Andrey A Gurtovenko

List of Publications by Year
in descending order

79	4,174	94269 37	114278 63
papers	citations	h-index	g-index

82	82	82	4237
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Modulating the Structure and Properties of Cell Membranes:â€‰ The Molecular Mechanism of Action of Dimethyl Sulfoxide. Journal of Physical Chemistry B, 2007, 111, 10453-10460.	1.2	354
2	Effect of NaCl and KCl on Phosphatidylcholine and Phosphatidylethanolamine Lipid Membranes:â€‰ Insight from Atomic-Scale Simulations for Understanding Salt-Induced Effects in the Plasma Membrane. Journal of Physical Chemistry B, 2008, 112, 1953-1962.	1.2	227
3	Pore Formation Coupled to Ion Transport through Lipid Membranes as Induced by Transmembrane Ionic Charge Imbalance:â€‰ Atomistic Molecular Dynamics Study. Journal of the American Chemical Society, 2005, 127, 17570-17571.	6.6	190
4	Atomic-Scale Structure and Electrostatics of Anionic Palmitoyloleoylphosphatidylglycerol Lipid Bilayers with Na+ Counterions. Biophysical Journal, 2007, 92, 1114-1124.	0.2	178
5	Defect-Mediated Trafficking across Cell Membranes: Insights from in Silico Modeling. Chemical Reviews, 2010, 110, 6077-6103.	23.0	171
6	Cationic DMPC/DMTAP Lipid Bilayers: Molecular Dynamics Study. Biophysical Journal, 2004, 86, 3461-3472.	0.2	156
7	Interaction of Ethanol with Biological Membranes: The Formation of Non-bilayer Structures within the Membrane Interior and their Significance. Journal of Physical Chemistry B, 2009, 113, 1983-1992.	1.2	144
8	Molecular Mechanism for Lipid Flip-Flops. Journal of Physical Chemistry B, 2007, 111, 13554-13559.	1.2	125
9	Generalized Gaussian Structures: Models for Polymer Systems with ComplexTopologies. Advances in Polymer Science, 2005, , 171-282.	0.4	113
10	Ion Leakage through Transient Water Pores in Protein-Free Lipid Membranes Driven by Transmembrane Ionic Charge Imbalance. Biophysical Journal, 2007, 92, 1878-1890.	0.2	108
11	Role of phosphatidylglycerols in the stability of bacterial membranes. Biochimie, 2008, 90, 930-938.	1.3	106
12	Asymmetry of lipid bilayers induced by monovalent salt: Atomistic molecular-dynamics study. Journal of Chemical Physics, 2005, 122, 244902.	1.2	105
13	Atomistic Simulations of Functional Au₁₄₄(SR)₆₀ Gold Nanoparticles in Aqueous Environment. Journal of Physical Chemistry C, 2012, 116, 9805-9815.	1.5	94
14	Membrane Potential and Electrostatics of Phospholipid Bilayers with Asymmetric Transmembrane Distribution of Anionic Lipids. Journal of Physical Chemistry B, 2008, 112, 4629-4634.	1.2	88
15	Lipid Transmembrane Asymmetry and Intrinsic Membrane Potential:Â Two Sides of the Same Coin. Journal of the American Chemical Society, 2007, 129, 5358-5359.	6.6	83
16	Microsecond Atomic-Scale Molecular Dynamics Simulations of Polyimides. Macromolecules, 2013, 46, 6357-6363.	2.2	80
17	l-Alanine in a Droplet of Water:Â A Density-Functional Molecular Dynamics Study. Journal of Physical Chemistry B, 2007, 111, 4227-4234.	1.2	76
18	Free Volume Properties of Sphingomyelin, DMPC, DPPC, and PLPC Bilayers. Journal of Computational and Theoretical Nanoscience, 2005, 2, 401-413.	0.4	75

