Pavel G Khalatur

List of Publications by Year
in descending order

98 papers	3,234 citations	126907 33 h-index	175258 52 g-index
98 all docs	98 docs citations	98 times ranked	2572 citing authors

#	Article	IF	Citations
1	Highly Cross-Linked Epoxy Resins:â€‰ An Atomistic Molecular Dynamics Simulation Combined with a Mapping/Reverse Mapping Procedure. Macromolecules, 2007, 40, 8104-8113.	4.8	181
2	Conformation-Dependent Sequence Design (Engineering) ofABCopolymers. Physical Review Letters, 1999, 82, 3456-3459.	7.8	164
3	Conformational Polymorphism of Amphiphilic Polymers in a Poor Solvent. Macromolecules, 2003, 36, 10103-10111.	4.8	139
4	Peptide nanofibrils boost retroviral gene transfer and provide a rapid means for concentrating viruses. Nature Nanotechnology, 2013, 8, 130-136.	31.5	125
5	Protein-like copolymers: computer simulation. Physica A: Statistical Mechanics and Its Applications, 1998, 249, 253-261.	2.6	122
6	Structural Organization of Water-Containing Nafion: The Integral Equation Theory. Macromolecular Theory and Simulations, 2002, 11, 566.	1.4	80
7	Title is missing!. Die Makromolekulare Chemie Rapid Communications, 1982, 3, 709-713.	1.1	78
8	Primary sequences of proteinlike copolymers:â€ƒLevy-flightâ€“type long-range correlations. Physical Review E, 2001, 64, 040903.	2.1	77
9	Impact of Hydrophobic Sequence Patterning on the Coil-to-Globule Transition of Protein-like Polymers. Macromolecules, 2012, 45, 5229-5236.	4.8	77
10	HA (Hydrophobic/Amphiphilic) Copolymer Model:Â Coilâ^'Globule Transition versus Aggregation. Macromolecules, 2004, 37, 5444-5460.	4.8	73
11	Thermal Properties and Topology of Epoxy Networks: A Multiscale Simulation Methodology. Macromolecules, 2015, 48, 206-212.	4.8	73
12	Study of the Mechanisms of Filler Reinforcement in Elastomer Nanocomposites. Macromolecules, 2014, 47, 5400-5408.	4.8	67
13	Large-scale atomistic and quantum-mechanical simulations of a Nafion membrane: Morphology, proton solvation and charge transport. Beilstein Journal of Nanotechnology, 2013, 4, 567-587.	2.8	64
14	Properties ofABcopolymers with a special adsorption-tuned primary structure. Physical Review E, 1999, 59, 3071-3078.	2.1	60
15	Structural Organization of Water-Containing Nafion: A Cellular-Automaton-Based Simulation. Macromolecular Theory and Simulations, 2002, 11, 587.	1.4	59
16	Microphase separation in regular and random Ñopolymer melts by DPD simulations. Chemical Physics Letters, 2011, 503, 277-282.	2.6	57
17	Molecular dynamics study of the solution of semiflexible telechelic polymer chains with strongly associating end-groups. Journal of Chemical Physics, 1999, 110, 6039-6049.	3.0	56
18	Orderâ^'Disorder Transition in Surface-Induced Nanopattern of Diblock Copolymer Films. Macromolecules, 2000, 33, 150-157.	4.8	53

