Juan J De Pablo

List of Publications by Year in descending order

235 papers	20,792 citations	8159 76 h-index	11288 136 g-index
237 all docs	237 docs citations	237 times ranked	13285 citing authors

#	Article	IF	Citations
1	Epitaxial self-assembly of block copolymers on lithographically defined nanopatterned substrates. Nature, 2003, 424, 411-414.	13.7	1,594
2	Density Multiplication and Improved Lithography by Directed Block Copolymer Assembly. Science, 2008, 321, 936-939.	6.0	1,099
3	Directed Assembly of Block Copolymer Blends into Nonregular Device-Oriented Structures. Science, 2005, 308, 1442-1446.	6.0	912
4	Dependence of the Glass Transition Temperature of Polymer Films on Interfacial Energy and Thickness. Macromolecules, 2001, 34, 5627-5634.	2.2	464
5	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
6	On the simulation of vaporâ€“liquid equilibria for alkanes. Journal of Chemical Physics, 1998, 108, 9905-9911.	1.2	418
7	Simulation of polyethylene above and below the melting point. Journal of Chemical Physics, 1992, 96, 2395-2403.	1.2	359
8	Endotoxin-Induced Structural Transformations in Liquid Crystalline Droplets. Science, 2011, 332, 1297-1300.	6.0	339
9	Thermal Probe Measurements of the Glass Transition Temperature for Ultrathin Polymer Films as a Function of Thickness. Macromolecules, 2000, 33, 6439-6447.	2.2	331
10	Hyper-parallel tempering Monte Carlo: Application to the Lennard-Jones fluid and the restricted primitive model. Journal of Chemical Physics, 1999, 111, 9509-9516.	1.2	300
11	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
12	A coarse grain model for DNA. Journal of Chemical Physics, 2007, 126, 084901.	1.2	271
13	Stochastic simulations of DNA in flow: Dynamics and the effects of hydrodynamic interactions. Journal of Chemical Physics, 2002, 116, 7752-7759.	1.2	252
14	Shear-induced migration in flowing polymer solutions: Simulation of long-chain DNA in microchannels. Journal of Chemical Physics, 2004, 120, 2513-2529.	1.2	228
15	3-D microwell culture of human embryonic stem cells. Biomaterials, 2006, 27, 6032-6042.	5.7	216
16	Simulation of phase equilibria for chain molecules. Journal of Chemical Physics, 1992, 97, 2817-2819.	1.2	213
17	Estimation of the chemical potential of chain molecules by simulation. Journal of Chemical Physics, 1992, 96, 6157-6162.	1.2	213
18	Topological defects in liquid crystals as templates for molecular self-assembly. Nature Materials, 2016, 15, 106-112.	13.3	211

#	Article	IF	Citations
19	Thermophysical properties of trehalose and its concentrated aqueous solutions. Pharmaceutical Research, 1997, 14, 578-590.	1.7	201
20	Chemical Patterns for Directed Self-Assembly of Lamellae-Forming Block Copolymers with Density Multiplication of Features. Macromolecules, 2013, 46, 1415-1424.	2.2	201
21	Molecular Simulation Study of Phospholipid Bilayers and Insights of the Interactions with Disaccharides. Biophysical Journal, 2003, 85, 2830-2844.	0.2	200
22	Monte Carlo Simulations of a Coarse Grain Model for Block Copolymers and Nanocomposites. Macromolecules, 2008, 41, 4989-5001.	2.2	198
23	Expanded grand canonical and Gibbs ensemble Monte Carlo simulation of polymers. Journal of Chemical Physics, 1996, 105, 4391-4394.	1.2	194
24	An experimentally-informed coarse-grained 3-site-per-nucleotide model of DNA: Structure, thermodynamics, and dynamics of hybridization. Journal of Chemical Physics, 2013, 139, 144903.	1.2	191
25	The microwell control of embryoid body size in order to regulate cardiac differentiation of human embryonic stem cells. Biomaterials, 2010, 31, 1885-1893.	5.7	184
