Marcus MÃ¹/₄ller

List of Publications by Year in descending order

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362 papers 20,982 citations

70 h-index 132 g-index

367 all docs

367 docs citations

367 times ranked

15609 citing authors

#	Article	IF	Citations
1	Is the "Bricks-and-Mortar―Mesophase Bicontinuous? Dynamic Simulations of Miktoarm Block Copolymer/Homopolymer Blends. Macromolecules, 2022, 55, 745-758.	4.8	3
2	Phase Separation of Regular, Quasi-Two-Dimensional <i>AB</i> Copolymer Networks. Macromolecules, 2022, 55, 1279-1294.	4.8	4
3	Memory in the relaxation of a polymer density modulation. Journal of Chemical Physics, 2022, 156, 124902.	3.0	4
4	A versatile setup for studying size and charge-state selected polyanionic nanoparticles. Review of Scientific Instruments, 2022, 93, 043301.	1.3	2
5	Phase Separation of Randomly Cross-Linked Diblock Copolymers. Macromolecules, 2022, 55, 5567-5580.	4.8	1
6	Wall-Spring Thermostat: A Novel Approach for Controlling the Dynamics of Soft Coarse-Grained Polymer Fluids at Surfaces. Macromolecules, 2022, 55, 5550-5566.	4.8	2
7	Molecular simulations and hydrodynamic theory of nonlocal shear-stress correlations in supercooled fluids. Journal of Chemical Physics, 2022, 157, .	3.0	5
8	Bottlebrush Block Copolymer Assembly in Ultraconfined Films: Effect of Substrate Selectivity. Macromolecules, 2021, 54, 2079-2089.	4.8	8
9	Lithographically Defined Cross-Linkable Top Coats for Nanomanufacturing with High-χ Block Copolymers. ACS Applied Materials & Samp; Interfaces, 2021, 13, 11224-11236.	8.0	10
10	How does curvature affect the free-energy barrier of stalk formation? Small vesicles vs apposing, planar membranes. European Biophysics Journal, 2021, 50, 253-264.	2.2	9
11	Dynamics and Rheology of Polymer Melts <i>via</i> Hierarchical Atomistic, Coarse-Grained, and Slip-Spring Simulations. Macromolecules, 2021, 54, 2740-2762.	4.8	40
12	The effect of polydispersity, shape fluctuations and curvature on small unilamellar vesicle small-angle X-ray scattering curves. Journal of Applied Crystallography, 2021, 54, 557-568.	4. 5	7
13	Cresting the Coulomb Barrier of Polyanionic Metal Clusters. Physical Review Letters, 2021, 126, 133001.	7.8	6
14	Nonequilibrium Processes in Polymer Membrane Formation: Theory and Experiment. Chemical Reviews, 2021, 121, 14189-14231.	47.7	63
15	Thermal Imaging of Block Copolymers with Sub-10 nm Resolution. ACS Nano, 2021, 15, 9005-9016.	14.6	4
16	Dynamics of Nonequilibrium Single-Chain Conformations in Triblock Copolymers. Macromolecules, 2021, 54, 6296-6311.	4.8	4
17	Dynamics of Long Entangled Polyisoprene Melts <i>via</i> Multiscale Modeling. Macromolecules, 2021, 54, 8693-8713.	4.8	14
18	Liquid and Droplet Transport in Brush-Coated Cylindrical Nanochannels: Brush-Assisted Droplet Formation. Journal of Physical Chemistry B, 2021, 125, 442-449.	2.6	2

