Nikolay Balabaev

List of Publications by Year
in descending order

121	1,931	304368 22	288905 40
papers	citations	h-index	g-index

121	121	121	1385
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	On The Berendsen Thermostat. Molecular Simulation, 1994, 13, 177-187.	0.9	156
2	Molecular dynamics simulation of a polymer chain in solution by collisional dynamics method. Journal of Computational Chemistry, 1996, 17, 1685-1695.	1.5	112
3	Strain softening and hardening of amorphous polymers: Atomistic simulation of bulk mechanics and local dynamics. Europhysics Letters, 2005, 71, 618-624.	0.7	110
4	Molecular Dynamics Simulation of Uniaxial Deformation of Glassy Amorphous Atactic Polystyrene. Macromolecules, 2004, 37, 8785-8793.	2.2	107
5	Effects of Strong Confinement on the Glass-Transition Temperature in Simulated Atactic Polystyrene Films. Macromolecules, 2011, 44, 2299-2310.	2.2	98
6	A Comparison Between Collisional Dynamics and Brownian Dynamics. Molecular Simulation, 1995, 15, 223-231.	0.9	96
7	Molecular-Weight and Cooling-Rate Dependence of SimulatedTgfor Amorphous Polystyrene. Macromolecules, 2003, 36, 8574-8575.	2.2	92
8	Correlated Segmental Dynamics in Amorphous Atactic Polystyrene:â€‰ A Molecular Dynamics Simulation Study. Macromolecules, 2002, 35, 9595-9604.	2.2	74
9	Simulated glass transition in freeâ€standing thin polystyrene films. Journal of Polymer Science, Part B: Polymer Physics, 2010, 48, 1160-1167.	2.4	49
10	Molecular Dynamics Simulation of Thermomechanical Properties of Montmorillonite Crystal. 1. Isolated Clay Nanoplate. Journal of Physical Chemistry B, 2008, 112, 2964-2969.	1.2	48
11	Investigation of Local Motions in Polymers by the Method of Molecular Dynamics. Macromolecules, 1980, 13, 602-608.	2.2	47
12	Molecular Dynamics Simulation of Thermomechanical Properties of Montmorillonite Crystal. II. Hydrated Montmorillonite Crystal. Journal of Physical Chemistry C, 2008, 112, 17056-17062.	1.5	42
13	Molecular dynamics simulations of hydrated unsaturated lipid bilayers in the liquid-crystal phase and comparison to self-consistent field modeling. Physical Review E, 2003, 67, 011909.	0.8	37
14	Molecular Dynamics Simulation of Thermomechanical Properties of Montmorillonite Crystal. 3. Montmorillonite Crystals with PEO Oligomer Intercalates. Journal of Physical Chemistry B, 2008, 112, 3597-3604.	1.2	37
15	Conformational mobility of carbosilane dendrimer: Molecular dynamics simulation. Physical Chemistry Chemical Physics, 2004, 6, 1285.	1.3	36
16	Self-consistent-field modeling of hydrated unsaturated lipid bilayers in the liquid-crystal phase and comparison to molecular dynamics simulations. Physical Review E, 2003, 67, 011910.	0.8	35
17	Computer simulation study of intermolecular voids in unsaturated phosphatidylcholine lipid bilayers. Journal of Chemical Physics, 2005, 122, 084906.	1.2	31
18	Molecular mechanisms of the chain diffusion between crystalline and amorphous fractions in polyethylene. Polymer, 2007, 48, 1802-1813.	1.8	29