26	Influence of Confinement on the Fragility of Antiplasticized and Pure Polymer Films. Physical Review Letters, 2006, 97, 045502.	2.9	181
27	A Microfluidic System for Large DNA Molecule Arrays. Analytical Chemistry, 2004, 76, 5293-5301.	3.2	175
28	Stabilization and Preservation of Lactobacillus acidophilus in Saccharide Matrices. Cryobiology, 2000, 41, 17-24.	0.3	170
29	DNA Dynamics in a Microchannel. Physical Review Letters, 2003, 91, 038102.	2.9	161
30	Effect of confinement on DNA dynamics in microfluidic devices. Journal of Chemical Physics, 2003, 119, 1165-1173.	1.2	160
31	The Materials Genome Initiative, the interplay of experiment, theory and computation. Current Opinion in Solid State and Materials Science, 2014, 18, 99-117.	5.6	160
32	Density-of-states Monte Carlo method for simulation of fluids. Journal of Chemical Physics, 2002, 116, 8745-8749.	1.2	159
33	Hydrodynamic interactions in long chain polymers: Application of the Chebyshev polynomial approximation in stochastic simulations. Journal of Chemical Physics, 2000, 113, 2894-2900.	1.2	153
34	Rapid Directed Assembly of Block Copolymer Films at Elevated Temperatures. Macromolecules, 2008, 41, 2759-2761.	2.2	145
35	Inhibition of human embryonic stem cell differentiation by mechanical strain. Journal of Cellular Physiology, 2006, 206, 126-137.	2.0	143
36	Extraordinary elevation of the glass transition temperature of thin polymer films grafted to silicon oxide substrates. Journal of Chemical Physics, 2001, 115, 9982-9990.	1.2	138

#	Article	IF	Citations
37	Dimensions and Shapes of Block Copolymer Domains Assembled on Lithographically Defined Chemically Patterned Substrates. Macromolecules, 2007, 40, 90-96.	2.2	137
38	Computer Simulation of the Cryoprotectant Disaccharide Î±,Î±-Trehalose in Aqueous Solution. Journal of Physical Chemistry A, 1999, 103, 4049-4055.	1.1	134
39	Morphology of multi-component polymer systems: single chain in mean field simulation studies. Soft Matter, 2006, 2, 573-583.	1.2	134
40	Fast Computation of Many-Particle Hydrodynamic and Electrostatic Interactions in a Confined Geometry. Physical Review Letters, 2007, 98, 140602.	2.9	134
41	Interpolation in the Directed Assembly of Block Copolymers on Nanopatterned Substrates: Simulation and Experiments. Macromolecules, 2010, 43, 3446-3454.	2.2	131
42	Hierarchical Assembly of Nanoparticle Superstructures from Block Copolymer-Nanoparticle Composites. Physical Review Letters, 2008, 100, 148303.	2.9	126
43	MonteÂCarlo Simulation of Coarse Grain Polymeric Systems. Physical Review Letters, 2009, 102, 197801.	2.9	126
44	Coarse-Grained Simulations of Macromolecules: From DNA to Nanocomposites. Annual Review of Physical Chemistry, 2011, 62, 555-574.	4.8	126
45	Rheology of Confined Polymer Melts. Macromolecules, 1996, 29, 7910-7918.	2.2	125
46	Cryopreservation of adherent human embryonic stem cells. Biotechnology and Bioengineering, 2004, 88, 299-312.	1.7	124
47	Extended continuum configurational bias Monte Carlo methods for simulation of flexible molecules. Journal of Chemical Physics, 1995, 102, 2636-2652.	1.2	123
48	Calorimetric Solution Properties of Simple Saccharides and Their Significance for the Stabilization of Biological Structure and Function. Journal of Physical Chemistry B, 2000, 104, 8876-8883.	1.2	120
49	Diffusion of Sucrose and Î±,Î±-Trehalose in Aqueous Solutions. Journal of Physical Chemistry A, 2003, 107, 936-943.	1.1	117
50	Engineering the Stem Cell Microenvironment. Biotechnology Progress, 2007, 23, 18-23.	1.3	114
51	Theoretically informed coarse grain simulations of polymeric systems. Journal of Chemical Physics, 2009, 131, 084903.	1.2	113