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19	Evaporation-Induced Liquid Expansion and Bubble Formation in Binary Mixtures. Physical Review Letters, 2021, 126, 028003.	7.8	5
20	Size and charge-state dependence of detachment energies of polyanionic silver clusters. Journal of Chemical Physics, 2021, 155, 164303.	3.0	3
21	Microscopic Model to Quantify the Difference of Energy-Transfer Rates between Bonded and Nonbonded Monomers in Polymers. Macromolecules, 2021, 54, 10969-10983.	4.8	6
22	Multifunctional Top-Coats Strategy for DSA of High-χ Block Copolymers. Journal of Photopolymer Science and Technology = [Fotoporima Konwakai Shi], 2021, 34, 11-16.	0.3	2
23	Selection of Advances in Theory and Simulation during the First Decade of <i>ACS Macro Letters</i> ACS Macro Letters, 2021, 10, 1629-1635.	4.8	2
24	Process-directed self-assembly of copolymers: Results of and challenges for simulation studies. Progress in Polymer Science, 2020, 101, 101198.	24.7	53
25	Selfâ€Assembly of Surfaceâ€Acylated Cellulose Nanowhiskers and Graphene Oxide for Multiresponsive Janusâ€Like Films with Timeâ€Dependent Dryâ€State Structures. Small, 2020, 16, e2004922.	10.0	7
26	Nonequilibrium Molecular Conformations in Polymer Self-Consistent Field Theory. Macromolecules, 2020, 53, 10457-10474.	4.8	9
27	Prediction of Kinetically Stable Nanotheranostic Superstructures: Integral of First-Passage Times from Constrained Simulations. Biomacromolecules, 2020, 21, 5008-5020.	5.4	4
28	Symmetric Diblock Copolymers in Cylindrical Confinement: A Way to Chiral Morphologies?. ACS Applied Materials & Diblock Copolymers in Cylindrical Confinement: A Way to Chiral Morphologies?. ACS Applied Materials & Diblock Copolymers in Cylindrical Confinement: A Way to Chiral Morphologies?. ACS Applied Materials & Diblock Copolymers in Cylindrical Confinement: A Way to Chiral Morphologies?. ACS Applied Materials & Diblock Copolymers in Cylindrical Confinement: A Way to Chiral Morphologies?. ACS Applied Materials & Diblock Copolymers in Cylindrical Confinement: A Way to Chiral Morphologies?. ACS Applied Materials & Diblock Copolymers in Cylindrical Confinement: A Way to Chiral Morphologies?.	8.0	4
29	Kinetic Pathways of Block Copolymer Directed Self-Assembly: Insights from Efficient Continuum Modeling. ACS Nano, 2020, 14, 13986-13994.	14.6	21
30	Cathodoluminescence nano-characterization of individual GaN/AlN quantum disks embedded in nanowires. Applied Physics Letters, 2020, 117, 133106.	3.3	3
31	Multiresponsive Janusâ€Like Films: Selfâ€Assembly of Surfaceâ€Acylated Cellulose Nanowhiskers and Graphene Oxide for Multiresponsive Janusâ€Like Films with Timeâ€Dependent Dryâ€State Structures (Small) Tj E	TQ ql ol 0.	7 8 4314 rg8
32	Quantitative Synaptic Biology: A Perspective on Techniques, Numbers and Expectations. International Journal of Molecular Sciences, 2020, 21, 7298.	4.1	3
33	Impact of Molecular Architecture on Defect Removal in Lamella-Forming Triblock Copolymers. Macromolecules, 2020, 53, 5337-5349.	4.8	7
34	Rheology of symmetric diblock copolymers. Computational Materials Science, 2019, 169, 109107.	3.0	9
35	Anomalous Ostwald Ripening Enables 2D Polymer Crystals via Fast Evaporation. Physical Review Letters, 2019, 123, 207801.	7.8	18
36	Processing Pathways Decide Polymer Properties at the Molecular Level. Macromolecules, 2019, 52, 7146-7156.	4.8	105

