

Pavel G Khalatur

List of Publications by Year in descending order

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times ranked

2572
citing authors

#	ARTICLE	IF	CITATIONS
1	Magnetoresponse smart nanocomposites with highly cross-linked polymer matrix. <i>Polymers for Advanced Technologies</i> , 2021, 32, 3922-3933.	3.2	14
2	Supramolecular polymerization: challenges and advantages of various methods in assessing the aggregation mechanism. <i>Nanoscale</i> , 2019, 11, 663-674.	5.6	7
3	Silicone-urea copolymer as a basis for self-organized multiphase nanomaterials. <i>Polymer</i> , 2018, 143, 200-211.	3.8	11
4	Filler reinforcement in cross-linked elastomer nanocomposites: insights from fully atomistic molecular dynamics simulation. <i>Soft Matter</i> , 2016, 12, 5402-5419.	2.7	47
5	Fully atomistic molecular dynamics simulation of nanosilica-filled crosslinked polybutadiene. <i>Chemical Physics Letters</i> , 2016, 653, 90-95.	2.6	38
6	Designing artificial enzymes from scratch: Experimental study and mesoscale simulation. <i>Chemical Physics Letters</i> , 2016, 661, 219-223.	2.6	3
7	A new concept for molecular engineering of artificial enzymes: a multiscale simulation. <i>Soft Matter</i> , 2016, 12, 689-704.	2.7	3
8	Thermal Properties and Topology of Epoxy Networks: A Multiscale Simulation Methodology. <i>Macromolecules</i> , 2015, 48, 206-212.	4.8	73
9	Self-organization of amphiphilic block copolymers in the presence of water: A mesoscale simulation. <i>Chemical Physics Letters</i> , 2014, 605-606, 22-27.	2.6	13
10	Study of the Mechanisms of Filler Reinforcement in Elastomer Nanocomposites. <i>Macromolecules</i> , 2014, 47, 5400-5408.	4.8	67
11	Self-organization of amphiphilic polymers. <i>Polimery</i> , 2014, 59, 74-79.	0.7	8
12	Structural Changes in Lamellar Diblock Copolymer Thin Films upon Swelling in Nonselective Solvents. <i>Macromolecules</i> , 2013, 46, 5786-5795.	4.8	40
13	Nonconventional scenarios of polymer self-assembly. <i>Soft Matter</i> , 2013, 9, 10943.	2.7	13
14	Peptide nanofibrils boost retroviral gene transfer and provide a rapid means for concentrating viruses. <i>Nature Nanotechnology</i> , 2013, 8, 130-136.	31.5	125
15	Effect of nanotube size on the mechanical properties of elastomeric composites. <i>Soft Matter</i> , 2013, 9, 4067.	2.7	29
16	Large-scale atomistic and quantum-mechanical simulations of a Nafion membrane: Morphology, proton solvation and charge transport. <i>Beilstein Journal of Nanotechnology</i> , 2013, 4, 567-587.	2.8	64
17	Impact of Hydrophobic Sequence Patterning on the Coil-to-Globule Transition of Protein-like Polymers. <i>Macromolecules</i> , 2012, 45, 5229-5236.	4.8	77
18	Perpendicular Domain Orientation in Dense Planar Brushes of Diblock Copolymers. <i>Macromolecules</i> , 2012, 45, 4870-4875.	4.8	24

