Andrey A Gurtovenko

List of Publications by Year
in descending order

79 papers	4,174 citations	94433 37 h-index	114465 63 g-index
82 all docs	82 docs citations	82 times ranked	4237 citing authors

#	Article	IF	Citations
1	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.	4.8	30
2	How to control interactions of cellulose-based biomaterials with skin: the role of acidity in the contact area. Soft Matter, 2021, 17, 6507-6518.	2.7	3
3	Asphaltenes as novel thermal conductivity enhancers for liquid paraffin: Insight from in silico modeling. Journal of Molecular Liquids, 2021, , 117112.	4.9	8
4	Molecular-Level Insight into the Interactions of DNA/Polycation Complexes with Model Cell Membranes. Journal of Physical Chemistry B, 2019, 123, 6505-6514.	2.6	14
5	Controlled Onâ€“Off Switching of Tight-Binding Hydrogen Bonds between Model Cell Membranes and Acetylated Cellulose Surfaces. Langmuir, 2019, 35, 13753-13760.	3.5	6
6	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.	4.6	13
7	Toward realistic computer modeling of paraffin-based composite materials: critical assessment of atomic-scale models of paraffins. RSC Advances, 2019, 9, 38834-38847.	3.6	39
8	Supramolecular complexes of DNA with cationic polymers: The effect of polymer concentration. Polymer, 2018, 142, 277-284.	3.8	16
9	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.	2.6	9
10	Toward Understanding Liposome-Based siRNA Delivery Vectors: Atomic-Scale Insight into siRNAâ€“Lipid Interactions. Langmuir, 2018, 34, 8685-8693.	3.5	10
11	Glycosylation and Lipids Working in Concert Direct CD2 Ectodomain Orientation and Presentation. Journal of Physical Chemistry Letters, 2017, 8, 1060-1066.	4.6	22
12	Molecular-Level Insight into the Interaction of Phospholipid Bilayers with Cellulose. Langmuir, 2017, 33, 12793-12803.	3.5	11
13	Independent adsorption of monovalent cations and cationic polymers at PE/PG lipid membranes. Journal of Physics: Conference Series, 2017, 794, 012010.	0.4	6
14	Molecular-level insight into the interactions of DNA with phospholipid bilayers: barriers and triggers. RSC Advances, 2016, 6, 36425-36432.	3.6	16
15	Adsorption of Synthetic Cationic Polymers on Model Phospholipid Membranes: Insight from Atomic-Scale Molecular Dynamics Simulations. Langmuir, 2016, 32, 10402-10414.	3.5	41
16	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.	4.6	19
17	Atomic-Scale Molecular Dynamics Simulations of DNAâ€“Polycation Complexes: Two Distinct Binding Patterns. Journal of Physical Chemistry B, 2016, 120, 6546-6554.	2.6	31
18	Molecular dynamics simulations of uniaxial deformation of thermoplastic polyimides. Soft Matter, 2016, 12, 3972-3981.	2.7	61