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37	Controlled Spacing between Nanopatterned Regions in Block Copolymer Films Obtained by Utilizing Substrate Topography for Local Film Thickness Differentiation. ACS Applied Materials & Samp; Interfaces, 2019, 11, 35247-35254.	8.0	18
38	Collective Short-Time Dynamics in Multicomponent Polymer Melts. Macromolecules, 2019, 52, 7704-7720.	4.8	19
39	Thermodynamically reversible paths of the first fusion intermediate reveal an important role for membrane anchors of fusion proteins. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 2571-2576.	7.1	65
40	Interface Repulsion and Lamellar Structures in Thin Films of Homopolymer Blends due to Thermal Oscillations. Physical Review Letters, 2019, 122, 237801.	7.8	3
41	Engineering Scale Simulation of Nonequilibrium Network Phases for Battery Electrolytes. Macromolecules, 2019, 52, 2050-2062.	4.8	13
42	Nanoscale mapping of carrier recombination in GaAs/AlGaAs core-multishell nanowires by cathodoluminescence imaging in a scanning transmission electron microscope. Applied Physics Letters, 2019, 115, 243102.	3.3	4
43	Role of Penetrability into a Brush-Coated Surface in Directed Self-Assembly of Block Copolymers. ACS Applied Materials & Samp; Interfaces, 2019, 11, 3571-3581.	8.0	7
44	Functional Macromolecular Systems: Kinetic Pathways to Obtain Tailored Structures. Macromolecular Chemistry and Physics, 2019, 220, 1800334.	2.2	29
45	Multi-architecture Monte-Carlo (MC) simulation of soft coarse-grained polymeric materials: SOft coarse grained Monte-Carlo Acceleration (SOMA). Computer Physics Communications, 2019, 235, 463-476.	7.5	38
46	Highly Ordered Mesoporous Hydroxide Thin Films through Self-Assembly of Size-Tailored Nanobuilding Blocks: A Theoretical-Experimental Approach. Chemistry of Materials, 2019, 31, 322-330.	6.7	23
47	Role of translational entropy in spatially inhomogeneous, coarse-grained models. Journal of Chemical Physics, 2018, 148, .	3.0	8
48	A Detailed Examination of the Topological Constraints of Lamellae-Forming Block Copolymers. Macromolecules, 2018, 51, 2110-2124.	4.8	19
49	Diblock Copolymers with Similar Glass Transition Temperatures in Both Blocks for Comparing Shear Orientation Processes with DPD Computer Simulations. Macromolecular Chemistry and Physics, 2018, 219, 1700559.	2.2	15
50	Nanomaterial interactions with biomembranes: Bridging the gap between soft matter models and biological context. Biointerphases, 2018, 13, 028501.	1.6	23
51	Continuum models for directed self-assembly. Molecular Systems Design and Engineering, 2018, 3, 295-313.	3.4	23
52	Metastable Prepores in Tension-Free Lipid Bilayers. Physical Review Letters, 2018, 120, 128103.	7.8	47
53	Fabrication of Ellipsoidal Mesostructures in Block Copolymers via a Step-Shear Deformation. Macromolecules, 2018, 51, 275-281.	4.8	7
54	Direct imaging of Indium-rich triangular nanoprisms self-organized formed at the edges of InGaN/GaN core-shell nanorods. Scientific Reports, 2018, 8, 16026.	3.3	19