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19	Mechanical unfolding of proteins L and G with constant force: Similarities and differences. Journal of Chemical Physics, 2009, 131, 045102.	1.2	29
20	Molecular dynamics study of a lipid bilayer and a polymer liquid. Molecular Physics, 1986, 59, 753-773.	0.8	25
21	Insight into the Structure of Polybutylcarbosilane Dendrimer Melts via Extensive Molecular Dynamics Simulations. Macromolecules, 2017, 50, 432-445.	2.2	25
22	Molecular Dynamics Simulation of Nanostructure of High Free Volume Polymers with SiMe₃ Side Groups. Macromolecules, 2018, 51, 1398-1408.	2.2	23
23	Available Instruments for Analyzing Molecular Dynamics Trajectories. The Open Biochemistry Journal, 2016, 10, 1-11.	0.3	23
24	Plastic deformation of glassy polymethylene: Computer-aided molecular-dynamic simulation. Polymer Science - Series A, 2010, 52, 633-644.	0.4	22
25	Interfacial and topological effects on the glass transition in free-standing polystyrene films. Journal of Chemical Physics, 2017, 146, 203314.	1.2	22
26	Investigating hydrogen bonds in liquid ethylene glycol structure by means of molecular dynamics. Russian Journal of Physical Chemistry A, 2014, 88, 94-102.	0.1	18
27	Efficient calculation of diffracted intensities in the case of nonstationary scattering by biological macromolecules under XFEL pulses. Acta Crystallographica Section D: Biological Crystallography, 2015, 71, 293-303.	2.5	18
28	Simulation of melting in crystalline polyethylene. Journal of Chemical Physics, 2012, 136, 224906.	1.2	17
29	Hybrid Polycarbosilane-Siloxane Dendrimers: Synthesis and Properties. Polymers, 2021, 13, 606.	2.0	17
30	Computer simulation of intramolecular mobility of dendrimers. Journal of Molecular Liquids, 1999, 82, 105-116.	2.3	15
31	Energy storage in plastic deformation of glassy polymethylene. Doklady Physical Chemistry, 2014, 457, 108-111.	0.2	14
32	Studying the cavities in liquid ethyleneglycol. Russian Journal of Physical Chemistry A, 2013, 87, 1145-1150.	0.1	13
33	Soliton solutions in polaron theory. Theoretical and Mathematical Physics(Russian Federation), 1980, 45, 936-938.	0.3	12
34	Molecular dynamics simulations of single siloxane dendrimers: Molecular structure and intramolecular mobility of terminal groups. Journal of Chemical Physics, 2018, 148, 014902.	1.2	12
35	Anisotropy of diffusion in a liquid crystalline system of semi-flexible polymer chains. Physical Chemistry Chemical Physics, 2003, 5, 2410-2416.	1.3	11
36	Properties of unsaturated phospholipid bilayers: Effect of cholesterol. Biochemistry (Moscow) Supplement Series A: Membrane and Cell Biology, 2007, 1, 343-357.	0.3	11

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37	Two-, Three-, and Four-State Events Occur in the Mechanical Unfolding of Small Protein L Using Molecular Dynamics Simulations. Protein and Peptide Letters, 2010, 17, 92-103.	0.4	11
38	Temperature dependence of the structure of a carbosilane dendrimer with terminal cyanobiphenyl groups: Molecular-dynamics simulation. Polymer Science - Series A, 2013, 55, 53-60.	0.4	11
39	A Comparative Study of Intramolecular Mobility of Single Siloxane and Carbosilane Dendrimers via Molecular Dynamics Simulations. Polymers, 2018, 10, 838.	2.0	11
40	Structure and Properties of High and Low Free Volume Polymers Studied by Molecular Dynamics Simulation. Computation, 2019, 7, 27.	1.0	11
41	The effect of a solid wall on polymer chain behavior under shear flow. Journal of Chemical Physics, 1998, 108, 797-806.	1.2	10
42	Right- and left-handed three-helix proteins. II. Similarity and differences in mechanical unfolding of proteins. Proteins: Structure, Function and Bioinformatics, 2014, 82, 90-102.	1.5	10
43	Modeling the structure of liquid monoethanolamine by molecular dynamics. Russian Journal of Physical Chemistry A, 2015, 89, 398-405.	0.1	10
44	Effects of generation number, spacer length and temperature on the structure and intramolecular dynamics of siloxane dendrimer melts: molecular dynamics simulations. Soft Matter, 2020, 16, 3792-3805.	1.2	10
45	Polaron nature of critical size of ammonia cluster. Chemical Physics Letters, 1995, 240, 585-588.	1.2	9
46	Vacancy mobility in polymer crystals. Journal of Experimental and Theoretical Physics, 1999, 88, 586-589.	0.2	9
47	Supersonic motion of vacancies in a polyethylene crystal. Physical Review E, 2001, 64, 036702.	0.8	9
48	Computer Simulation of Gas-Phase Neutralization of Electrospray-Generated Protein Macroions. Journal of Physical Chemistry B, 2012, 116, 5872-5881.	1.2	9
49	Comparative mechanical unfolding studies of spectrin domains R15, R16 and R17. Journal of Structural Biology, 2018, 201, 162-170.	1.3	9
50	Dynamics of Soliton-Like Excitations in a Chain of a Polymer Crystal: Influence of Neighbouring Chains Mobility. Journal of Nonlinear Mathematical Physics, 2001, 8, 305.	0.8	8
51	Extension of chains composed of freely joined elastic segments. Russian Journal of Physical Chemistry B, 2009, 3, 242-246.	0.2	8
52	Molecular dynamic simulation of motion in solid polymers. Rotator phase of n-alkane. Polymer Bulletin, 1984, 12, 303-309.	1.7	7
53	Diffusion of topological solitons and dielectric Î±c relaxation in a polymeric crystal. Journal of Experimental and Theoretical Physics, 2002, 94, 759-769.	0.2	7
54	Molecular dynamics investigation of bond ordering of unsaturated lipids in monolayers. Journal of Biological Physics, 1999, 25, 245-262.	0.7	6

