical Physics, 2018, 148, 195101.	1.2	16
63	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.	2.3	16
64	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.	1.5	15
65	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.	1.2	15
66	Multi-shell model of ion-induced nucleic acid condensation. Journal of Chemical Physics, 2016, 144, 155101.	1.2	13
67	Strongly Bent Double-Stranded DNA: Reconciling Theory and Experiment. Frontiers in Physics, 2019, 7, .	1.0	12
68	Melting Points of OPC and OPC3 Water Models. ACS Omega, 2020, 5, 25087-25094.	1.6	12
69	Three-dimensional Organization of Polytene Chromosomes in Somatic and Germline Tissues of Malaria Mosquitoes. Cells, 2020, 9, 339.	1.8	11
70	Multidimensional Global Optimization and Robustness Analysis in the Context of Proteinâ€“Ligand Binding. Journal of Chemical Theory and Computation, 2020, 16, 4669-4684.	2.3	11
71	Quantified effects of chromosome-nuclear envelope attachments on 3D organization of chromosomes. Nucleus, 2015, 6, 212-224.	0.6	10
72	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.	2.4	7

#	Article	IF	Citations
73	Linear relationship between peak and season-long abundances in insects. PLoS ONE, 2018, 13, e0193110.	1.1	6
74	Bounds on Absolute Gypsy Moth (Lymantria dispar dispar) (Lepidoptera: Erebidae) Population Density as Derived from Counts in Single Milk Carton Traps. Insects, 2020, 11, 673.	1.0	5
75	Validation and Estimation of Parameters for a General Probabilistic Model of the PCR Process. Journal of Computational Biology, 2007, 14, 97-112.	0.8	4
76	Exploring optimization strategies for improving explicit water models: Rigid n-point model and polarizable model based on Drude oscillator. PLoS ONE, 2019, 14, e0224991.	1.1	4
77	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.	2.0	4
78	Insights from All-Atom Molecular Dynamics Simulations of 40 Nucleosome Chromatin Fiber. Biophysical Journal, 2015, 108, 319a.	0.2	2
79	Stretching of Long Double-Stranded DNA and RNA Described by the Same Approach. Journal of Chemical Theory and Computation, 2022, 18, 3911-3920.	2.3	2
80	Estimating Persistence Length of DNA from Molecular Dynamics Simulations. Biophysical Journal, 2015, 108, 233a.	0.2	1
81	How to Count Bugs: A Method to Estimate the Most Probable Absolute Population Density and Its Statistical Bounds from a Single Trap Catch. Insects, 2021, 12, 932.	1.0	1
82	Correlation between computed equilibrium secondary structure free energy and siRNA efficiency. , 2009, , .		0
83	Low Order Physical Multipoles. Biophysical Journal, 2011, 100, 614a.	0.2	0
84	A Model of Nuclear Organization Demonstrates the Effect of Nuclear Envelope - Chromosome Contacts on 3D Organization of Chromosomes. Biophysical Journal, 2013, 104, 551a.	0.2	0
85	Molecular Dynamics Study of Cobalt(III) Hexammine Counter-Ion Distributions around B-DNA and A-RNA Duplexes. Biophysical Journal, 2013, 104, 423a.	0.2	0
86	Introducing Charge Hydration Asymmetry in the Realm of Continuum Solvation. Biophysical Journal, 2013, 104, 35a.	0.2	0
87	The Physics of DNA Bending. Biophysical Journal, 2013, 104, 15a-16a.	0.2	0
88	Strongly Bent DNA: Reconciling Theory and Experiment. Biophysical Journal, 2014, 106, 280a.	0.2	0
89	Nucleosome Stability is Controlled by the Charge of its Globular Core: Implications for the Biological Function. Biophysical Journal, 2014, 106, 75a.	0.2	0
90	Chromosome-Nuclear Envelope Interactions Have Multiple Effects on Chromosome Folding Dynamics in Simulation. Biophysical Journal, 2015, 108, 537a.	0.2	0

#	Article	IF	Citations
91	From Small to Large to Very Large: Modeling of Biomolecular Structures in Implicit Solvent. Biophysical Journal, 2015, 108, 208a.	0.2	0
92	Multiscale Approximation with Graphical Processing Units for Multiplicative Speedup in Molecular Dynamics. , 2016, , .		0
93	Condensation of Nucleic Acids by Multivalent Ions: Sequence Dependence and the Curious Case of RNA. Biophysical Journal, 2016, 110, 409a.	0.2	0
94	Modulation of the DNA Accessibility in the Nucleosome -- Insights from Physics Models. Biophysical Journal, 2019, 116, 71a.	0.2	0
95	The Curious Case of Strongly Bent DNA. Biophysical Journal, 2020, 118, 377a.	0.2	0
96	The Effect of Nuclear Envelope on Chromatin Architecture in Drosophila Melanogaster: Modeling of Three-Dimensional Interphase Chromosome Organization. Biophysical Journal, 2020, 118, 551a.	0.2	0