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19	Scattering Study of the Conformational Structure and Aggregation Behavior of a Conjugated Polymer Solution. Langmuir, 2009, 25, 4668-4677.	3.5	51
20	Adsorption of multiblock copolymers onto a chemically heterogeneous surface: A model of pattern recognition. Journal of Chemical Physics, 2005, 122, 114703.	3.0	49
21	Mesoscale simulation of polymer electrolyte membranes based on sulfonated poly(ether ether ketone) and Nafion. Soft Matter, 2010, 6, 3939.	2.7	48
22	Parallel Algorithm for 3D SCF Simulation of Copolymers With Flexible and Rigid Blocks. Macromolecular Theory and Simulations, 2012, 21, 382-399.	1.4	48
23	Filler reinforcement in cross-linked elastomer nanocomposites: insights from fully atomistic molecular dynamics simulation. Soft Matter, 2016, 12, 5402-5419.	2.7	47
24	Aggregation and counterion condensation in solution of charged proteinlike copolymers: A molecular-dynamics study. Journal of Chemical Physics, 2003, 119, 1232-1247.	3.0	45
25	Microphase separation in diblock copolymers with amphiphilic block: Local chemical structure can dictate global morphology. Chemical Physics Letters, 2008, 461, 58-63.	2.6	43
26	Conformational properties and dynamics of molecular bottle-brushes: A cellular-automaton-based simulation. Macromolecular Theory and Simulations, 2000, 9, 141-155.	1.4	41
27	Self-Assembling Nanofibers from Thiopheneâ€“Peptide Diblock Oligomers: A Combined Experimental and Computer Simulations Study. ACS Nano, 2011, 5, 6894-6909.	14.6	41
28	Effect of Comonomer Sequence Distribution on the Adsorption of Random Copolymers onto Impenetrable Flat Surfaces. Macromolecules, 2009, 42, 2843-2853.	4.8	40
29	Structural Changes in Lamellar Diblock Copolymer Thin Films upon Swelling in Nonselective Solvents. Macromolecules, 2013, 46, 5786-5795.	4.8	40
30	Computer-Aided Conformation-Dependent Design of Copolymer Sequences. , 0, , 1-100.		39
31	Fully atomistic molecular dynamics simulation of nanosilica-filled crosslinked polybutadiene. Chemical Physics Letters, 2016, 653, 90-95.	2.6	38
32	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
33	Nonconventional morphologies in two-length scale block copolymer systems beyond the weak segregation theory. Journal of Chemical Physics, 2008, 128, 244903.	3.0	37
34	Computer modeling of synthesis of proteinlike copolymer via copolymerization with simultaneous globule formation. Journal of Chemical Physics, 2003, 118, 8049-8060.	3.0	36
35	Biomimetic sequence design in functional copolymers. Current Opinion in Solid State and Materials Science, 2004, 8, 3-10.	11.5	35
36	Microphase separation of diblock copolymers with amphiphilic segment. Soft Matter, 2009, 5, 2896.	2.7	35

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37	Conformation-dependent evolution of copolymer sequences. Physical Review E, 2003, 67, 051901.	2.1	34
38	Computer modeling of radical copolymerization under unusual conditions. Journal of Polymer Science Part A, 2004, 42, 5339-5353.	2.3	34
39	Solution properties of charged hydrophobic/hydrophilic copolymers. Current Opinion in Colloid and Interface Science, 2005, 10, 22-29.	7.4	33
40	Directed Assembly of Block Copolymers by Sparsely Patterned Substrates. Journal of Physical Chemistry C, 2011, 115, 25185-25200.	3.1	32
41	Semiflexible amphiphilic polymers: Cylindrical-shaped, collagenlike, and toroidal structures. Journal of Chemical Physics, 2006, 124, 144914.	3.0	30
42	Effect of nanotube size on the mechanical properties of elastomeric composites. Soft Matter, 2013, 9, 4067.	2.7	29
43	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
44	Computer simulation of solutions of telechelic polymers with associating end-groups. Macromolecular Theory and Simulations, 1996, 5, 877-899.	1.4	28
45	Selfâ€Assembled Polythiopheneâ€Based Nanostructures: Numerical Studies. Macromolecular Theory and Simulations, 2009, 18, 219-246.	1.4	26
46	Conformation of a polymer chain near the solvent critical region. I. The integral equation theory. Journal of Chemical Physics, 1998, 109, 5108-5118.	3.0	25
47	Self-Assembled Monolayers of Î²-Alkylated Oligothiophenes on Graphite Substrate:â€‰ Molecular Dynamics Simulation. Journal of Physical Chemistry C, 2007, 111, 7165-7174.	3.1	25
48	Molecular dynamics simulation of the synthesis of protein-like copolymers via conformation-dependent design. New Journal of Physics, 2004, 6, 44-44.	2.9	24
49	Perpendicular Domain Orientation in Dense Planar Brushes of Diblock Copolymers. Macromolecules, 2012, 45, 4870-4875.	4.8	24
50	Solution properties of charged quasi-random copolymers: Integral equation theory. Journal of Chemical Physics, 2003, 119, 6959-6972.	3.0	21
51	Silk-inspired â€˜molecular chimerasâ€™: Atomistic simulation of nanoarchitectures based on thiopheneâ€“peptide copolymers. Chemical Physics Letters, 2008, 461, 64-70.	2.6	19
52	Computer simulation studies of aggregates of associating polymers: Influence of low-molecular-weight additives solubilizing the aggregates. Macromolecular Theory and Simulations, 1998, 7, 299-316.	1.4	17
53	Hybrid MC/RISM technique for simulation of polymer solutions: Monte Carlo+ RISM integral equations. Molecular Physics, 1998, 93, 555-572.	1.7	17
54	Conformation of a polymer chain near the solvent critical region. II. Monte Carlo simulation. Journal of Chemical Physics, 1998, 109, 5119-5125.	3.0	17