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55	Dynamics of twist point defects with stretching in a polymer crystal. Journal of Experimental and Theoretical Physics, 2000, 91, 515-523.	0.2	6
56	Molecular dynamics simulations of unsaturated lipid bilayers. , 2001, 4348, 215.		6
57	High-temperature quasi-hexagonal phase in the simplest model of a polymer crystal. Doklady Physical Chemistry, 2008, 418, 15-18.	0.2	6
58	Stretching of a semiflexible chain composed of elastic bonds. Polymer Science - Series A, 2010, 52, 655-661.	0.4	6
59	Analysis of local rearrangements in chains during simulation of the plastic deformation of glassy polymethylene. Polymer Science - Series A, 2014, 56, 219-227.	0.4	6
60	Mechanical stability analysis of the protein L immunoglobulinâ€binding domain by full alanine screening using molecular dynamics simulations. Biotechnology Journal, 2015, 10, 386-394.	1.8	6
61	Molecular-dynamic study of liquid ethylenediamine. Russian Journal of Physical Chemistry A, 2016, 90, 1986-1992.	0.1	6
62	Computer Simulation of High-Frequency Heating of a Protonated Poly(ethylene oxide) Chain in a Vacuum. Polymer Science - Series A, 2018, 60, 404-416.	0.4	6
63	Description of Mixed Networks of Đ•Bonds in a Waterâ€“Ethylene Glycol System by Methods of Graph Theory and Delaunay Simplices. Russian Journal of Physical Chemistry A, 2021, 95, 1283-1290.	0.1	6
64	Molecular dynamics simulation of ferredoxin in different electronic states. , 1993, 1921, 375.		5
65	Comparative investigation of lipid membrane systems. , 2002, , .		5
66	Molecular dynamics simulation of a flexible polymer network in a liquid crystal solvent; structure and equilibrium properties. Polymer, 2004, 45, 4857-4866.	1.8	5
67	Molecular Dynamic Simulation of Side-Chain Liquid Crystalline Elastomer Under Load. Macromolecular Symposia, 2007, 252, 101-109.	0.4	5
68	New possibilities of X-ray nanocrystallography of biological macromolecules based on X-ray free-electron lasers. Russian Journal of Physical Chemistry B, 2014, 8, 457-463.	0.2	5
69	Computer simulation of rearrangements in chains of glassy polymethylene subjected at low temperature inelastic deformation. Polymer Science - Series A, 2014, 56, 511-521.	0.4	5
70	Modeling of plastic deformation of glasses in creeping and stress relaxation regimes. Polymer Science - Series D, 2015, 8, 85-91.	0.2	5
71	Structure of a Liquid Monoethanolamineâ€“Water System: Describing Networks of Mixed Hydrogen Bonds. Russian Journal of Physical Chemistry A, 2021, 95, 974-982.	0.1	5
72	Spectral properties of the polaron model of a protein. , 1991, , .		4