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55	Numerical algorithms for solving self-consistent field theory reversely for block copolymer systems. Journal of Chemical Physics, 2018, 149, 214104.	3.0	6
56	Step-Shear Deformation of Block Copolymers. Macromolecules, 2018, 51, 8386-8405.	4.8	3
57	Kinetics of pattern formation in symmetric diblock copolymer melts. Journal of Chemical Physics, 2018, 148, 204908.	3.0	19
58	Phase separation in mixed polymer brushes on nanoparticle surfaces enables the generation of anisotropic nanoarchitectures. Soft Matter, 2018, 14, 4551-4557.	2.7	21
59	Nanopatterning of Solvent between Apposing Planar Brushes under Pressure. Macromolecules, 2018, 51, 6387-6394.	4.8	2
60	Transitions between Lamellar Orientations in Shear Flow. Macromolecules, 2018, 51, 4642-4659.	4.8	21
61	A multi-chain polymer slip-spring model with fluctuating number of entanglements: Density fluctuations, confinement, and phase separation. Journal of Chemical Physics, 2017, 146, 014903.	3.0	34
62	Process-Accessible States of Block Copolymers. Physical Review Letters, 2017, 118, 067801.	7.8	23
63	Uniform Distance Scaling Behavior of Planet–Satellite Nanostructures Made by Star Polymers. Langmuir, 2017, 33, 2017-2026.	3.5	28
64	Membrane stress profiles from self-consistent field theory. Journal of Chemical Physics, 2017, 146, 104901.	3.0	16
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66	Molecular Dynamics Simulation of Alkylthiol Self-Assembled Monolayers on Liquid Mercury. Langmuir, 2017, 33, 744-754.	3.5	6
67	Formation of ordered mesostructured TiO ₂ thin films: a soft coarse-grained simulation study. Physical Chemistry Chemical Physics, 2017, 19, 28249-28262.	2.8	18
68	Rupturing the hemi-fission intermediate in membrane fission under tension: Reaction coordinates, kinetic pathways, and free-energy barriers. Journal of Chemical Physics, 2017, 147, 064906.	3.0	12
69	Generalization of the swelling method to measure the intrinsic curvature of lipids. Journal of Chemical Physics, 2017, 147, 224902.	3.0	1
70	Functional Poly(<i>N</i> -isopropylacrylamide)/Poly(acrylic acid) Mixed Brushes for Controlled Manipulation of Nanoparticles. Macromolecules, 2016, 49, 5256-5265.	4.8	13
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74	eMC: A Monte Carlo scheme with energy conservation. Europhysics Letters, 2016, 114, 20001.	2.0	4
75	Thermodynamics and Kinetics of Defect Motion and Annihilation in the Self-Assembly of Lamellar Diblock Copolymers. Macromolecules, 2016, 49, 6126-6138.	4.8	38
76	Process-directed self-assembly of multiblock copolymers: Solvent casting vs spray coating. European Physical Journal: Special Topics, 2016, 225, 1785-1803.	2.6	8
77	Dynamics and Structure of Monolayer Polymer Crystallites on Graphene. Nano Letters, 2016, 16, 6994-7000.	9.1	21
78	Alkyl-Based Surfactants at a Liquid Mercury Surface: Computer Simulation of Structure, Self-Assembly, and Phase Behavior. Journal of Physical Chemistry Letters, 2016, 7, 1546-1553.	4.6	6
79	Directed self-assembly of block copolymers by chemical or topographical guiding patterns: Optimizing molecular architecture, thin-film properties, and kinetics. Progress in Polymer Science, 2016, 54-55, 47-75.	24.7	122
80	Kinetics of Nanoscale Self-Assembly Measured on Liquid Drops by Macroscopic Optical Tensiometry: From Mercury to Water and Fluorocarbons. Journal of the American Chemical Society, 2016, 138, 2585-2591.	13.7	5
81	Defect annihilation in chemo-epitaxial directed self-assembly: Computer simulation and Self-Consistent Field Theory. Materials Research Society Symposia Proceedings, 2015, 1750, 12.	0.1	2
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83	Calculation of membrane bending rigidity using field-theoretic umbrella sampling. Journal of Chemical Physics, 2015, 143, 243155.	3.0	14
84	Mechanism of the Cassie-Wenzel transition via the atomistic and continuum string methods. Journal of Chemical Physics, 2015, 142, 104701.	3.0	35
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86	Kinetics of directed self-assembly of block copolymers on chemically patterned substrates. Journal of Physics: Conference Series, 2015, 640, 012010.	0.4	16
87	Morphology Modulation of Multicomponent Polymer Brushes in Selective Solvent by Patterned Surfaces. Macromolecules, 2015, 48, 213-228.	4.8	6
88	Mechanics of membrane fusion/pore formation. Chemistry and Physics of Lipids, 2015, 185, 109-128.	3.2	50
89	Poly($\langle i \rangle N \langle l \rangle$ -isopropylacrylamide)-Based Mixed Brushes: A Computer Simulation Study. ACS Applied Materials & Samp; Interfaces, 2015, 7, 12450-12462.	8.0	36
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93	Defects in the Self-Assembly of Block Copolymers and Their Relevance for Directed Self-Assembly. Annual Review of Chemical and Biomolecular Engineering, 2015, 6, 187-216.	6.8	114
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101	Defect Removal in the Course of Directed Self-Assembly is Facilitated in the Vicinity of the Order-Disorder Transition. Physical Review Letters, 2014, 113, 168301.	7.8	97
102	Mixed brush of chemically and physically adsorbed polymers under shear: Inverse transport of the physisorbed species. Journal of Chemical Physics, 2014, 140, 014901.	3.0	12
103	Collective Lipid Bilayer Dynamics Excited by Surface Acoustic Waves. Physical Review Letters, 2014, 113, 118102.	7.8	16
104	Measuring the composition-curvature coupling in binary lipid membranes by computer simulations. Journal of Chemical Physics, 2014, 141, 194902.	3.0	13
105	Arm Retraction Dynamics and Bistability of a Three-Arm Star Polymer in a Nanopore. Macromolecules, 2014, 47, 2156-2168.	4.8	8
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107	Directed transport of polymer drops on vibrating superhydrophobic substrates: a molecular dynamics study. Soft Matter, 2014, 10, 4373.	2.7	18
108	Conformational Properties of Semiflexible Chains at Nematic Ordering Transitions in Thin Films: A Monte Carlo Simulation. Macromolecules, 2014, 47, 1206-1220.	4.8	32