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55	Computer simulation of globules with microstructure. Macromolecular Symposia, 1999, 146, 259-265.	0.7	17
56	Phase behavior of comblike copolymers: The integral equation theory. Journal of Chemical Physics, 2000, 112, 4849-4861.	3.0	17
57	Self-Consistent Integral Equation Theory for Semiflexible Polyelectrolytes in Poor Solvent. Macromolecular Theory and Simulations, 2003, 12, 339-353.	1.4	17
58	Recognition of complex patterned substrates by heteropolymer chains consisting of multiple monomer types. Journal of Chemical Physics, 2006, 124, 174904.	3.0	17
59	Nonmonotonic incommensurability effects in lamellar-in-lamellar self-assembled multiblock copolymers. Journal of Chemical Physics, 2009, 130, 204901.	3.0	17
60	Reconstruction of Protein-Like Globular Structure for Random and Designed Copolymers. Macromolecular Theory and Simulations, 2002, 11, 213-221.	1.4	15
61	Pattern multiplication by template-guided self-assembly of cylinder-forming copolymers: Field-theoretic and particle-based simulations. Chemical Physics Letters, 2010, 492, 103-108.	2.6	15
62	Molecular Dispenser:Â Conformation-Dependent Design Approach. Macromolecules, 2003, 36, 5047-5050.	4.8	14
63	Magnetoresponsive smart nanocomposites with highly crossâ€linked polymer matrix. Polymers for Advanced Technologies, 2021, 32, 3922-3933.	3.2	14
64	The critical micelle concentration for the solution of polyelectrolyte/neutral blockâ€copolymers. Zeitschrift Fur Elektrotechnik Und Elektrochemie, 1996, 100, 857-862.	0.9	13
65	Rheological properties of self-associating polymer systems: nonequilibrium molecular dynamics simulation. Journal of Molecular Liquids, 2001, 91, 205-217.	4.9	13
66	Nonconventional scenarios of polymer self-assembly. Soft Matter, 2013, 9, 10943.	2.7	13
67	Self-organization of amphiphilic block copolymers in the presence of water: A mesoscale simulation. Chemical Physics Letters, 2014, 605-606, 22-27.	2.6	13
68	Template copolymerization near a patterned surface: Computer simulation. Journal of Chemical Physics, 2004, 121, 6011-6020.	3.0	12
69	Modeling of Radical Copolymerization near a Selectively Adsorbing Surface:â€‰ Design of Gradient Copolymers with Long-Range Correlations. Macromolecules, 2005, 38, 2419-2430.	4.8	12
70	Block Copolymer Based Molecular Motor. Macromolecular Rapid Communications, 2007, 28, 977-980.	3.9	12
71	Diagram of State of Stiff Amphiphilic Macromolecules. Macromolecular Symposia, 2007, 252, 24-35.	0.7	11
72	Silicone-urea copolymer as a basis for self-organized multiphase nanomaterials. Polymer, 2018, 143, 200-211.	3.8	11