52	Monte Carlo simulation of the chemical potential of polymers in an expanded ensemble. Journal of Chemical Physics, 1995, 103, 2703-2710.	1.2	110
53	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
54	Hyperparallel tempering Monte Carlo simulation of polymeric systems. Journal of Chemical Physics, 2000, 113, 1276-1282.	1.2	107

#	Article	IF	Citations
55	Free Energy of Defects in Ordered Assemblies of Block Copolymer Domains. ACS Macro Letters, 2012, 1, 418-422.	2.3	107
56	Molecular pathways for defect annihilation in directed self-assembly. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, 14144-14149.	3.3	98
57	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.	2.9	97
58	Calculation of local mechanical properties of filled polymers. Physical Review E, 2007, 75, 031803.	0.8	96
59	SIMULATION OFPHASETRANSITIONS INFLUIDS. Annual Review of Physical Chemistry, 1999, 50, 377-411.	4.8	94
60	Theoretically informed coarse grain simulations of block copolymer melts: method and applications. Soft Matter, 2009, 5, 4858.	1.2	91
61	Influence of Nanorod Inclusions on Structure and Primitive Path Network of Polymer Nanocomposites at Equilibrium and Under Deformation. Macromolecules, 2011, 44, 1034-1045.	2.2	91
62	Parallel Î²-Sheet Vibrational Couplings Revealed by 2D IR Spectroscopy of an Isotopically Labeled Macrocycle: Quantitative Benchmark for the Interpretation of Amyloid and Protein Infrared Spectra. Journal of the American Chemical Society, 2012, 134, 19118-19128.	6.6	91
63	Simulation and prediction of vapour-liquid equilibria for chain molecules. Molecular Physics, 1996, 87, 347-366.	0.8	90
64	Potential of mean force between a spherical particle suspended in a nematic liquid crystal and a substrate. Journal of Chemical Physics, 2002, 117, 7781-7787.	1.2	89
65	Mechanism and kinetics of ordering in diblock copolymer thin films on chemically nanopatterned substrates. Journal of Polymer Science, Part B: Polymer Physics, 2005, 43, 3444-3459.	2.4	89
66	Stabilization of lactate dehydrogenase following freeze thawing and vacuum-drying in the presence of trehalose and borate. Pharmaceutical Research, 1998, 15, 1215-1221.	1.7	87
67	Molecular Simulation Study on the Influence of Dimethylsulfoxide on the Structure of Phospholipid Bilayers. Biophysical Journal, 2003, 85, 3636-3645.	0.2	87
68	Relationship between polymer chain conformation and phase boundaries in a supercritical fluid. Journal of Chemical Physics, 1997, 107, 10782-10792.	1.2	85
69	Molecular Simulation of Sucrose Solutions near the Glass Transition Temperature. Journal of Physical Chemistry A, 2001, 105, 734-742.	1.1	85
70	Symmetric diblock copolymer thin films confined between homogeneous and patterned surfaces: Simulations and theory. Journal of Chemical Physics, 2000, 112, 9996-10010.	1.2	84
71	Evidence for size-dependent mechanical properties from simulations of nanoscopic polymeric structures. Journal of Chemical Physics, 2002, 116, 9939-9951.	1.2	84
72	SSAGES: Software Suite for Advanced General Ensemble Simulations. Journal of Chemical Physics, 2018, 148, 044104.	1.2	83

#	Article	IF	Citations
73	Multicanonical parallel tempering. Journal of Chemical Physics, 2002, 116, 5419-5423.	1.2	82
74	Remediation of Line Edge Roughness in Chemical Nanopatterns by the Directed Assembly of Overlying Block Copolymer Films. Macromolecules, 2010, 43, 2334-2342.	2.2	81
75	Concentration dependence of shear and extensional rheology of polymer solutions: Brownian dynamics simulations. Journal of Rheology, 2006, 50, 137-167.	1.3	80
76	A molecular view of vapor deposited glasses. Journal of Chemical Physics, 2011, 134, 194903.	1.2	80