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73	Computer modelling of structure and dynamics of C-50 n-paraffin crystal, hexagonal phase of C-50 crystal and ethylene/propylene statistical copolymers. Macromolecular Symposia, 1999, 146, 133-143.	0.4	4
74	Molecular dynamics investigation of polar diacylglycerolipid monolayers: bond ordering properties. , 2000, 4064, 144.		4
75	Modeling of Screw Dislocation Dynamics in Crystalline Polyethylene. Doklady Physical Chemistry, 2002, 384, 101-103.	0.2	4
76	<title>Molecular dynamics study of phosphatidylcholine and diacylglycerolipid bilayers in the liquid crystal phase</title>. , 2003, , .		4
77	Computer simulation of the liquid crystal formation in a semi-flexible polymer system. Macromolecular Symposia, 2003, 191, 191-200.	0.4	4
78	Molecular dynamics simulation of a flexible polymer network in a liquid crystalline solvent; dynamical properties. Polymer, 2004, 45, 8901-8911.	1.8	4
79	Molecular Dynamic Simulation of Side-Chain Liquid Crystalline Elastomer. Macromolecular Symposia, 2006, 237, 119-127.	0.4	4
80	Viscoelasticity of stretched polymer chains: Analytical theory and computer-aided simulation. Polymer Science - Series A, 2008, 50, 1238-1247.	0.4	4
81	Comparison of transition states obtained upon modeling of unfolding of immunoglobulin-binding domains of proteins L and G caused by external action with transition states obtained in the absence of force probed by experiments. Biochemistry (Moscow), 2009, 74, 316-328.	0.7	4
82	On the structures of ethylene glycol, monoethanolamine, and ethylenediamine in the liquid phase. Russian Journal of Physical Chemistry A, 2016, 90, 1000-1005.	0.1	4
83	Molecular dynamics models of pores in the liquid monoethanolamine structure. Russian Journal of Physical Chemistry A, 2016, 90, 100-104.	0.1	4
84	Elastic and Non-elastic Properties of Cadherin Ectodomain: Comparison with Mechanical System. Advances in Intelligent Systems and Computing, 2020, , 555-566.	0.5	4
85	Adsorption of Silicon-Containing Dendrimers: Effects of Chemical Composition, Structure, and Generation Number. Polymers, 2021, 13, 552.	2.0	4
86	Molecular dynamics simulation of a polymer chain in solution by collisional dynamics method. Journal of Computational Chemistry, 1996, 17, 1685-1695.	1.5	4
87	Signal transfer in human protein tyrosine phosphatase PTP1B from allosteric inhibitor P00058. Journal of Biomolecular Structure and Dynamics, 2022, 40, 13823-13832.	2.0	4
88	Simulation of the Drift of a Macromolecular Ion in a Gas under the Action of an Electric Field. Polymer Science - Series A, 2021, 63, 891-901.	0.4	4
89	Selfâ€assembly of domain wall of molecular twist defects in polyethylene crystal. Macromolecular Symposia, 1996, 106, 31-39.	0.4	3
90	Molecular dynamics simulation of thermo-mechanical properties of montmorillonite crystal. Nanotechnologies in Russia, 2009, 4, 676-699.	0.7	3

