

# Juan J De Pablo

## List of Publications by Year in descending order

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235  
papers

20,792  
citations

9428

76  
h-index

12940

136  
g-index

237  
all docs

237  
docs citations

237  
times ranked

15337  
citing authors

#	ARTICLE	IF	CITATIONS
1	Autonomous materials systems from active liquid crystals. <i>Nature Reviews Materials</i> , 2021, 6, 437-453.	23.3	53
2	Transformation between elastic dipoles, quadrupoles, octupoles, and hexadecapoles driven by surfactant self-assembly in nematic emulsion. <i>Science Advances</i> , 2021, 7, .	4.7	9
3	Combining Particle-Based Simulations and Machine Learning to Understand Defect Kinetics in Thin Films of Symmetric Diblock Copolymers. <i>Macromolecules</i> , 2021, 54, 10074-10085.	2.2	11
4	Prolate and oblate chiral liquid crystal spheroids. <i>Science Advances</i> , 2020, 6, eaba6728.	4.7	27
5	Formation, Stability, and Annihilation of the Stitched Morphology in Block Copolymer Thin Films. <i>Macromolecules</i> , 2020, 53, 10446-10456.	2.2	3
6	Cuboidal liquid crystal phases under multiaxial geometrical frustration. <i>Soft Matter</i> , 2020, 16, 870-880.	1.2	8
7	Soft crystal martensites: An in situ resonant soft x-ray scattering study of a liquid crystal martensitic transformation. <i>Science Advances</i> , 2020, 6, eaay5986.	4.7	20
8	Fluctuations and phase transitions of uniaxial and biaxial liquid crystals using a theoretically informed Monte Carlo and a Landau free energy density. <i>Journal of Physics Condensed Matter</i> , 2019, 31, 175101.	0.7	1
9	Free energy of metal-organic framework self-assembly. <i>Journal of Chemical Physics</i> , 2019, 150, 104502.	1.2	18
10	Influence of Homopolymer Addition in Templated Assembly of Cylindrical Block Copolymers. <i>ACS Nano</i> , 2019, 13, 4073-4082.	7.3	3
11	Structure and proton conduction in sulfonated poly(ether ether ketone) semi-permeable membranes: a multi-scale computational approach. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 9362-9375.	1.3	4
12	Thermally reconfigurable Janus droplets with nematic liquid crystalline and isotropic perfluorocarbon oil compartments. <i>Soft Matter</i> , 2019, 15, 2580-2590.	1.2	19
13	Reconfigurable Multicompartment Emulsion Drops Formed by Nematic Liquid Crystals and Immiscible Perfluorocarbon Oils. <i>Langmuir</i> , 2019, 35, 16312-16323.	1.6	12
14	SSAGES: Software Suite for Advanced General Ensemble Simulations. <i>Journal of Chemical Physics</i> , 2018, 148, 044104.	1.2	83
15	<i>In Silico</i> Measurement of Elastic Moduli of Nematic Liquid Crystals. <i>Physical Review Letters</i> , 2018, 120, 107801.	2.9	16
16	A Detailed Examination of the Topological Constraints of Lamellae-Forming Block Copolymers. <i>Macromolecules</i> , 2018, 51, 2110-2124.	2.2	19
17	Light-activated helical inversion in cholesteric liquid crystal microdroplets. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2018, 115, 4334-4339.	3.3	30
18	Optimizing self-consistent field theory block copolymer models with X-ray metrology. <i>Molecular Systems Design and Engineering</i> , 2018, 3, 376-389.	1.7	13