77	A new united atom force field for Î±-olefins. Journal of Chemical Physics, 2001, 114, 3612-3616.	1.2	79
78	Liquid Crystal Enabled Early Stage Detection of Beta Amyloid Formation on Lipid Monolayers. Advanced Functional Materials, 2015, 25, 6050-6060.	7.8	79
79	Effects of trehalose on the phase behavior of DPPCâ€“cholesterol unilamellar vesicles. Biochimica Et Biophysica Acta - Biomembranes, 2006, 1758, 65-73.	1.4	77
80	Local dynamic mechanical properties in model free-standing polymer thin films. Journal of Chemical Physics, 2005, 122, 144712.	1.2	75
81	Computational Approaches for the Dynamics of Structure Formation in Self-Assembling Polymeric Materials. Annual Review of Materials Research, 2013, 43, 1-34.	4.3	75
82	Elongation and migration of single DNA molecules in microchannels using oscillatory shear flows. Lab on A Chip, 2009, 9, 2348.	3.1	74
83	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
84	Phase behavior of freeze-dried phospholipidâ€“cholesterol mixtures stabilized with trehalose. Biochimica Et Biophysica Acta - Biomembranes, 2005, 1713, 57-64.	1.4	72
85	Molecular plasticity of polymeric glasses in the elastic regime. Physical Review E, 2008, 77, 041502.	0.8	71
86	Directed Copolymer Assembly on Chemical Substrate Patterns:â€‰ 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
87	Monte Carlo simulation of branched and crosslinked polymers. Journal of Chemical Physics, 1996, 104, 4788-4801.	1.2	69
88	Simulation of vapour-liquid equilibria for branched alkanes. Molecular Physics, 2000, 98, 231-238.	0.8	69
89	Modulation of Wnt/Î²-catenin signaling in human embryonic stem cells using a 3-D microwell array. Biomaterials, 2012, 33, 2041-2049.	5.7	68
90	Computer Simulation of the Mechanical Properties of Amorphous Polymer Nanostructures. Nano Letters, 2003, 3, 1405-1410.	4.5	67

#	Article	IF	Citations
91	Cross-Stream Migration of Flexible Molecules in a Nanochannel. Physical Review Letters, 2006, 96, 224505.	2.9	66
92	Threeâ€dimensional Directed Assembly of Block Copolymers together with Twoâ€dimensional Square and Rectangular Nanolithography. Advanced Materials, 2011, 23, 3692-3697.	11.1	66
93	Structural Transitions in Cholesteric Liquid Crystal Droplets. ACS Nano, 2016, 10, 6484-6490.	7.3	66
94	Evolutionary Optimization of Directed Self-Assembly of Triblock Copolymers on Chemically Patterned Substrates. ACS Macro Letters, 2014, 3, 747-752.	2.3	64
95	Modulating Membrane Properties:Â The Effect of Trehalose and Cholesterol on a Phospholipid Bilayer. Journal of Physical Chemistry B, 2005, 109, 24173-24181.	1.2	63
96	Mechanical properties of antiplasticized polymer nanostructures. Soft Matter, 2010, 6, 2475.	1.2	63
97	Phase Equilibria of Charge-, Size-, and Shape-Asymmetric Model Electrolytes. Physical Review Letters, 2002, 88, 095504.	2.9	62
98	Predictive Molecular Model for the Thermodynamic and Transport Properties of Triacylglycerols. Journal of Physical Chemistry B, 2003, 107, 14443-14451.	1.2	61
99	Simulations of the Morphology of Cylinder-Forming Asymmetric Diblock Copolymer Thin Films on Nanopatterned Substrates. Macromolecules, 2003, 36, 1731-1740.	2.2	61
100	Cavitation and Crazing in Rod-Containing Nanocomposites. Macromolecules, 2011, 44, 5498-5509.	2.2	61
101	Phase Equilibria of Size-Asymmetric Primitive Model Electrolytes. Physical Review Letters, 2001, 86, 2054-2057.	2.9	60
102	Ethylene and 1-Hexene Sorption in LLDPE under Typical Gas Phase Reactor Conditions:Â A Priori Simulation and Modeling for Prediction of Experimental Observations. Macromolecules, 2004, 37, 9139-9150.	2.2	59
