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	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
2	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
3	Binding of regulatory proteins to nucleosomes is modulated by dynamic histone tails. Nature Communications, 2021, 12, 5280.	5.8	43
4	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
5	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
6	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
7	Melting Points of OPC and OPC3 Water Models. ACS Omega, 2020, 5, 25087-25094.	1.6	12
8	The Curious Case of Strongly Bent DNA. Biophysical Journal, 2020, 118, 377a.	0.2	0
9	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
10	Three-dimensional Organization of Polytene Chromosomes in Somatic and Germline Tissues of Malaria Mosquitoes. Cells, 2020, 9, 339.	1.8	11
11	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
12	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
13	The nucleosome: from structure to function through physics. Current Opinion in Structural Biology, 2019, 56, 119-130.	2.6	52
14	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
15	Modulation of the DNA Accessibility in the Nucleosome -- Insights from Physics Models. Biophysical Journal, 2019, 116, 71a.	0.2	0
16	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
17	Generalized Born Implicit Solvent Models for Biomolecules. Annual Review of Biophysics, 2019, 48, 275-296.	4.5	155
18	Strongly Bent Double-Stranded DNA: Reconciling Theory and Experiment. Frontiers in Physics, 2019, 7, .	1.0	12

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19	Why Computed Protein Folding Landscapes Are Sensitive to the Water Model. Journal of Chemical Theory and Computation, 2019, 15, 625-636.	2.3	31
20	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
21	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
22	Water models for biomolecular simulations. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2018, 8, e1347.	6.2	140
23	Explicit ions/implicit water generalized Born model for nucleic acids. Journal of Chemical Physics, 2018, 148, 195101.	1.2	16
24	Modulation of nucleosomal DNA accessibility via charge-altering post-translational modifications in histone core. Epigenetics and Chromatin, 2018, 11, 11.	1.8	73
25	Chromosomeâ€“nuclear envelope attachments affect interphase chromosome territories and entanglement. Epigenetics and Chromatin, 2018, 11, 3.	1.8	23
26	Linear relationship between peak and season-long abundances in insects. PLoS ONE, 2018, 13, e0193110.	1.1	6
27	Spermine Condenses DNA, but Not RNA Duplexes. Biophysical Journal, 2017, 112, 22-30.	0.2	48
28	Partially Assembled Nucleosome Structures atÂAtomic Detail. Biophysical Journal, 2017, 112, 460-472.	0.2	50
29	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
30	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
31	Multi-shell model of ion-induced nucleic acid condensation. Journal of Chemical Physics, 2016, 144, 155101.	1.2	13
32	Multiscale Approximation with Graphical Processing Units for Multiplicative Speedup in Molecular Dynamics. , 2016, , .		0
33	Accuracy limit of rigid 3-point water models. Journal of Chemical Physics, 2016, 145, 074501.	1.2	195
34	Condensation of Nucleic Acids by Multivalent Ions: Sequence Dependence and the Curious Case of RNA. Biophysical Journal, 2016, 110, 409a.	0.2	0
35	Opposing Effects of Multivalent Ions on the Flexibility of DNA and RNA. Physical Review Letters, 2016, 117, 028101.	2.9	47
36	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

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37	The Role of Correlation and Solvation in Ion Interactions with B-DNA. Biophysical Journal, 2016, 110, 315-326.	0.2	33
38	Chromosome-Nuclear Envelope Interactions Have Multiple Effects on Chromosome Folding Dynamics in Simulation. Biophysical Journal, 2015, 108, 537a.	0.2	0
39	Insights from All-Atom Molecular Dynamics Simulations of 40 Nucleosome Chromatin Fiber. Biophysical Journal, 2015, 108, 319a.	0.2	2
40	Accurate Evaluation of Charge Asymmetry in Aqueous Solvation. Journal of Physical Chemistry B, 2015, 119, 6092-6100.	1.2	16
41	From Small to Large to Very Large: Modeling of Biomolecular Structures in Implicit Solvent. Biophysical Journal, 2015, 108, 208a.	0.2	0
42	Speed of Conformational Change: Comparing Explicit and Implicit Solvent Molecular Dynamics Simulations. Biophysical Journal, 2015, 108, 1153-1164.	0.2	158
43	Estimating Persistence Length of DNA from Molecular Dynamics Simulations. Biophysical Journal, 2015, 108, 233a.	0.2	1
44	Quantified effects of chromosome-nuclear envelope attachments on 3D organization of chromosomes. Nucleus, 2015, 6, 212-224.	0.6	10
45	Proteinâ€“Ligand Electrostatic Binding Free Energies from Explicit and Implicit Solvation. Journal of Chemical Theory and Computation, 2015, 11, 4450-4459.	2.3	32
46	Accuracy of continuum electrostatic calculations based on three common dielectric boundary definitions. Journal of Theoretical and Computational Chemistry, 2014, 13, 1440006.	1.8	22
47	Why double-stranded RNA resists condensation. Nucleic Acids Research, 2014, 42, 10823-10831.	6.5	67
48	Strongly Bent DNA: Reconciling Theory and Experiment. Biophysical Journal, 2014, 106, 280a.	0.2	0
49	Building Water Models: A Different Approach. Journal of Physical Chemistry Letters, 2014, 5, 3863-3871.	2.1	640
50	Introducing Charge Hydration Asymmetry into the Generalized Born Model. Journal of Chemical Theory and Computation, 2014, 10, 1788-1794.	2.3	30
51	Nucleosome Stability is Controlled by the Charge of its Globular Core: Implications for the Biological Function. Biophysical Journal, 2014, 106, 75a.	0.2	0
52	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
53	Protonation and pK changes in proteinâ€“ligand binding. Quarterly Reviews of Biophysics, 2013, 46, 181-209.	2.4	151
54	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