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19	Interplay of structure, elasticity, and dynamics in actin-based nematic materials. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, E124-E133.	3.3	73
20	Mechanisms of Directed Self-Assembly in Cylindrical Hole Confinements. Macromolecules, 2018, 51, 2418-2427.	2.2	4
21	Amphiphile-Induced Phase Transition of Liquid Crystals at Aqueous Interfaces. ACS Applied Materials & Interfaces, 2018, 10, 37618-37624.	4.0	23
22	Defect Annihilation Pathways in Directed Assembly of Lamellar Block Copolymer Thin Films. ACS Nano, 2018, 12, 9974-9981.	7.3	38
23	Layered nested Markov chain Monte Carlo. Journal of Chemical Physics, 2018, 149, 072326.	1.2	9
24	Molecular Structure of Canonical Liquid Crystal Interfaces. Journal of the American Chemical Society, 2017, 139, 3841-3850.	6.6	56
25	Segregation of liquid crystal mixtures in topological defects. Nature Communications, 2017, 8, 15064.	5.8	25
26	Spherical nematic shells with a prolate ellipsoidal core. Soft Matter, 2017, 13, 7465-7472.	1.2	13
27	Derivation of Multiple Covarying Material and Process Parameters Using Physics-Based Modeling of X-ray Data. Macromolecules, 2017, 50, 7783-7793.	2.2	26
28	Water Flux Induced Reorientation of Liquid Crystals. ACS Central Science, 2017, 3, 1345-1349.	5.3	9
29	Electrostatic confinement and manipulation of DNA molecules for genome analysis. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, 13400-13405.	3.3	25
30	Parallel $O(N)$ Stokes <sup>TM</sup> solver towards scalable Brownian dynamics of hydrodynamically interacting objects in general geometries. Journal of Chemical Physics, 2017, 146, 244114.	1.2	14
31	Educating local radial basis functions using the highest gradient of interest in three dimensional geometries. International Journal for Numerical Methods in Engineering, 2017, 110, 603-617.	1.5	1
32	Understanding Atomic-Scale Behavior of Liquid Crystals at Aqueous Interfaces. Journal of Chemical Theory and Computation, 2017, 13, 237-244.	2.3	31
33	Design of surface patterns with optimized thermodynamic driving forces for the directed self-assembly of block copolymers in lithographic applications. Molecular Systems Design and Engineering, 2017, 2, 567-580.	1.7	11
34	Lattice Boltzmann simulation of asymmetric flow in nematic liquid crystals with finite anchoring. Journal of Chemical Physics, 2016, 144, 084905.	1.2	30
35	Directed self-assembly of nematic liquid crystals on chemically patterned surfaces: morphological states and transitions. Soft Matter, 2016, 12, 8595-8605.	1.2	23
36	Structural Transitions in Cholesteric Liquid Crystal Droplets. ACS Nano, 2016, 10, 6484-6490.	7.3	66

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37	Topological defects in liquid crystals as templates for molecular self-assembly. <i>Nature Materials</i> , 2016, 15, 106-112.	13.3	211
38	Sculpting bespoke mountains: Determining free energies with basis expansions. <i>Journal of Chemical Physics</i> , 2015, 143, 044101.	1.2	11
39	Stimuli-Responsive Cubosomes Formed from Blue Phase Liquid Crystals. <i>Advanced Materials</i> , 2015, 27, 6892-6898.	11.1	44
40	Graphoepitaxial assembly of cylinder forming block copolymers in cylindrical holes. <i>Journal of Polymer Science, Part B: Polymer Physics</i> , 2015, 53, 430-441.	2.4	7
41	Liquid Crystal Enabled Early Stage Detection of Beta Amyloid Formation on Lipid Monolayers. <i>Advanced Functional Materials</i> , 2015, 25, 6050-6060.	7.8	79
42	Homeotropic nano-particle assembly on degenerate planar nematic interfaces: films and droplets. <i>Soft Matter</i> , 2015, 11, 5067-5076.	1.2	12
43	The effects of geometry and chemistry of nanopatterned substrates on the directed self-assembly of block-copolymer melts. , 2015, , .		2
44	Interplay of Surface Energy and Bulk Thermodynamic Forces in Ordered Block Copolymer Droplets. <i>Macromolecules</i> , 2015, 48, 4717-4723.	2.2	11
45	Molecular pathways for defect annihilation in directed self-assembly. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2015, 112, 14144-14149.	3.3	98
46	Theoretically informed Monte Carlo simulation of liquid crystals by sampling of alignment-tensor fields. <i>Journal of Chemical Physics</i> , 2015, 143, 044107.	1.2	22
47	Self-consistent description of electrokinetic phenomena in particle-based simulations. <i>Journal of Chemical Physics</i> , 2015, 143, 014108.	1.2	8
48	Liquid crystal free energy relaxation by a theoretically informed Monte Carlo method using a finite element quadrature approach. <i>Journal of Chemical Physics</i> , 2015, 143, 243157.	1.2	13
49	Defect Removal in the Course of Directed Self-Assembly is Facilitated in the Vicinity of the Order-Disorder Transition. <i>Physical Review Letters</i> , 2014, 113, 168301.	2.9	97
50	Surface Adsorption in Nonpolarizable Atomic Models. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 5616-5624.	2.3	4
51	Measuring liquid crystal elastic constants with free energy perturbations. <i>Soft Matter</i> , 2014, 10, 882-893.	1.2	42
52	Basis Function Sampling: A New Paradigm for Material Property Computation. <i>Physical Review Letters</i> , 2014, 113, 190602.	2.9	17
53	Free energy landscapes of the encapsulation mechanism of DNA nucleobases onto carbon nanotubes. <i>RSC Advances</i> , 2014, 4, 1310-1321.	1.7	15
54	Evolutionary Optimization of Directed Self-Assembly of Triblock Copolymers on Chemically Patterned Substrates. <i>ACS Macro Letters</i> , 2014, 3, 747-752.	2.3	64