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19	Parallel Algorithm for 3D SCF Simulation of Copolymers With Flexible and Rigid Blocks. <i>Macromolecular Theory and Simulations</i> , 2012, 21, 382-399.	1.4	48
20	Self-Assembling Nanofibers from Thiophene- α -Peptide Diblock Oligomers: A Combined Experimental and Computer Simulations Study. <i>ACS Nano</i> , 2011, 5, 6894-6909.	14.6	41
21	Directed Assembly of Block Copolymers by Sparsely Patterned Substrates. <i>Journal of Physical Chemistry C</i> , 2011, 115, 25185-25200.	3.1	32
22	Self-organizing bioinspired oligothiophene- α -oligopeptide hybrids. <i>Beilstein Journal of Nanotechnology</i> , 2011, 2, 525-544.	2.8	10
23	Microphase separation in regular and random \tilde{N} opolymer melts by DPD simulations. <i>Chemical Physics Letters</i> , 2011, 503, 277-282.	2.6	57
24	A novel strategy for controlling the orientation of cylindrical domains in thin blend copolymer films via α -double phase separation α TM . <i>Chemical Physics Letters</i> , 2010, 487, 297-302.	2.6	10
25	Pattern multiplication by template-guided self-assembly of cylinder-forming copolymers: Field-theoretic and particle-based simulations. <i>Chemical Physics Letters</i> , 2010, 492, 103-108.	2.6	15
26	Mesoscale simulation of polymer electrolyte membranes based on sulfonated poly(ether ether ketone) and Nafion. <i>Soft Matter</i> , 2010, 6, 3939.	2.7	48
27	Large-scale atomistic simulation of a nanosized fibril formed by thiophene- α -peptide α -molecular chimeras α . <i>Soft Matter</i> , 2010, 6, 1453.	2.7	7
28	Self-Assembled Polythiophene- α -Based Nanostructures: Numerical Studies. <i>Macromolecular Theory and Simulations</i> , 2009, 18, 219-246.	1.4	26
29	Effect of Comonomer Sequence Distribution on the Adsorption of Random Copolymers onto Impenetrable Flat Surfaces. <i>Macromolecules</i> , 2009, 42, 2843-2853.	4.8	40
30	Scattering Study of the Conformational Structure and Aggregation Behavior of a Conjugated Polymer Solution. <i>Langmuir</i> , 2009, 25, 4668-4677.	3.5	51
31	Computer Simulation Study of Model Nafion Membrane in Water/Methanol Solvent. <i>Composite Interfaces</i> , 2009, 16, 547-577.	2.3	5
32	Morphology of Nafion Membranes: Microscopic and Mesoscopic Modeling. <i>Topics in Applied Physics</i> , 2009, , 453-483.	0.8	8
33	Microphase separation of diblock copolymers with amphiphilic segment. <i>Soft Matter</i> , 2009, 5, 2896.	2.7	35
34	Nonmonotonic incommensurability effects in lamellar-in-lamellar self-assembled multiblock copolymers. <i>Journal of Chemical Physics</i> , 2009, 130, 204901.	3.0	17
35	Microphase separation in diblock copolymers with amphiphilic block: Local chemical structure can dictate global morphology. <i>Chemical Physics Letters</i> , 2008, 461, 58-63.	2.6	43
36	Silk-inspired α -molecular chimeras α TM : Atomistic simulation of nanoarchitectures based on thiophene- α -peptide copolymers. <i>Chemical Physics Letters</i> , 2008, 461, 64-70.	2.6	19

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37	Nonconventional morphologies in two-length scale block copolymer systems beyond the weak segregation theory. <i>Journal of Chemical Physics</i> , 2008, 128, 244903.	3.0	37
38	Computer simulation of the assembly of gold nanoparticles on DNA fragments via electrostatic interaction. <i>Journal of Chemical Physics</i> , 2008, 128, 124909.	3.0	10
39	Evolutionary Approach in Copolymer Sequence Design. <i>Macromolecular Symposia</i> , 2007, 252, 36-46.	0.7	6
40	Computer Design of Copolymers with Desired Functionalities: Microphase Separation in Diblock Copolymers with Amphiphilic Block. <i>AIP Conference Proceedings</i> , 2007, , .	0.4	1
41	Molecular Bottle Brushes in a Solution of Semiflexible Polyelectrolytes and Block Copolymers with an Oppositely Charged Block: A Molecular Dynamics Simulation. <i>Journal of Physical Chemistry B</i> , 2007, 111, 8360-8368.	2.6	9
42	Diagram of State of Stiff Amphiphilic Macromolecules. <i>Macromolecular Symposia</i> , 2007, 252, 24-35.	0.7	11
43	Highly Cross-Linked Epoxy Resins: An Atomistic Molecular Dynamics Simulation Combined with a Mapping/Reverse Mapping Procedure. <i>Macromolecules</i> , 2007, 40, 8104-8113.	4.8	181
44	Self-Assembled Monolayers of \hat{I}^2 -Alkylated Oligothiophenes on Graphite Substrate: Molecular Dynamics Simulation. <i>Journal of Physical Chemistry C</i> , 2007, 111, 7165-7174.	3.1	25
45	Block Copolymer Based Molecular Motor. <i>Macromolecular Rapid Communications</i> , 2007, 28, 977-980.	3.9	12
46	Semiflexible amphiphilic polymers: Cylindrical-shaped, collagenlike, and toroidal structures. <i>Journal of Chemical Physics</i> , 2006, 124, 144914.	3.0	30
47	Simulation of Gradient Copolymers Synthesis via Conformation-Dependent Graft Copolymerization near a Uniform Adsorbing Surface. <i>Macromolecules</i> , 2006, 39, 8808-8815.	4.8	9
48	Ribbonlike nanostructures from stiff polyanions and short cationic chains. <i>Chemical Physics Letters</i> , 2006, 420, 29-34.	2.6	4
49	The formation of planar ribbonlike aggregates from stiff polyanions in the presence of anisotropic cations. <i>Journal of Chemical Physics</i> , 2006, 125, 154906.	3.0	4
50	Recognition of complex patterned substrates by heteropolymer chains consisting of multiple monomer types. <i>Journal of Chemical Physics</i> , 2006, 124, 174904.	3.0	17
51	Solution properties of charged hydrophobic/hydrophilic copolymers. <i>Current Opinion in Colloid and Interface Science</i> , 2005, 10, 22-29.	7.4	33
52	Adsorption of multiblock copolymers onto a chemically heterogeneous surface: A model of pattern recognition. <i>Journal of Chemical Physics</i> , 2005, 122, 114703.	3.0	49
53	Modeling of Radical Copolymerization near a Selectively Adsorbing Surface: Design of Gradient Copolymers with Long-Range Correlations. <i>Macromolecules</i> , 2005, 38, 2419-2430.	4.8	12
54	Molecular dynamics simulation of the synthesis of protein-like copolymers via conformation-dependent design. <i>New Journal of Physics</i> , 2004, 6, 44-44.	2.9	24