103	Investigation of Transition States in Bulk and Freestanding Film Polymer Glasses. Physical Review Letters, 2004, 92, 155505.	2.9	59
104	Cross-stream-line migration in confined flowing polymer solutions: Theory and simulation. Physics of Fluids, 2006, 18, 123101.	1.6	59
105	Dynamical Simulations of Coarse Grain Polymeric Systems: Rouse and Entangled Dynamics. Macromolecules, 2013, 46, 6287-6299.	2.2	59
106	The effect of hydrodynamic interactions on the dynamics of DNA translocation through pores. Journal of Chemical Physics, 2008, 128, 085102.	1.2	57
107	Directed Assembly of a Cylinder-Forming Diblock Copolymer: Topographic and Chemical Patterns. Macromolecules, 2010, 43, 6495-6504.	2.2	57
108	Evolutionary pattern design for copolymer directed self-assembly. Soft Matter, 2013, 9, 11467.	1.2	57

#	Article	IF	Citations
109	Molecular Structure of Canonical Liquid Crystal Interfaces. Journal of the American Chemical Society, 2017, 139, 3841-3850.	6.6	56
110	Vapor-liquid equilibria for polyatomic fluids from site-site computer simulations: pure hydrocarbons and binary mixtures containing methane. Fluid Phase Equilibria, 1992, 73, 187-210.	1.4	55
111	Equilibrated Adsorption of CO on Silica-Supported Pt Catalysts. Journal of Physical Chemistry B, 2000, 104, 4169-4180.	1.2	55
112	Density of states of a binary Lennard-Jones glass. Journal of Chemical Physics, 2003, 119, 4405-4408.	1.2	55
113	Density of Statesâ€"Based Molecular Simulations. Annual Review of Chemical and Biomolecular Engineering, 2012, 3, 369-394.	3.3	55
114	Viscosity and Glass Transition Temperature of Aqueous Mixtures of Trehalose with Borax and Sodium Chloride. Journal of Physical Chemistry B, 1999, 103, 10243-10249.	1.2	54
115	A new double-rebridging technique for linear polyethylene. Journal of Chemical Physics, 2003, 119, 2456-2462.	1.2	54
116	A coarse-grain three-site-per-nucleotide model for DNA with explicit ions. Journal of Chemical Physics, 2011, 135, 165104.	1.2	54
117	Effect of pH, Counter Ion, and Phosphate Concentration on the Glass Transition Temperature of Freeze-Dried Sugar-Phosphate Mixtures. Pharmaceutical Research, 2004, 21, 1615-1621.	1.7	53
118	Simulations of theoretically informed coarse grain models of polymeric systems. Faraday Discussions, 2010, 144, 111-125.	1.6	53
119	Autonomous materials systems from active liquid crystals. Nature Reviews Materials, 2021, 6, 437-453.	23.3	53
120	A biased Monte Carlo technique for calculation of the density of states of polymer films. Journal of Chemical Physics, 2002, 116, 7238-7243.	1.2	52
121	Block Copolymer Assembly on Nanoscale Patterns of Polymer Brushes Formed by Electrohydrodynamic Jet Printing. ACS Nano, 2014, 8, 6606-6613.	7.3	52
122	Monte Carlo Simulation of Free-Standing Polymer Films near the Glass Transition Temperature. Macromolecules, 2002, 35, 2167-2176.	2.2	51
123	Solution Structures of Rat Amylin Peptide: Simulation, Theory, and Experiment. Biophysical Journal, 2010, 98, 443-451.	0.2	51
124	Morphologies of Linear Triblock Copolymers from Monte Carlo Simulations. Macromolecules, 2011, 44, 5490-5497.	2.2	51
125	Directed Assembly of Non-equilibrium ABA Triblock Copolymer Morphologies on Nanopatterned Substrates. ACS Nano, 2012, 6, 5440-5448.	7.3	50
126	Nematic-Field-Driven Positioning of Particles in Liquid Crystal Droplets. Physical Review Letters, 2013, 111, 227801.	2.9	50

#	Article	IF	Citations
127	An immersed boundary method for Brownian dynamics simulation of polymers in complex geometries: Application to DNA flowing through a nanoslit with embedded nanopits. Journal of Chemical Physics, 2012, 136, 014901.	1.2	48