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55	Control of Directed Self-Assembly in Block Polymers by Polymeric Topcoats. <i>Macromolecules</i> , 2014, 47, 3520-3527.	2.2	36
56	Reversible Switching of Liquid Crystalline Order Permits Synthesis of Homogeneous Populations of Dipolar Patchy Microparticles. <i>Advanced Functional Materials</i> , 2014, 24, 6219-6226.	7.8	26
57	The Materials Genome Initiative, the interplay of experiment, theory and computation. <i>Current Opinion in Solid State and Materials Science</i> , 2014, 18, 99-117.	5.6	160
58	Block Copolymer Assembly on Nanoscale Patterns of Polymer Brushes Formed by Electrohydrodynamic Jet Printing. <i>ACS Nano</i> , 2014, 8, 6606-6613.	7.3	52
59	Dynamical Simulations of Coarse Grain Polymeric Systems: Rouse and Entangled Dynamics. <i>Macromolecules</i> , 2013, 46, 6287-6299.	2.2	59
60	Computational Approaches for the Dynamics of Structure Formation in Self-Assembling Polymeric Materials. <i>Annual Review of Materials Research</i> , 2013, 43, 1-34.	4.3	75
61	Colloid-Liquid Crystal Gels that Respond to Biomolecular Interactions. <i>Small</i> , 2013, 9, 2785-2792.	5.2	18
62	Presentation of Large DNA Molecules for Analysis as Nanoconfined Dumbbells. <i>Macromolecules</i> , 2013, 46, 8356-8368.	2.2	39
63	An experimentally-informed coarse-grained 3-site-per-nucleotide model of DNA: Structure, thermodynamics, and dynamics of hybridization. <i>Journal of Chemical Physics</i> , 2013, 139, 144903.	1.2	191
64	Evolutionary pattern design for copolymer directed self-assembly. <i>Soft Matter</i> , 2013, 9, 11467.	1.2	57
65	Nematic-Field-Driven Positioning of Particles in Liquid Crystal Droplets. <i>Physical Review Letters</i> , 2013, 111, 227801.	2.9	50
66	Chemical Patterns for Directed Self-Assembly of Lamellae-Forming Block Copolymers with Density Multiplication of Features. <i>Macromolecules</i> , 2013, 46, 1415-1424.	2.2	201
67	Scalable simulations for directed self-assembly patterning with the use of GPU parallel computing. , 2012, , .		1
68	Directed Assembly of Non-equilibrium ABA Triblock Copolymer Morphologies on Nanopatterned Substrates. <i>ACS Nano</i> , 2012, 6, 5440-5448.	7.3	50
69	Parallel $\hat{I}^2$ -Sheet Vibrational Couplings Revealed by 2D IR Spectroscopy of an Isotopically Labeled Macrocycle: Quantitative Benchmark for the Interpretation of Amyloid and Protein Infrared Spectra. <i>Journal of the American Chemical Society</i> , 2012, 134, 19118-19128.	6.6	91
70	Free Energy of Defects in Ordered Assemblies of Block Copolymer Domains. <i>ACS Macro Letters</i> , 2012, 1, 418-422.	2.3	107
71	An immersed boundary method for Brownian dynamics simulation of polymers in complex geometries: Application to DNA flowing through a nanoslit with embedded nanopits. <i>Journal of Chemical Physics</i> , 2012, 136, 014901.	1.2	48
72	Morphology of Lamellae-Forming Block Copolymer Films between Two Orthogonal Chemically Nanopatterned Striped Surfaces. <i>Physical Review Letters</i> , 2012, 108, 065502.	2.9	34