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55	Computer modeling of radical copolymerization under unusual conditions. <i>Journal of Polymer Science Part A</i> , 2004, 42, 5339-5353.	2.3	34
56	Template copolymerization near a patterned surface: Computer simulation. <i>Journal of Chemical Physics</i> , 2004, 121, 6011-6020.	3.0	12
57	HA (Hydrophobic/Amphiphilic) Copolymer Model: A Coil-Globule Transition versus Aggregation. <i>Macromolecules</i> , 2004, 37, 5444-5460.	4.8	73
58	Biomimetic sequence design in functional copolymers. <i>Current Opinion in Solid State and Materials Science</i> , 2004, 8, 3-10.	11.5	35
59	Charged designed copolymers in the presence of multivalent counterions: a molecular dynamics study. <i>New Journal of Physics</i> , 2004, 6, 133-133.	2.9	10
60	Segmentation of Heteropolymer Sequences Specifying Subsequences with Different Composition and Statistical Properties. <i>Macromolecular Theory and Simulations</i> , 2003, 12, 604-613.	1.4	7
61	Self-Consistent Integral Equation Theory for Semiflexible Polyelectrolytes in Poor Solvent. <i>Macromolecular Theory and Simulations</i> , 2003, 12, 339-353.	1.4	17
62	Aggregation and counterion condensation in solution of charged proteinlike copolymers: A molecular-dynamics study. <i>Journal of Chemical Physics</i> , 2003, 119, 1232-1247.	3.0	45
63	Molecular Dispenser: A Conformation-Dependent Design Approach. <i>Macromolecules</i> , 2003, 36, 5047-5050.	4.8	14
64	Solution properties of charged quasi-random copolymers: Integral equation theory. <i>Journal of Chemical Physics</i> , 2003, 119, 6959-6972.	3.0	21
65	Conformational Polymorphism of Amphiphilic Polymers in a Poor Solvent. <i>Macromolecules</i> , 2003, 36, 10103-10111.	4.8	139
66	Computer modeling of synthesis of proteinlike copolymer via copolymerization with simultaneous globule formation. <i>Journal of Chemical Physics</i> , 2003, 118, 8049-8060.	3.0	36
67	Conformation-dependent evolution of copolymer sequences. <i>Physical Review E</i> , 2003, 67, 051901.	2.1	34
68	The influence of hydrogen bonds on the globular structure of HP-copolymers. <i>Macromolecular Symposia</i> , 2003, 201, 29-46.	0.7	5
69	Reconstruction of Protein-Like Globular Structure for Random and Designed Copolymers. <i>Macromolecular Theory and Simulations</i> , 2002, 11, 213-221.	1.4	15
70	Structural Organization of Water-Containing Nafion: The Integral Equation Theory. <i>Macromolecular Theory and Simulations</i> , 2002, 11, 566.	1.4	80
71	Structural Organization of Water-Containing Nafion: A Cellular-Automaton-Based Simulation. <i>Macromolecular Theory and Simulations</i> , 2002, 11, 587.	1.4	59
72	Conformation-Dependent Sequence Design of Copolymers. , 2002, , 333-350.		1