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109	Rigorous simulation and optimization of the lithography/directed self-assembly co-process. Proceedings of SPIE, 2014, , .	0.8	O
110	Dynamical Simulations of Coarse Grain Polymeric Systems: Rouse and Entangled Dynamics. Macromolecules, 2013, 46, 6287-6299.	4.8	59
111	Computational Approaches for the Dynamics of Structure Formation in Self-Assembling Polymeric Materials. Annual Review of Materials Research, 2013, 43, 1-34.	9.3	75
112	Interbilayer repulsion forces between tension-free lipid bilayers from simulation. Soft Matter, 2013, 9, 10705.	2.7	22
113	Fusion Proteins - Different Tools for Different Jobs?. Biophysical Journal, 2013, 104, 664a.	0.5	0
114	Correlation between surface topography and slippage: a Molecular Dynamics study. Soft Matter, 2013, 9, 3613.	2.7	32
115	Theoretically informed entangled polymer simulations: linear and non-linear rheology of melts. Soft Matter, 2013, 9, 2030.	2.7	43
116	Exploring thermodynamic stability of the stalk fusion-intermediate with three-dimensional self-consistent field theory calculations. Soft Matter, 2013, 9, 4097.	2.7	13
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118	Mechanisms of Vesicle Spreading on Surfaces: Coarse-Grained Simulations. Langmuir, 2013, 29, 4335-4349.	3.5	34
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121	The role of inertia and coarse-graining on the transverse modes of lipid bilayers. Europhysics Letters, 2012, 97, 68010.	2.0	15
122	Random Block Copolymers: Structure, Dynamics, and Mechanical Properties in the Bulk and at Selective Substrates. Macromolecules, 2012, 45, 9841-9853.	4.8	19
123	Polymers at Interfaces and Surfaces and in Confined Geometries. , 2012, , 387-416.		7
124	Properties of Random Block Copolymer Morphologies: Molecular Dynamics and Single-Chain-in-Mean-Field Simulations. Macromolecules, 2012, 45, 1107-1117.	4.8	37
125	Directed Assembly of Non-equilibrium ABA Triblock Copolymer Morphologies on Nanopatterned Substrates. ACS Nano, 2012, 6, 5440-5448.	14.6	50
126	Translationally Invariant Slip-Spring Model for Entangled Polymer Dynamics. Physical Review Letters, 2012, 109, 148302.	7.8	102