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73	Symmetric Diblock Copolymers Confined by Two Nanopatterned Surfaces. <i>Macromolecules</i> , 2012, 45, 2588-2596.	2.2	25
74	Nonequilibrium Simulations of Lamellae Forming Block Copolymers under Steady Shear: A Comparison of Dissipative Particle Dynamics and Brownian Dynamics. <i>Macromolecules</i> , 2012, 45, 8109-8116.	2.2	32
75	Nonbulk Complex Structures in Thin Films of Symmetric Block Copolymers on Chemically Nanopatterned Surfaces. <i>Macromolecules</i> , 2012, 45, 3986-3992.	2.2	40
76	Effects of 3D microwell culture on growth kinetics and metabolism of human embryonic stem cells. <i>Biotechnology and Applied Biochemistry</i> , 2012, 59, 88-96.	1.4	15
77	Density of States-Based Molecular Simulations. <i>Annual Review of Chemical and Biomolecular Engineering</i> , 2012, 3, 369-394.	3.3	55
78	Modulation of Wnt/ $\beta$ -catenin signaling in human embryonic stem cells using a 3-D microwell array. <i>Biomaterials</i> , 2012, 33, 2041-2049.	5.7	68
79	Pattern Dimensions and Feature Shapes of Ternary Blends of Block Copolymer and Low Molecular Weight Homopolymers Directed To Assemble on Chemically Nanopatterned Surfaces. <i>ACS Nano</i> , 2011, 5, 5673-5682.	7.3	35
80	Morphologies of Linear Triblock Copolymers from Monte Carlo Simulations. <i>Macromolecules</i> , 2011, 44, 5490-5497.	2.2	51
81	Influence of Nanorod Inclusions on Structure and Primitive Path Network of Polymer Nanocomposites at Equilibrium and Under Deformation. <i>Macromolecules</i> , 2011, 44, 1034-1045.	2.2	91
82	Cavitation and Crazeing in Rod-Containing Nanocomposites. <i>Macromolecules</i> , 2011, 44, 5498-5509.	2.2	61
83	Coarse-Grained Simulations of Macromolecules: From DNA to Nanocomposites. <i>Annual Review of Physical Chemistry</i> , 2011, 62, 555-574.	4.8	126
84	A coarse-grain three-site-per-nucleotide model for DNA with explicit ions. <i>Journal of Chemical Physics</i> , 2011, 135, 165104.	1.2	54
85	Endotoxin-Induced Structural Transformations in Liquid Crystalline Droplets. <i>Science</i> , 2011, 332, 1297-1300.	6.0	339
86	Effect of trehalose on the interaction of Alzheimer's A $\beta$ -peptide and anionic lipid monolayers. <i>Biochimica Et Biophysica Acta - Biomembranes</i> , 2011, 1808, 26-33.	1.4	17
87	Flux Tempered Metadynamics. <i>Journal of Statistical Physics</i> , 2011, 145, 932-945.	0.5	32
88	Three-dimensional Directed Assembly of Block Copolymers together with Two-dimensional Square and Rectangular Nanolithography. <i>Advanced Materials</i> , 2011, 23, 3692-3697.	11.1	66
89	Monte-Carlo simulation of ternary blends of block copolymers and homopolymers. <i>Journal of Chemical Physics</i> , 2011, 135, 114904.	1.2	13
90	A molecular view of vapor deposited glasses. <i>Journal of Chemical Physics</i> , 2011, 134, 194903.	1.2	80