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73	Charged designed copolymers in the presence of multivalent counterions: a molecular dynamics study. New Journal of Physics, 2004, 6, 133-133.	2.9	10
74	Computer simulation of the assembly of gold nanoparticles on DNA fragments via electrostatic interaction. Journal of Chemical Physics, 2008, 128, 124909.	3.0	10
75	A novel strategy for controlling the orientation of cylindrical domains in thin blend copolymer films via â€˜double phase separationâ€™. Chemical Physics Letters, 2010, 487, 297-302.	2.6	10
76	Self-organizing bioinspired oligothiopheneâ€“oligopeptide hybrids. Beilstein Journal of Nanotechnology, 2011, 2, 525-544.	2.8	10
77	Simulation of Gradient Copolymers Synthesis via Conformation-Dependent Graft Copolymerization near a Uniform Adsorbing Surface. Macromolecules, 2006, 39, 8808-8815.	4.8	9
78	Molecular Bottle Brushes in a Solution of Semiflexible Polyelectrolytes and Block Copolymers with an Oppositely Charged Block:Â A Molecular Dynamics Simulationâ€. Journal of Physical Chemistry B, 2007, 111, 8360-8368.	2.6	9
79	Molecular motions in a liquid-crystalline lipid bilayer. Molecular dynamics simulation. Die Makromolekulare Chemie, 1987, 188, 3029-3040.	1.1	8
80	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
81	Morphology of Nafion Membranes: Microscopic and Mesoscopic Modeling. Topics in Applied Physics, 2009, , 453-483.	0.8	8
82	Self-organization of amphiphilic polymers. Polimery, 2014, 59, 74-79.	0.7	8
83	Computer simulation of irreversible gelation of polymers with stickers. Macromolecular Theory and Simulations, 1997, 6, 317-338.	1.4	7
84	Self-organization of comblike copolymers with end-functionalized side chains: A cellular-automaton-based simulation. Journal of Chemical Physics, 2000, 112, 11069-11079.	3.0	7
85	Segmentation of Heteropolymer Sequences Specifying Subsequences with Different Composition and Statistical Properties. Macromolecular Theory and Simulations, 2003, 12, 604-613.	1.4	7
86	Large-scale atomistic simulation of a nanosized fibril formed by thiopheneâ€“peptide â€œmolecular chimerasâ€• Soft Matter, 2010, 6, 1453.	2.7	7
87	Supramolecular polymerization: challenges and advantages of various methods in assessing the aggregation mechanism. Nanoscale, 2019, 11, 663-674.	5.6	7
88	Evolutionary Approach in Copolymer Sequence Design. Macromolecular Symposia, 2007, 252, 36-46.	0.7	6
89	Phase behavior of polymer containing colloidal dispersions: The integral equation theory. Journal of Chemical Physics, 2000, 113, 7006-7012.	3.0	5
90	The influence of hydrogen bonds on the globular structure of HP-copolymers. Macromolecular Symposia, 2003, 201, 29-46.	0.7	5

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91	Computer Simulation Study of Model Nafion Membrane in Water/Methanol Solvent. Composite Interfaces, 2009, 16, 547-577.	2.3	5
92	Ribbonlike nanostructures from stiff polyanions and short cationic chains. Chemical Physics Letters, 2006, 420, 29-34.	2.6	4
93	The formation of planar ribbonlike aggregates from stiff polyanions in the presence of anisotropic cations. Journal of Chemical Physics, 2006, 125, 154906.	3.0	4
94	Designing artificial enzymes from scratch: Experimental study and mesoscale simulation. Chemical Physics Letters, 2016, 661, 219-223.	2.6	3
95	A new concept for molecular engineering of artificial enzymes: a multiscale simulation. Soft Matter, 2016, 12, 689-704.	2.7	3
96	Association of diphilic chains near the solvent critical region. Journal of Chemical Physics, 1999, 111, 2340-2344.	3.0	1
97	Computer Design of Copolymers with Desired Functionalities: Microphase Separation in Diblock Copolymers with Amphiphilic Block. AIP Conference Proceedings, 2007, , .	0.4	1
98	Conformation-Dependent Sequence Design of Copolymers. , 2002, , 333-350.		1