#	Article	IF	Citations
19	Molecular dynamics study of charged dendrimers in salt-free solution: Effect of counterions. Journal of Chemical Physics, 2006, 124, 094904.	1.2	73
20	Cationic Au Nanoparticle Binding with Plasma Membrane-like Lipid Bilayers: Potential Mechanism for Spontaneous Permeation to Cells Revealed by Atomistic Simulations. Journal of Physical Chemistry C, 2014, 118, 11131-11141.	1.5	69
21	Thermal properties of bulk polyimides: insights from computer modeling versus experiment. Soft Matter, 2014, 10, 1224.	1.2	68
22	Effect of Monovalent Salt on Cationic Lipid Membranes As Revealed by Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2005, 109, 21126-21134.	1.2	67
23	Dynamics of dendrimer-based polymer networks. Journal of Chemical Physics, 2003, 119, 7579-7590.	1.2	63
24	Calculation of the electrostatic potential of lipid bilayers from molecular dynamics simulations: Methodological issues. Journal of Chemical Physics, 2009, 130, 215107.	1.2	63
25	Molecular dynamics simulations of uniaxial deformation of thermoplastic polyimides. Soft Matter, 2016, 12, 3972-3981.	1.2	61
26	Molecular-dynamics simulation of polyimide matrix pre-crystallization near the surface of a single-walled carbon nanotube. RSC Advances, 2014, 4, 830-844.	1.7	51
27	Viscoelastic Dynamic Properties of Meshlike Polymer Networks:Â Contributions of Intra- and Interchain Relaxation Processes. Macromolecules, 2000, 33, 6578-6587.	2.2	50
28	Intra- and Interchain Relaxation Processes in Meshlike Polymer Networks. Macromolecules, 1998, 31, 5756-5770.	2.2	49
29	Dynamics of inhomogeneous cross-linked polymers consisting of domains of different sizes. Journal of Chemical Physics, 2001, 115, 6785-6793.	1.2	48
30	Complexes Comprised of Charged Dendrimers, Linear Polyelectrolytes, and Counterions: Insight through Coarse-Grained Molecular Dynamics Simulations. Macromolecules, 2008, 41, 4961-4968.	2.2	48
31	Rouse Dynamics of Polymer Networks Bearing Dendritic Wedges. Macromolecules, 2002, 35, 7481-7491.	2.2	46
32	Atomistic simulations of anionic Au144(SR)60 nanoparticles interacting with asymmetric model lipid membranes. Biochimica Et Biophysica Acta - Biomembranes, 2014, 1838, 2852-2860.	1.4	46
33	Influence of the electrostatic interactions on thermophysical properties of polyimides: Molecularâ€dynamics simulations. Journal of Polymer Science, Part B: Polymer Physics, 2014, 52, 640-646.	2.4	45
34	Electroporation of Asymmetric Phospholipid Membranes. Journal of Physical Chemistry B, 2014, 118, 9909-9918.	1.2	45
35	Adsorption of Synthetic Cationic Polymers on Model Phospholipid Membranes: Insight from Atomic-Scale Molecular Dynamics Simulations. Langmuir, 2016, 32, 10402-10414.	1.6	41
36	Toward realistic computer modeling of paraffin-based composite materials: critical assessment of atomic-scale models of paraffins. RSC Advances, 2019, 9, 38834-38847.	1.7	39

#	Article	IF	Citations
37	Ion Dynamics in Cationic Lipid Bilayer Systems in Saline Solutions. Journal of Physical Chemistry B, 2009, 113, 9226-9234.	1.2	38
38	Effect of the SO2 group in the diamine fragment of polyimides on their structural, thermophysical, and mechanical properties. Polymer Science - Series A, 2012, 54, 631-643.	0.4	37
39	Chemically Induced Phospholipid Translocation Across Biological Membranes. Langmuir, 2008, 24, 9656-9660.	1.6	36
40	Parameterization of electrostatic interactions for molecular dynamics simulations of heterocyclic polymers. Journal of Polymer Science, Part B: Polymer Physics, 2015, 53, 912-923.	2.4	36
41	Relaxation of disordered polymer networks: Regular lattice made up of small-world Rouse networks. Journal of Chemical Physics, 2001, 115, 4924-4929.	1.2	33
42	Ion Transport through Chemically Induced Pores in Protein-Free Phospholipid Membranes. Journal of Physical Chemistry B, 2007, 111, 13379-13382.	1.2	33
43	Molecular Mechanism of Calcium-Induced Adsorption of DNA on Zwitterionic Phospholipid Membranes. Journal of Physical Chemistry B, 2015, 119, 6638-6645.	1.2	32
44	Atomic-Scale Molecular Dynamics Simulations of DNAâ€“Polycation Complexes: Two Distinct Binding Patterns. Journal of Physical Chemistry B, 2016, 120, 6546-6554.	1.2	31
45	Evaluation of thermal conductivity of organic phase-change materials from equilibrium and non-equilibrium computer simulations: Paraffin as a test case. International Journal of Heat and Mass Transfer, 2021, 165, 120639.	2.5	30
46	Anomalous diffusion and relaxation in macromolecular systems. Journal of Non-Crystalline Solids, 2002, 305, 71-80.	1.5	25
47	Cationic Dimyristoylphosphatidylcholine and Dioleoyloxytrimethylammonium Propane Lipid Bilayers: Atomistic Insight for Structure and Dynamics. Journal of Physical Chemistry B, 2012, 116, 269-276.	1.2	25
48	Intrinsic Potential of Cell Membranes: Opposite Effects of Lipid Transmembrane Asymmetry and Asymmetric Salt Ion Distribution. Journal of Physical Chemistry B, 2009, 113, 7194-7198.	1.2	23
49	Glycosylation and Lipids Working in Concert Direct CD2 Ectodomain Orientation and Presentation. Journal of Physical Chemistry Letters, 2017, 8, 1060-1066.	2.1	22
50	What Can We Learn about Cholesterolâ€™s Transmembrane Distribution Based on Cholesterol-Induced Changes in Membrane Dipole Potential?. Journal of Physical Chemistry Letters, 2016, 7, 4585-4590.	2.1	19
51	The Aqueous and Crystalline Forms of L-Alanine Zwitterion. Journal of Computational and Theoretical Nanoscience, 2008, 5, 277-285.	0.4	19
52	Viscoelastic dynamic properties of heterogeneous polymer networks with domain structure. Macromolecular Theory and Simulations, 2000, 9, 388-397.	0.6	18
53	Response of Disordered Polymer Networks to External Fields:Â Regular Lattices Built from Complex Subunits. Macromolecules, 2002, 35, 3288-3295.	2.2	18
54	Dimethyl sulfoxide enhances GLUT4 translocation through a reduction in GLUT4 endocytosis in insulin-stimulated 3T3-L1 adipocytes. Biochimie, 2011, 93, 697-709.	1.3	18