128	Simulation of Vaporâ"Liquid Equilibria for Alkane Mixtures. Industrial & Engineering Chemistry Research, 1998, 37, 3195-3202.	1.8	47
129	Molecular and multiscale modeling in chemical engineering - current view and future perspectives. AICHE Journal, 2005, 51, 2371-2376.	1.8	47
130	Molecular simulations in chemical engineering: Present and future. AICHE Journal, 2002, 48, 2716-2721.	1.8	46
131	Stimuliâ€Responsive Cubosomes Formed from Blue Phase Liquid Crystals. Advanced Materials, 2015, 27, 6892-6898.	11.1	44
132	Phase equilibria and clustering in size-asymmetric primitive model electrolytes. Journal of Chemical Physics, 2001, 114, 1727-1731.	1.2	43
133	Polymer chain collapse near the lower critical solution temperature. Chemical Physics Letters, 1997, 278, 302-306.	1.2	42
134	Solubility of Small Molecules and Their Mixtures in Polyethylene. Journal of Physical Chemistry B, 1999, 103, 3539-3544.	1.2	42
135	Simulation of the effects of chain architecture on the sorption of ethylene in polyethylene. Journal of Chemical Physics, 2004, 120, 11304-11315.	1.2	42
136	Measuring liquid crystal elastic constants with free energy perturbations. Soft Matter, 2014, 10, 882-893.	1.2	42
137	Simulation of structure and interaction forces for surfaces coated with grafted chains in a compressible solvent. Journal of Chemical Physics, 1998, 109, 6424-6434.	1.2	41
138	Nonbulk Complex Structures in Thin Films of Symmetric Block Copolymers on Chemically Nanopatterned Surfaces. Macromolecules, 2012, 45, 3986-3992.	2.2	40
139	Simulation of Ternary Mixtures of Ethylene, 1-Hexene, and Polyethylene. Macromolecules, 2001, 34, 7841-7848.	2.2	39
140	Presentation of Large DNA Molecules for Analysis as Nanoconfined Dumbbells. Macromolecules, 2013, 46, 8356-8368.	2.2	39
141	Structure of binary polymer blends: Multiple time step hybrid Monte Carlo simulations and selfâ€consistent integralâ€equation theory. Journal of Chemical Physics, 1995, 103, 8247-8256.	1.2	38
142	Defect Annihilation Pathways in Directed Assembly of Lamellar Block Copolymer Thin Films. ACS Nano, 2018, 12, 9974-9981.	7.3	38
143	Pseudo-ensemble simulations and Gibbsâ€"Duhem integrations for polymers. Journal of Chemical Physics, 1997, 106, 2911-2923.	1.2	37
144	Simulation of Vaporâ"Liquid Phase Equilibria of Primary Alcohols and Alcoholâ"Alkane Mixtures. Journal of Physical Chemistry B, 2004, 108, 10071-10076.	1.2	37

#	Article	IF	Citations
145	Influence of confinement on the vibrational density of states and the Boson peak in a polymer glass. Journal of Chemical Physics, 2004, 120, 9371-9375.	1.2	36
146	Tethered DNA dynamics in shear flow. Journal of Chemical Physics, 2009, 130, 234902.	1.2	36
147	Control of Directed Self-Assembly in Block Polymers by Polymeric Topcoats. Macromolecules, 2014, 47, 3520-3527.	2.2	36
148	Pattern Dimensions and Feature Shapes of Ternary Blends of Block Copolymer and Low Molecular Weight Homopolymers Directed To Assemble on Chemically Nanopatterned Surfaces. ACS Nano, 2011, 5, 5673-5682.	7.3	35
149	Nanoparticles in nematic liquid crystals: Interactions with nanochannels. Journal of Chemical Physics, 2007, 127, 124702.	1.2	34
150	Morphology of Lamellae-Forming Block Copolymer Films between Two Orthogonal Chemically Nanopatterned Striped Surfaces. Physical Review Letters, 2012, 108, 065502.	2.9	34
151	Local elastic constants in thin films of an fcc crystal. Physical Review E, 2003, 67, 031601.	0.8	32
152	Effect of sugarâ€“phosphate mixtures on the stability of DPPC membranes in dehydrated systems. Cryobiology, 2004, 48, 81-89.	0.3	32
153	NlogN method for hydrodynamic interactions of confined polymer systems: Brownian dynamics. Journal of Chemical Physics, 2006, 125, 164906.	1.2	32