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19	Molecular Mechanism of Calcium-Induced Adsorption of DNA on Zwitterionic Phospholipid Membranes. Journal of Physical Chemistry B, 2015, 119, 6638-6645.	2.6	32
20	Parameterization of electrostatic interactions for molecular dynamics simulations of heterocyclic polymers. Journal of Polymer Science, Part B: Polymer Physics, 2015, 53, 912-923.	2.1	36
21	Molecular Dynamics Simulations of Hyperbranched PAMAM Vicsek Fractals. Macromolecular Theory and Simulations, 2015, 24, 100-109.	1.4	7
22	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.	2.1	45
23	Thermal properties of bulk polyimides: insights from computer modeling versus experiment. Soft Matter, 2014, 10, 1224.	2.7	68
24	Molecular-dynamics simulation of polyimide matrix pre-crystallization near the surface of a single-walled carbon nanotube. RSC Advances, 2014, 4, 830-844.	3.6	51
25	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.	1.0	12
26	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.	3.1	69
27	Electroporation of Asymmetric Phospholipid Membranes. Journal of Physical Chemistry B, 2014, 118, 9909-9918.	2.6	45
28	Atomistic simulations of anionic Au144(SR)60 nanoparticles interacting with asymmetric model lipid membranes. Biochimica Et Biophysica Acta - Biomembranes, 2014, 1838, 2852-2860.	2.6	46
29	Microsecond Atomic-Scale Molecular Dynamics Simulations of Polyimides. Macromolecules, 2013, 46, 6357-6363.	4.8	80
30	Atomistic Simulations of Functional Gold Nanoparticles Au144(Sr)60 Interacting with Membranes. Biophysical Journal, 2013, 104, 664a.	0.5	0
31	Structure of Glycocalyx. Biophysical Journal, 2013, 104, 251a.	0.5	16
32	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.	1.0	37
33	Cationic Dimyristoylphosphatidylcholine and Dioleoyloxytrimethylammonium Propane Lipid Bilayers: Atomistic Insight for Structure and Dynamics. Journal of Physical Chemistry B, 2012, 116, 269-276.	2.6	25
34	Atomistic Simulations of Functional Au₁₄₄(SR)₆₀ Gold Nanoparticles in Aqueous Environment. Journal of Physical Chemistry C, 2012, 116, 9805-9815.	3.1	94
35	Dimethyl sulfoxide enhances GLUT4 translocation through a reduction in GLUT4 endocytosis in insulin-stimulated 3T3-L1 adipocytes. Biochimie, 2011, 93, 697-709.	2.6	18
36	Defect-Mediated Trafficking across Cell Membranes: Insights from in Silico Modeling. Chemical Reviews, 2010, 110, 6077-6103.	47.7	171

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37	Calculation of the electrostatic potential of lipid bilayers from molecular dynamics simulations: Methodological issues. Journal of Chemical Physics, 2009, 130, 215107.	3.0	63
38	Ion Dynamics in Cationic Lipid Bilayer Systems in Saline Solutions. Journal of Physical Chemistry B, 2009, 113, 9226-9234.	2.6	38
39	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.	2.6	23
40	Collective Dynamics in Lipid Membranes: From Pore Formation to Flip-Flops. , 2009, , 121-139.		3
41	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.	2.6	144
42	Complexes Comprised of Charged Dendrimers, Linear Polyelectrolytes, and Counterions: Insight through Coarse-Grained Molecular Dynamics Simulations. Macromolecules, 2008, 41, 4961-4968.	4.8	48
43	Chemically Induced Phospholipid Translocation Across Biological Membranes. Langmuir, 2008, 24, 9656-9660.	3.5	36
44	Role of phosphatidylglycerols in the stability of bacterial membranes. Biochimie, 2008, 90, 930-938.	2.6	106
45	Membrane Potential and Electrostatics of Phospholipid Bilayers with Asymmetric Transmembrane Distribution of Anionic Lipids. Journal of Physical Chemistry B, 2008, 112, 4629-4634.	2.6	88
46	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.	2.6	227
47	The Aqueous and Crystalline Forms of L-Alanine Zwitterion. Journal of Computational and Theoretical Nanoscience, 2008, 5, 277-285.	0.4	19
48	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.	2.6	354
49	l-Alanine in a Droplet of Water:Â A Density-Functional Molecular Dynamics Study. Journal of Physical Chemistry B, 2007, 111, 4227-4234.	2.6	76
50	Atomic-Scale Structure and Electrostatics of Anionic Palmitoyloleoylphosphatidylglycerol Lipid Bilayers with Na+ Counterions. Biophysical Journal, 2007, 92, 1114-1124.	0.5	178
51	Ion Leakage through Transient Water Pores in Protein-Free Lipid Membranes Driven by Transmembrane Ionic Charge Imbalance. Biophysical Journal, 2007, 92, 1878-1890.	0.5	108
52	Lipid Transmembrane Asymmetry and Intrinsic Membrane Potential:Â Two Sides of the Same Coin. Journal of the American Chemical Society, 2007, 129, 5358-5359.	13.7	83
53	Molecular Mechanism for Lipid Flip-Flops. Journal of Physical Chemistry B, 2007, 111, 13554-13559.	2.6	125
54	Ion Transport through Chemically Induced Pores in Protein-Free Phospholipid Membranes. Journal of Physical Chemistry B, 2007, 111, 13379-13382.	2.6	33