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91	Viscoelasticity of a stretched polymer chain with ends exposed to a constant force. Polymer Science - Series A, 2011, 53, 1086-1096.	0.4	3
92	Experimental and theoretical studies of mechanical unfolding of different proteins. Biochemistry (Moscow), 2013, 78, 1216-1227.	0.7	3
93	Femtosecond X-ray free-electron lasers: A new tool for studying nanocrystals and single macromolecules. Russian Journal of Physical Chemistry B, 2014, 8, 445-456.	0.2	3
94	Glass-Transition Temperature of Cyclic Polystyrene: A Computational Study. Polymer Science - Series A, 2021, 63, 356-362.	0.4	3
95	Is It Possible to Find an Antimicrobial Peptide That Passes the Membrane Bilayer with Minimal Force Resistance? An Attempt at a Predictive Approach by Molecular Dynamics Simulation. International Journal of Molecular Sciences, 2022, 23, 5997.	1.8	3
96	Molecular dynamics simulations of monolayers containing polyene lipids of biomembranes. , 1998, , .		2
97	Molecular dynamics simulations of unsaturated lipids in monolayers: an investigation of bond ordering. , 1999, , .		2
98	Melting of Crystals Composed of Elastic and Lennard-Jones Particles. Doklady Physical Chemistry, 2002, 382, 66-69.	0.2	2
99	Simulation of the Mechanical Unfolding of the Ubiquitin by Pulling in Different Directions with Constant Speed. Macromolecular Symposia, 2009, 278, 105-113.	0.4	2
100	V-structures of ethylene glycol and monoethanolamine in the temperature range of the liquid phase. Russian Journal of Physical Chemistry A, 2017, 91, 195-200.	0.1	2
101	Description of the hydrogen bond network in liquid 3-amino-1-propanol by graph theory and percolation methods. Radioelektronika, Nanosistemy, Informacionnye Tehnologii, 2020, 12, 61-68.	0.2	2
102	Describing Mixed Networks of Hydrogen Bonds in 1,3-Propanediolâ€“Water Systems. Russian Journal of Physical Chemistry A, 2022, 96, 985-992.	0.1	2
103	<title>Simulation of spin label behavior on a model surface</title>. , 1991, , .		1
104	Molecular dynamics study of C-C bond ordering in diacylglycerolipid monolayers. , 2001, 4348, 207.		1
105	Coarse-grained polyethylene: 1. The simplest model for the orthorhombic crystal. Polymer Science - Series A, 2017, 59, 149-158.	0.4	1
106	Resonance Effects in Highâ€Frequency Heating of Isolated Protonated Poly(ethylene oxide) Chains in a Vacuum. Macromolecular Theory and Simulations, 2019, 28, 1800056.	0.6	1
107	Molecular Simulation of Plastic Deformation of Oligomer Systems. Advanced Structured Materials, 2019, , 303-312.	0.3	1
108	Structure Description of Liquid 1,3-Propanediol and Ethylene Glycol by Graph Theory and Percolation Methods. Russian Journal of Physical Chemistry A, 2020, 94, 1143-1148.	0.1	1

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109	Molecular dynamics simulations of isolated molecules of polyunsaturated lipids. , 1998, 3345, 202.		0
110	Numerical simulation of plastic deformation in polymer crystals. , 1999, , .		0
111	Molecular dynamics study of monolayers consisting of polyunsaturated diacylglycerolipids. , 2002, 4627, 129.		0
112	Molecular Dynamics Simulation of Liquid Crystalline Polymer Networks and Flexible Polymer Network in Liquid Crystal Solution. AIP Conference Proceedings, 2004, , .	0.3	0
113	To the memory of Ãˆmmanuil Ãˆl'evich Shnol'. Russian Mathematical Surveys, 2017, 72, 185-198.	0.2	0
114	Repeated Elements of the Structure of Liquid Monoethanolamine. Doklady Physical Chemistry, 2018, 479, 47-51.	0.2	0
115	Describing the Structure of Spatial Networks of Hydrogen Bonds in Liquids Using the Voronoiâ€“Delaunay Approach. Russian Journal of Physical Chemistry A, 2019, 93, 1082-1087.	0.1	0
116	Viscoelasticity of a Stretched Semiflexible Polymer Chain with Fixed Ends. Polymer Science - Series A, 2021, 63, 180-195.	0.4	0
117	Models of Extended Electron States in Proteins. Topics in Molecular Organization and Engineering, 1991, , 31-40.	0.1	0
118	Microrheological Properties in Polymeric Heterogeneous Media by Collision Dynamics Simulation. , 1998, , 347-348.		0
119	High-Frequency Heating of a Multiply Protonated Poly(ethylene oxide) Chain in a Vacuum. Polymer Science - Series A, 2020, 62, 578-587.	0.4	0
120	Dynamics of Soliton-Like Excitations in a Chain of a Polymer Crystal: Influence of Neighbouring Chains Mobility. Journal of Nonlinear Mathematical Physics, 2001, 8, 305.	0.8	0
121	Simulations of the Stretching of Two Models of Filamentous Actin at a Constant Velocity Using Method of Molecular Dynamics. Lecture Notes on Data Engineering and Communications Technologies, 2022, , 379-385.	0.5	0