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55	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
56	Introducing Charge Hydration Asymmetry in the Realm of Continuum Solvation. Biophysical Journal, 2013, 104, 35a.	0.2	0
57	The Physics of DNA Bending. Biophysical Journal, 2013, 104, 15a-16a.	0.2	0
58	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
59	Point Charges Optimally Placed to Represent the Multipole Expansion of Charge Distributions. PLoS ONE, 2013, 8, e67715.	1.1	25
60	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
61	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
62	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
63	AnnlognGeneralized Born Approximation. Journal of Chemical Theory and Computation, 2011, 7, 544-559.	2.3	18
64	Low Order Physical Multipoles. Biophysical Journal, 2011, 100, 614a.	0.2	0
65	Heat conductivity of the DNA double helix. Physical Review B, 2011, 83, .	1.1	41
66	A strategy for reducing gross errors in the generalized Born models of implicit solvation. Journal of Chemical Physics, 2011, 134, 164104.	1.2	23
67	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
68	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
69	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
70	Statistics and Physical Origins of pK and Ionization State Changes upon Protein-Ligand Binding. Biophysical Journal, 2010, 98, 872-880.	0.2	46
71	Charge State of the Globular Histone Core Controls Stability of the Nucleosome. Biophysical Journal, 2010, 99, 1577-1585.	0.2	65
72	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

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73	Correlation between computed equilibrium secondary structure free energy and siRNA efficiency. , 2009, , .		0
74	An analytical approach to computing biomolecular electrostatic potential. I. Derivation and analysis. Journal of Chemical Physics, 2008, 129, 075101.	1.2	27
75	Implicit Solvent Models in Molecular Dynamics Simulations: A Brief Overview. Annual Reports in Computational Chemistry, 2008, 4, 125-137.	0.9	82
76	An analytical approach to computing biomolecular electrostatic potential. II. Validation and applications. Journal of Chemical Physics, 2008, 129, 075102.	1.2	27
77	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
78	Analysis of Basic Clustering Algorithms for Numerical Estimation of Statistical Averages in Biomolecules. Journal of Computational Biology, 2008, 15, 165-184.	0.8	39
79	Analysis of integral expressions for effective Born radii. Journal of Chemical Physics, 2007, 127, 185101.	1.2	54
80	Generalized Born Model with a Simple, Robust Molecular Volume Correction. Journal of Chemical Theory and Computation, 2007, 3, 156-169.	2.3	334
81	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
82	A Computational Study of Nucleosomal DNA Flexibility. Biophysical Journal, 2006, 91, 4121-4132.	0.2	72
83	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
84	Analytical electrostatics for biomolecules: Beyond the generalizedâ€‡ Born approximation. Journal of Chemical Physics, 2006, 124, 124902.	1.2	113
85	The Amber biomolecular simulation programs. Journal of Computational Chemistry, 2005, 26, 1668-1688.	1.5	7,742
86	H++: a server for estimating pKas and adding missing hydrogens to macromolecules. Nucleic Acids Research, 2005, 33, W368-W371.	6.5	1,295
87	Incorporating variable dielectric environments into the generalized Born model. Journal of Chemical Physics, 2005, 122, 094511.	1.2	82
88	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
89	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
90	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

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91	Structural Details, Pathways, and Energetics of Unfolding Apomyoglobin. Journal of Molecular Biology, 2003, 325, 555-567.	2.0	52
92	Modeling of Flap Endonuclease Interactions with DNA Substrate. Journal of Molecular Biology, 2003, 328, 537-554.	2.0	36
93	Proton Affinity Changes Driving Unidirectional Proton Transport in the Bacteriorhodopsin Photocycle. Journal of Molecular Biology, 2003, 332, 1183-1193.	2.0	63
94	Effective Born radii in the generalized Born approximation: The importance of being perfect. Journal of Computational Chemistry, 2002, 23, 1297-1304.	1.5	412
95	A Novel View of pH Titration in Biomoleculesâ€. Biochemistry, 2001, 40, 3413-3419.	1.2	183
96	Modification of the Generalized Born Model Suitable for Macromolecules. Journal of Physical Chemistry B, 2000, 104, 3712-3720.	1.2	973