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91	The microwell control of embryoid body size in order to regulate cardiac differentiation of human embryonic stem cells. <i>Biomaterials</i> , 2010, 31, 1885-1893.	5.7	184
92	Mechanism and dynamics of block copolymer directed assembly with density multiplication on chemically patterned surfaces. <i>Journal of Vacuum Science and Technology B: Nanotechnology and Microelectronics</i> , 2010, 28, C6B13-C6B19.	0.6	10
93	Shape control and density multiplication of cylinder-forming ternary block copolymer-homopolymer blend thin films on chemical patterns. <i>Journal of Vacuum Science and Technology B: Nanotechnology and Microelectronics</i> , 2010, 28, C6B24-C6B29.	0.6	7
94	Graphoepitaxial assembly of asymmetric ternary blends of block copolymers and homopolymers. <i>Nanotechnology</i> , 2010, 21, 495301.	1.3	14
95	Solution Structures of Rat Amylin Peptide: Simulation, Theory, and Experiment. <i>Biophysical Journal</i> , 2010, 98, 443-451.	0.2	51
96	Interpolation in the Directed Assembly of Block Copolymers on Nanopatterned Substrates: Simulation and Experiments. <i>Macromolecules</i> , 2010, 43, 3446-3454.	2.2	131
97	Remediation of Line Edge Roughness in Chemical Nanopatterns by the Directed Assembly of Overlying Block Copolymer Films. <i>Macromolecules</i> , 2010, 43, 2334-2342.	2.2	81
98	Simulations of theoretically informed coarse grain models of polymeric systems. <i>Faraday Discussions</i> , 2010, 144, 111-125.	1.6	53
99	Mechanical properties of antiplasticized polymer nanostructures. <i>Soft Matter</i> , 2010, 6, 2475.	1.2	63
100	Directed Assembly of a Cylinder-Forming Diblock Copolymer: Topographic and Chemical Patterns. <i>Macromolecules</i> , 2010, 43, 6495-6504.	2.2	57
101	Hydrodynamic effects on the translocation rate of a polymer through a pore. <i>Journal of Chemical Physics</i> , 2009, 131, 044904.	1.2	27
102	Theoretically informed coarse grain simulations of polymeric systems. <i>Journal of Chemical Physics</i> , 2009, 131, 084903.	1.2	113
103	Association of Helical $\beta$ -Peptides and their Aggregation Behavior from the Potential of Mean Force in Explicit Solvent. <i>Biophysical Journal</i> , 2009, 96, 4349-4362.	0.2	15
104	Tethered DNA dynamics in shear flow. <i>Journal of Chemical Physics</i> , 2009, 130, 234902.	1.2	36
105	Monte Carlo Simulation of Coarse Grain Polymeric Systems. <i>Physical Review Letters</i> , 2009, 102, 197801.	2.9	126
106	Theoretically informed coarse grain simulations of block copolymer melts: method and applications. <i>Soft Matter</i> , 2009, 5, 4858.	1.2	91
107	Fluorinated Quaternary Ammonium Salts as Dissolution Aids for Polar Polymers in Environmentally Benign Supercritical Carbon Dioxide. <i>Chemistry of Materials</i> , 2009, 21, 3125-3135.	3.2	13
108	Multiple free energy minima in systems of confined tethered polymers toward soft nanomechanical bistable elements. <i>Soft Matter</i> , 2009, 5, 3694.	1.2	4