154	Flux Tempered Metadynamics. Journal of Statistical Physics, 2011, 145, 932-945.	0.5	32
155	Nonequilibrium Simulations of Lamellae Forming Block Copolymers under Steady Shear: A Comparison of Dissipative Particle Dynamics and Brownian Dynamics. Macromolecules, 2012, 45, 8109-8116.	2.2	32
156	Understanding Atomic-Scale Behavior of Liquid Crystals at Aqueous Interfaces. Journal of Chemical Theory and Computation, 2017, 13, 237-244.	2.3	31
157	Calculation of interfacial tension from density of states. Journal of Chemical Physics, 2003, 118, 4226-4229.	1.2	30
158	Lattice Boltzmann simulation of asymmetric flow in nematic liquid crystals with finite anchoring. Journal of Chemical Physics, 2016, 144, 084905.	1.2	30
159	Light-activated helical inversion in cholesteric liquid crystal microdroplets. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, 4334-4339.	3.3	30
160	Continuum configurational bias Monte-Carlo studies of alkanes and polyethylene. Fluid Phase Equilibria, 1993, 83, 323-331.	1.4	29
161	DFT Calculations and Monte Carlo Simulations of the Co-Adsorption of Hydrogen Atoms and Ethylidyne Species on Pt(111). Journal of Physical Chemistry B, 2001, 105, 8550-8562.	1.2	27
162	Hydrodynamic effects on the translocation rate of a polymer through a pore. Journal of Chemical Physics, 2009, 131, 044904.	1.2	27

#	Article	IF	Citations
163	Prolate and oblate chiral liquid crystal spheroids. Science Advances, 2020, 6, eaba6728.	4.7	27
164	Reversible Switching of Liquid Crystalline Order Permits Synthesis of Homogeneous Populations of Dipolar Patchy Microparticles. Advanced Functional Materials, 2014, 24, 6219-6226.	7.8	26
165	Derivation of Multiple Covarying Material and Process Parameters Using Physics-Based Modeling of X-ray Data. Macromolecules, 2017, 50, 7783-7793.	2.2	26
166	Electrical Conductivity of Supercooled Aqueous Mixtures of Trehalose with Sodium Chloride. Journal of Physical Chemistry B, 2000, 104, 10419-10425.	1.2	25
167	Symmetric Diblock Copolymers Confined by Two Nanopatterned Surfaces. Macromolecules, 2012, 45, 2588-2596.	2.2	25
168	Segregation of liquid crystal mixtures in topological defects. Nature Communications, 2017, 8, 15064.	5.8	25
169	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
170	Directed self-assembly of nematic liquid crystals on chemically patterned surfaces: morphological states and transitions. Soft Matter, 2016, 12, 8595-8605.	1.2	23
171	Amphiphile-Induced Phase Transition of Liquid Crystals at Aqueous Interfaces. ACS Applied Materials & Interfaces, 2018, 10, 37618-37624.	4.0	23
172	Monte Carlo Simulations of Reaction Kinetics for Ethane Hydrogenolysis over Pt. Journal of Physical Chemistry B, 2002, 106, 9604-9612.	1.2	22
173	Theoretically informed Monte Carlo simulation of liquid crystals by sampling of alignment-tensor fields. Journal of Chemical Physics, 2015, 143, 044107.	1.2	22
174	Simulation of phase equilibria for chain molecules. Fluid Phase Equilibria, 1995, 104, 195-206.	1.4	20
175	Interactions of Liquid Crystal-Forming Molecules with Phospholipid Bilayers Studied by Molecular Dynamics Simulations. Biophysical Journal, 2005, 89, 3141-3158.	0.2	20
176	Soft crystal martensites: An in situ resonant soft x-ray scattering study of a liquid crystal martensitic transformation. Science Advances, 2020, 6, eaay5986.	4.7	20
177	Comment on the accuracy of Wertheimâ€™s theory of associating fluids. Journal of Chemical Physics, 1995, 103, 3868-3869.	1.2	19
178	On the calculation of transport properties of polymer melts from nonequilibrium molecular dynamics. Journal of Chemical Physics, 1997, 106, 8285-8286.	1.2	19