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127	Free Energy of Defects in Ordered Assemblies of Block Copolymer Domains. ACS Macro Letters, 2012, 1, 418-422.	4.8	107
128	Geometry-Controlled Interface Localization-Delocalization Transition in Block Copolymers. Physical Review Letters, 2012, 109, 087801.	7.8	12
129	Test of a scaling hypothesis for the structure factor of disordered diblock copolymer melts. Soft Matter, 2012, 8, 11310.	2.7	34
130	Nonequilibrium Simulations of Lamellae Forming Block Copolymers under Steady Shear: A Comparison of Dissipative Particle Dynamics and Brownian Dynamics. Macromolecules, 2012, 45, 8109-8116.	4.8	32
131	Transition Path from Two Apposed Membranes to a Stalk Obtained by a Combination of Particle Simulations and String Method. Physical Review Letters, 2012, 108, 228103.	7.8	47
132	Line-Tension Controlled Mechanism for Influenza Fusion. PLoS ONE, 2012, 7, e38302.	2.5	63
133	Polymer–solid contacts described by soft, coarse-grained models. Physical Chemistry Chemical Physics, 2011, 13, 10491.	2.8	38
134	Molecular transport and flow past hard and soft surfaces: computer simulation of model systems. Journal of Physics Condensed Matter, 2011, 23, 184105.	1.8	11
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136	Quasi-Block Copolymers: Design, Synthesis, and Evidence for Their Formation in Solution and in the Melt. Macromolecules, 2011, 44, 9773-9781.	4.8	18
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140	Phase Behavior of Polymerâ€Containing Systems: Recent Advances Through Computer Simulation. Macromolecular Theory and Simulations, 2011, 20, 600-613.	1.4	9
141	An Alternate Path for Fusion and its Exploration by Field-Theoretic Means. Current Topics in Membranes, 2011, 68, 295-323.	0.9	8
142	Monte-Carlo simulation of ternary blends of block copolymers and homopolymers. Journal of Chemical Physics, 2011, 135, 114904.	3.0	13
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145	Photovoltaically rechargeable fuel cell accumulator for energy self-sufficient microsystems., 2011,,.		1
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155	Remediation of Line Edge Roughness in Chemical Nanopatterns by the Directed Assembly of Overlying Block Copolymer Films. Macromolecules, 2010, 43, 2334-2342.	4.8	81
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157	Simulations of theoretically informed coarse grain models of polymeric systems. Faraday Discussions, 2010, 144, 111-125.	3.2	53
158	Self-Assembly in Thin Films of Mixtures of Block Copolymers and Homopolymers Interacting by Hydrogen Bonds. Macromolecules, 2010, 43, 7734-7743.	4.8	35
159	Theoretically informed coarse grain simulations of polymeric systems. Journal of Chemical Physics, 2009, 131, 084903.	3.0	113
160	Nucleation in A/B/AB blends: Interplay between microphase assembly and macrophase separation. Journal of Chemical Physics, 2009, 130, 154902.	3.0	24
161	Hydrodynamic boundary condition of polymer melts at simple and complex surfaces. Computer Physics Communications, 2009, 180, 600-604.	7. 5	10
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164	Microphase Separation of Mixed Polymer Brushes: Dependence of the Morphology on Grafting Density, Composition, Chain-Length Asymmetry, Solvent Quality, and Selectivity. Journal of Physical Chemistry B, 2009, 113, 11384-11402.	2.6	78
165	Microphase Separation of Diblock Copolymer Brushes in Selective Solvents: Single-Chain-in-Mean-Field Simulations and Integral Geometry Analysis. Macromolecules, 2009, 42, 2251-2264.	4.8	51
166	Coarse-grained models for fluids and their mixtures: Comparison of Monte Carlo studies of their phase behavior with perturbation theory and experiment. Journal of Chemical Physics, 2009, 130, 044101.	3.0	51
167	Comparison of Simulations of Lipid Membranes with Membranes of Block Copolymers. Advances in Polymer Science, 2009, , 43-85.	0.8	10
168	Conformational Changes of a Single Semiflexible Macromolecule Near an Adsorbing Surface: A Monte Carlo Simulation. Journal of Physical Chemistry B, 2009, 113, 3653-3668.	2.6	28
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170	MonteÂCarlo Simulation of Coarse Grain Polymeric Systems. Physical Review Letters, 2009, 102, 197801.	7.8	126
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