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109	Elongation and migration of single DNA molecules in microchannels using oscillatory shear flows. Lab on A Chip, 2009, 9, 2348.	3.1	74
110	Molecular plasticity of polymeric glasses in the elastic regime. Physical Review E, 2008, 77, 041502.	0.8	71
111	Directed Copolymer Assembly on Chemical Substrate Patterns: A Phenomenological and Single-Chain-in-Mean-Field Simulations Study of the Influence of Roughness in the Substrate Pattern. Langmuir, 2008, 24, 1284-1295.	1.6	70
112	The effect of hydrodynamic interactions on the dynamics of DNA translocation through pores. Journal of Chemical Physics, 2008, 128, 085102.	1.2	57
113	Hierarchical Assembly of Nanoparticle Superstructures from Block Copolymer-Nanoparticle Composites. Physical Review Letters, 2008, 100, 148303.	2.9	126
114	Monte Carlo Simulations of a Coarse Grain Model for Block Copolymers and Nanocomposites. Macromolecules, 2008, 41, 4989-5001.	2.2	198
115	Density Multiplication and Improved Lithography by Directed Block Copolymer Assembly. Science, 2008, 321, 936-939.	6.0	1,099
116	Rapid Directed Assembly of Block Copolymer Films at Elevated Temperatures. Macromolecules, 2008, 41, 2759-2761.	2.2	145
117	A single-molecule barcoding system using nanoslits for DNA analysis. Proceedings of the National Academy of Sciences of the United States of America, 2007, 104, 2673-2678.	3.3	285
118	A coarse grain model for DNA. Journal of Chemical Physics, 2007, 126, 084901.	1.2	271
119	Nanoparticles in nematic liquid crystals: Interactions with nanochannels. Journal of Chemical Physics, 2007, 127, 124702.	1.2	34
120	Directed Self-Assembly of Block Copolymers for Nanolithography: Fabrication of Isolated Features and Essential Integrated Circuit Geometries. ACS Nano, 2007, 1, 168-175.	7.3	424
121	Fast Computation of Many-Particle Hydrodynamic and Electrostatic Interactions in a Confined Geometry. Physical Review Letters, 2007, 98, 140602.	2.9	134
122	Calculation of local mechanical properties of filled polymers. Physical Review E, 2007, 75, 031803.	0.8	96
123	Dimensions and Shapes of Block Copolymer Domains Assembled on Lithographically Defined Chemically Patterned Substrates. Macromolecules, 2007, 40, 90-96.	2.2	137
124	Engineering the Stem Cell Microenvironment. Biotechnology Progress, 2007, 23, 18-23.	1.3	114
125	Concentration dependence of shear and extensional rheology of polymer solutions: Brownian dynamics simulations. Journal of Rheology, 2006, 50, 137-167.	1.3	80
126	Fabrication of Complex Three-Dimensional Nanostructures from Self-Assembling Block Copolymer Materials on Two-Dimensional Chemically Patterned Templates with Mismatched Symmetry. Physical Review Letters, 2006, 96, 036104.	2.9	110



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127	Cross-stream-line migration in confined flowing polymer solutions: Theory and simulation. <i>Physics of Fluids</i> , 2006, 18, 123101.	1.6	59
128	Cross-Stream Migration of Flexible Molecules in a Nanochannel. <i>Physical Review Letters</i> , 2006, 96, 224505.	2.9	66
129	Effects of trehalose on the phase behavior of DPPC-cholesterol unilamellar vesicles. <i>Biochimica Et Biophysica Acta - Biomembranes</i> , 2006, 1758, 65-73.	1.4	77
130	Directed assembly of copolymer materials on patterned substrates: Balance of simple symmetries in complex structures. <i>Journal of Polymer Science, Part B: Polymer Physics</i> , 2006, 44, 2589-2604.	2.4	19
131	Morphology of multi-component polymer systems: single chain in mean field simulation studies. <i>Soft Matter</i> , 2006, 2, 573-583.	1.2	134
132	3-D microwell culture of human embryonic stem cells. <i>Biomaterials</i> , 2006, 27, 6032-6042.	5.7	216
133	Inhibition of human embryonic stem cell differentiation by mechanical strain. <i>Journal of Cellular Physiology</i> , 2006, 206, 126-137.	2.0	143
134	Influence of Confinement on the Fragility of Antiplasticized and Pure Polymer Films. <i>Physical Review Letters</i> , 2006, 97, 045502.	2.9	181
135	NlogN method for hydrodynamic interactions of confined polymer systems: Brownian dynamics. <i>Journal of Chemical Physics</i> , 2006, 125, 164906.	1.2	32
136	Platelet cryopreservation using a trehalose and phosphate formulation. <i>Biotechnology and Bioengineering</i> , 2005, 92, 79-90.	1.7	19
137	Molecular and multiscale modeling in chemical engineering - current view and future perspectives. <i>AIChE Journal</i> , 2005, 51, 2371-2376.	1.8	47
138	Mechanism and kinetics of ordering in diblock copolymer thin films on chemically nanopatterned substrates. <i>Journal of Polymer Science, Part B: Polymer Physics</i> , 2005, 43, 3444-3459.	2.4	89
139	Local dynamic mechanical properties in model free-standing polymer thin films. <i>Journal of Chemical Physics</i> , 2005, 122, 144712.	1.2	75
140	Modulating Membrane Properties: The Effect of Trehalose and Cholesterol on a Phospholipid Bilayer. <i>Journal of Physical Chemistry B</i> , 2005, 109, 24173-24181.	1.2	63
141	Phase behavior of freeze-dried phospholipid-cholesterol mixtures stabilized with trehalose. <i>Biochimica Et Biophysica Acta - Biomembranes</i> , 2005, 1713, 57-64.	1.4	72
142	Interactions of Liquid Crystal-Forming Molecules with Phospholipid Bilayers Studied by Molecular Dynamics Simulations. <i>Biophysical Journal</i> , 2005, 89, 3141-3158.	0.2	20
143	Directed Assembly of Block Copolymer Blends into Nonregular Device-Oriented Structures. <i>Science</i> , 2005, 308, 1442-1446.	6.0	912
144	Influence of confinement on the vibrational density of states and the Boson peak in a polymer glass. <i>Journal of Chemical Physics</i> , 2004, 120, 9371-9375.	1.2	36