#	Article	IF	Citations
55	Dielectric relaxation of polymer networks built from macromolecules with dipole moment directed along the end-to-end chain vector. Macromolecular Theory and Simulations, 1996, 5, 969-986.	0.6	17
56	Structure of Glycocalyx. Biophysical Journal, 2013, 104, 251a.	0.2	16
57	Molecular-level insight into the interactions of DNA with phospholipid bilayers: barriers and triggers. RSC Advances, 2016, 6, 36425-36432.	1.7	16
58	Supramolecular complexes of DNA with cationic polymers: The effect of polymer concentration. Polymer, 2018, 142, 277-284.	1.8	16
59	The model theory of viscoelastic relaxation properties of bulk cross-linked polymers. Interchain friction effects. Macromolecular Theory and Simulations, 1997, 6, 523-551.	0.6	15
60	Viscoelastic Relaxation of Cross-Linked, Alternating Copolymers in the Free-Draining Limit. Macromolecules, 2003, 36, 486-494.	2.2	14
61	Molecular-Level Insight into the Interactions of DNA/Polycation Complexes with Model Cell Membranes. Journal of Physical Chemistry B, 2019, 123, 6505-6514.	1.2	14
62	The Devil Is in the Details: What Do We Really Track in Single-Particle Tracking Experiments of Diffusion in Biological Membranes?. Journal of Physical Chemistry Letters, 2019, 10, 1005-1011.	2.1	13
63	Computer simulation of the heat-resistant polyimides ULTEMâ„¢ and EXTEMâ„¢ with the use of GROMOS53a6 and AMBER99 force fields. Polymer Science - Series A, 2014, 56, 558-567.	0.4	12
64	Molecular-Level Insight into the Interaction of Phospholipid Bilayers with Cellulose. Langmuir, 2017, 33, 12793-12803.	1.6	11
65	Toward Understanding Liposome-Based siRNA Delivery Vectors: Atomic-Scale Insight into siRNAâ€“Lipid Interactions. Langmuir, 2018, 34, 8685-8693.	1.6	10
66	Relaxation of Copolymeric Dendrimers Built from Alternating Monomers. Macromolecular Theory and Simulations, 2004, 13, 487-496.	0.6	9
67	Phospholipidâ€“Cellulose Interactions: Insight from Atomistic Computer Simulations for Understanding the Impact of Cellulose-Based Materials on Plasma Membranes. Journal of Physical Chemistry B, 2018, 122, 9973-9981.	1.2	9
68	The relaxation spectra of polymer networks with different types of topology, ordering, heterogeneity. Macromolecular Symposia, 2003, 191, 131-140.	0.4	8
69	Asphaltenes as novel thermal conductivity enhancers for liquid paraffin: Insight from in silico modeling. Journal of Molecular Liquids, 2021, , 117112.	2.3	8
70	Theory of relaxation properties of two-dimensional polymer networks, 2. Local dynamic characteristics. Macromolecular Theory and Simulations, 2000, 9, 416-427.	0.6	7
71	Molecular Dynamics Simulations of Hyperbranched PAMAM Vicsek Fractals. Macromolecular Theory and Simulations, 2015, 24, 100-109.	0.6	7
72	Independent adsorption of monovalent cations and cationic polymers at PE/PG lipid membranes. Journal of Physics: Conference Series, 2017, 794, 012010.	0.3	6

#	Article	IF	Citations
73	Controlled Onâ€“Off Switching of Tight-Binding Hydrogen Bonds between Model Cell Membranes and Acetylated Cellulose Surfaces. Langmuir, 2019, 35, 13753-13760.	1.6	6
74	Unsolved problems in the theory of dynamics in homogeneous and heterogeneous polymer networks. Macromolecular Symposia, 2001, 171, 69-78.	0.4	5
75	Collective Dynamics in Lipid Membranes: From Pore Formation to Flip-Flops. , 2009, , 121-139.		3
76	How to control interactions of cellulose-based biomaterials with skin: the role of acidity in the contact area. Soft Matter, 2021, 17, 6507-6518.	1.2	3
77	Theory of long-scale cooperative relaxation of polymer networks. Hydrodynamic interaction effects. , 2000, 7, 11-23.		2
78	Anomalous dynamics of model polymer systems. Journal of Luminescence, 2001, 94-95, 437-440.	1.5	1
79	Atomistic Simulations of Functional Gold Nanoparticles Au144(Sr)60 Interacting with Membranes. Biophysical Journal, 2013, 104, 664a.	0.2	0