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55	Molecular dynamics study of charged dendrimers in salt-free solution: Effect of counterions. Journal of Chemical Physics, 2006, 124, 094904.	3.0	73
56	Generalized Gaussian Structures: Models for Polymer Systems with ComplexTopologies. Advances in Polymer Science, 2005, , 171-282.	0.8	113
57	Effect of Monovalent Salt on Cationic Lipid Membranes As Revealed by Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2005, 109, 21126-21134.	2.6	67
58	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.	13.7	190
59	Asymmetry of lipid bilayers induced by monovalent salt: Atomistic molecular-dynamics study. Journal of Chemical Physics, 2005, 122, 244902.	3.0	105
60	Free Volume Properties of Sphingomyelin, DMPC, DPPC, and PLPC Bilayers. Journal of Computational and Theoretical Nanoscience, 2005, 2, 401-413.	0.4	75
61	Relaxation of Copolymeric Dendrimers Built from Alternating Monomers. Macromolecular Theory and Simulations, 2004, 13, 487-496.	1.4	9
62	Cationic DMPC/DMTAP Lipid Bilayers: Molecular Dynamics Study. Biophysical Journal, 2004, 86, 3461-3472.	0.5	156
63	Viscoelastic Relaxation of Cross-Linked, Alternating Copolymers in the Free-Draining Limit. Macromolecules, 2003, 36, 486-494.	4.8	14
64	Dynamics of dendrimer-based polymer networks. Journal of Chemical Physics, 2003, 119, 7579-7590.	3.0	63
65	The relaxation spectra of polymer networks with different types of topology, ordering, heterogeneity. Macromolecular Symposia, 2003, 191, 131-140.	0.7	8
66	Response of Disordered Polymer Networks to External Fields:Â Regular Lattices Built from Complex Subunits. Macromolecules, 2002, 35, 3288-3295.	4.8	18
67	Rouse Dynamics of Polymer Networks Bearing Dendritic Wedges. Macromolecules, 2002, 35, 7481-7491.	4.8	46
68	Anomalous diffusion and relaxation in macromolecular systems. Journal of Non-Crystalline Solids, 2002, 305, 71-80.	3.1	25
69	Unsolved problems in the theory of dynamics in homogeneous and heterogeneous polymer networks. Macromolecular Symposia, 2001, 171, 69-78.	0.7	5
70	Anomalous dynamics of model polymer systems. Journal of Luminescence, 2001, 94-95, 437-440.	3.1	1
71	Relaxation of disordered polymer networks: Regular lattice made up of small-world Rouse networks. Journal of Chemical Physics, 2001, 115, 4924-4929.	3.0	33
72	Dynamics of inhomogeneous cross-linked polymers consisting of domains of different sizes. Journal of Chemical Physics, 2001, 115, 6785-6793.	3.0	48

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73	Viscoelastic dynamic properties of heterogeneous polymer networks with domain structure. Macromolecular Theory and Simulations, 2000, 9, 388-397.	1.4	18
74	Theory of relaxation properties of two-dimensional polymer networks, 2. Local dynamic characteristics. Macromolecular Theory and Simulations, 2000, 9, 416-427.	1.4	7
75	Theory of long-scale cooperative relaxation of polymer networks. Hydrodynamic interaction effects. , 2000, 7, 11-23.		2
76	Viscoelastic Dynamic Properties of Meshlike Polymer Networks:Â Contributions of Intra- and Interchain Relaxation Processes. Macromolecules, 2000, 33, 6578-6587.	4.8	50
77	Intra- and Interchain Relaxation Processes in Meshlike Polymer Networks. Macromolecules, 1998, 31, 5756-5770.	4.8	49
78	The model theory of viscoelastic relaxation properties of bulk cross-linked polymers. Interchain friction effects. Macromolecular Theory and Simulations, 1997, 6, 523-551.	1.4	15
79	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.	1.4	17