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145	Shear-induced migration in flowing polymer solutions: Simulation of long-chain DNA in microchannels. <i>Journal of Chemical Physics</i> , 2004, 120, 2513-2529.	1.2	228
146	Simulation of the effects of chain architecture on the sorption of ethylene in polyethylene. <i>Journal of Chemical Physics</i> , 2004, 120, 11304-11315.	1.2	42
147	Effect of pH, Counter Ion, and Phosphate Concentration on the Glass Transition Temperature of Freeze-Dried Sugar-Phosphate Mixtures. <i>Pharmaceutical Research</i> , 2004, 21, 1615-1621.	1.7	53
148	Cryopreservation of adherent human embryonic stem cells. <i>Biotechnology and Bioengineering</i> , 2004, 88, 299-312.	1.7	124
149	Ethylene and 1-Hexene Sorption in LLDPE under Typical Gas Phase Reactor Conditions: A Priori Simulation and Modeling for Prediction of Experimental Observations. <i>Macromolecules</i> , 2004, 37, 9139-9150.	2.2	59
150	A Microfluidic System for Large DNA Molecule Arrays. <i>Analytical Chemistry</i> , 2004, 76, 5293-5301.	3.2	175
151	Simulation of Vapor-Liquid Phase Equilibria of Primary Alcohols and Alcohol-Alkane Mixtures. <i>Journal of Physical Chemistry B</i> , 2004, 108, 10071-10076.	1.2	37
152	Investigation of Transition States in Bulk and Freestanding Film Polymer Glasses. <i>Physical Review Letters</i> , 2004, 92, 155505.	2.9	59
153	Effect of sugar-phosphate mixtures on the stability of DPPC membranes in dehydrated systems. <i>Cryobiology</i> , 2004, 48, 81-89.	0.3	32
154	Epitaxial self-assembly of block copolymers on lithographically defined nanopatterned substrates. <i>Nature</i> , 2003, 424, 411-414.	18.7	1,594
155	Diffusion of Sucrose and $\pm$ -Trehalose in Aqueous Solutions. <i>Journal of Physical Chemistry A</i> , 2003, 107, 936-943.	1.1	117
156	Calculation of interfacial tension from density of states. <i>Journal of Chemical Physics</i> , 2003, 118, 4226-4229.	1.2	30
157	Computer Simulation of the Mechanical Properties of Amorphous Polymer Nanostructures. <i>Nano Letters</i> , 2003, 3, 1405-1410.	4.5	67
158	DNA Dynamics in a Microchannel. <i>Physical Review Letters</i> , 2003, 91, 038102.	2.9	161
159	Predictive Molecular Model for the Thermodynamic and Transport Properties of Triacylglycerols. <i>Journal of Physical Chemistry B</i> , 2003, 107, 14443-14451.	1.2	61
160	Simulations of the Morphology of Cylinder-Forming Asymmetric Diblock Copolymer Thin Films on Nanopatterned Substrates. <i>Macromolecules</i> , 2003, 36, 1731-1740.	2.2	61
161	Molecular Simulation Study of Phospholipid Bilayers and Insights of the Interactions with Disaccharides. <i>Biophysical Journal</i> , 2003, 85, 2830-2844.	0.2	200
162	Molecular Simulation Study on the Influence of Dimethylsulfoxide on the Structure of Phospholipid Bilayers. <i>Biophysical Journal</i> , 2003, 85, 3636-3645.	0.2	87

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163	Density of states of a binary Lennard-Jones glass. <i>Journal of Chemical Physics</i> , 2003, 119, 4405-4408.	1.2	55
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