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73	Rheological properties of self-associating polymer systems: nonequilibrium molecular dynamics simulation. <i>Journal of Molecular Liquids</i> , 2001, 91, 205-217.	4.9	13
74	Primary sequences of proteinlike copolymers: "Levy-flight" type long-range correlations. <i>Physical Review E</i> , 2001, 64, 040903.	2.1	77
75	Conformational properties and dynamics of molecular bottle-brushes: A cellular-automaton-based simulation. <i>Macromolecular Theory and Simulations</i> , 2000, 9, 141-155.	1.4	41
76	Phase behavior of polymer containing colloidal dispersions: The integral equation theory. <i>Journal of Chemical Physics</i> , 2000, 113, 7006-7012.	3.0	5
77	Phase behavior of comblike copolymers: The integral equation theory. <i>Journal of Chemical Physics</i> , 2000, 112, 4849-4861.	3.0	17
78	Self-organization of comblike copolymers with end-functionalized side chains: A cellular-automaton-based simulation. <i>Journal of Chemical Physics</i> , 2000, 112, 11069-11079.	3.0	7
79	Order-Disorder Transition in Surface-Induced Nanopattern of Diblock Copolymer Films. <i>Macromolecules</i> , 2000, 33, 150-157.	4.8	53
80	Association of diphilic chains near the solvent critical region. <i>Journal of Chemical Physics</i> , 1999, 111, 2340-2344.	3.0	1
81	Properties of ABCopolymers with a special adsorption-tuned primary structure. <i>Physical Review E</i> , 1999, 59, 3071-3078.	2.1	60
82	Molecular dynamics study of the solution of semiflexible telechelic polymer chains with strongly associating end-groups. <i>Journal of Chemical Physics</i> , 1999, 110, 6039-6049.	3.0	56
83	Conformation-Dependent Sequence Design (Engineering) of ABCopolymers. <i>Physical Review Letters</i> , 1999, 82, 3456-3459.	7.8	164
84	Computer simulation of globules with microstructure. <i>Macromolecular Symposia</i> , 1999, 146, 259-265.	0.7	17
85	Computer simulation studies of aggregates of associating polymers: Influence of low-molecular-weight additives solubilizing the aggregates. <i>Macromolecular Theory and Simulations</i> , 1998, 7, 299-316.	1.4	17
86	Protein-like copolymers: computer simulation. <i>Physica A: Statistical Mechanics and Its Applications</i> , 1998, 249, 253-261.	2.6	122
87	Hybrid MC/RISM technique for simulation of polymer solutions: Monte Carlo+ RISM integral equations. <i>Molecular Physics</i> , 1998, 93, 555-572.	1.7	17
88	Conformation of a polymer chain near the solvent critical region. I. The integral equation theory. <i>Journal of Chemical Physics</i> , 1998, 109, 5108-5118.	3.0	25
89	Conformation of a polymer chain near the solvent critical region. II. Monte Carlo simulation. <i>Journal of Chemical Physics</i> , 1998, 109, 5119-5125.	3.0	17
90	Computer simulation of irreversible gelation of polymers with stickers. <i>Macromolecular Theory and Simulations</i> , 1997, 6, 317-338.	1.4	7

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91	The critical micelle concentration for the solution of polyelectrolyte/neutral block copolymers. Zeitschrift Fur Elektrotechnik Und Elektrochemie, 1996, 100, 857-862.	0.9	13
92	Aggregation processes in self-associating polymer systems: Computer simulation study of micelles in the superstrong segregation regime. Macromolecular Theory and Simulations, 1996, 5, 713-747.	1.4	37
93	Aggregation processes in self-associating polymer systems: A comparative analysis of theoretical and computer simulation data for micelles in the superstrong segregation regime. Macromolecular Theory and Simulations, 1996, 5, 749-757.	1.4	28
94	Computer simulation of solutions of telechelic polymers with associating end-groups. Macromolecular Theory and Simulations, 1996, 5, 877-899.	1.4	28
95	Computer simulation analysis of microstructure formation in monomer and polymer blends involving a glassy component. Macromolecular Theory and Simulations, 1994, 3, 939-961.	1.4	8
96	Molecular motions in a liquid-crystalline lipid bilayer. Molecular dynamics simulation. Die Makromolekulare Chemie, 1987, 188, 3029-3040.	1.1	8
97	Title is missing!. Die Makromolekulare Chemie Rapid Communications, 1982, 3, 709-713.	1.1	78
98	Computer-Aided Conformation-Dependent Design of Copolymer Sequences. , 0, , 1-100.		39