179	Effects of charge, size, and shape-asymmetry on the phase behavior of model electrolytes. Journal of Chemical Physics, 2002, 116, 2967-2972.	1.2	19
180	Platelet cryopreservation using a trehalose and phosphate formulation. Biotechnology and Bioengineering, 2005, 92, 79-90.	1.7	19

#	Article	IF	Citations
181	Directed assembly of copolymer materials on patterned substrates: Balance of simple symmetries in complex structures. Journal of Polymer Science, Part B: Polymer Physics, 2006, 44, 2589-2604.	2.4	19
182	A Detailed Examination of the Topological Constraints of Lamellae-Forming Block Copolymers. Macromolecules, 2018, 51, 2110-2124.	2.2	19
183	Thermally reconfigurable Janus droplets with nematic liquid crystalline and isotropic perfluorocarbon oil compartments. Soft Matter, 2019, 15, 2580-2590.	1.2	19
184	Study of acid diffusion in resist near the glass transition temperature. Journal of Vacuum Science & Technology an Official Journal of the American Vacuum Society B, Microelectronics Processing and Phenomena, 1999, 17, 3351.	1.6	18
185	Molecular Simulation of Physical Properties of Hindered-Amine Light Stabilizers in Polyethylene. Journal of the American Chemical Society, 1999, 121, 4252-4261.	6.6	18
186	Segmental dynamics in a blend of alkanes: Nuclear magnetic resonance experiments and molecular dynamics simulation. Journal of Chemical Physics, 2002, 116, 8209-8217.	1.2	18
187	A method for multiscale simulation of flowing complex fluids. Journal of Non-Newtonian Fluid Mechanics, 2002, 108, 123-142.	1.0	18
188	Colloidâ€inâ€Liquid Crystal Gels that Respond to Biomolecular Interactions. Small, 2013, 9, 2785-2792.	5.2	18
189	Free energy of metal-organic framework self-assembly. Journal of Chemical Physics, 2019, 150, 104502.	1.2	18
190	An effective-colloid pair potential for Lennard-Jones colloidâ€“polymer mixtures. Journal of Chemical Physics, 2003, 118, 2392-2397.	1.2	17
191	Effect of trehalose on the interaction of Alzheimer's AÎ²-peptide and anionic lipid monolayers. Biochimica Et Biophysica Acta - Biomembranes, 2011, 1808, 26-33.	1.4	17
192	Basis Function Sampling: A New Paradigm for Material Property Computation. Physical Review Letters, 2014, 113, 190602.	2.9	17
193	In Silico Measurement of Elastic Moduli of Nematic Liquid Crystals. Physical Review Letters, 2018, 120, 107801.	2.9	16
194	Phase equilibria in binary polymer blends: Integral equation approach. Journal of Chemical Physics, 1998, 109, 10042-10052.	1.2	15
195	Association of Helical Î²-Peptides and their Aggregation Behavior from the Potential of Mean Force in Explicit Solvent. Biophysical Journal, 2009, 96, 4349-4362.	0.2	15
196	Effects of 3D microwell culture on growth kinetics and metabolism of human embryonic stem cells. Biotechnology and Applied Biochemistry, 2012, 59, 88-96.	1.4	15
197	Free energy landscapes of the encapsulation mechanism of DNA nucleobases onto carbon nanotubes. RSC Advances, 2014, 4, 1310-1321.	1.7	15
198	Graphoepitaxial assembly of asymmetric ternary blends of block copolymers and homopolymers. Nanotechnology, 2010, 21, 495301.	1.3	14

#	Article	IF	Citations
199	Parallel O(N) Stokesâ€™ solver towards scalable Brownian dynamics of hydrodynamically interacting objects in general geometries. Journal of Chemical Physics, 2017, 146, 244114.	1.2	14
200	The effect of solvation on the conformation of freely jointed repulsive trimers. Journal of Chemical Physics, 1994, 101, 6013-6023.	1.2	13
201	Fluorinated Quaternary Ammonium Salts as Dissolution Aids for Polar Polymers in Environmentally Benign Supercritical Carbon Dioxide. Chemistry of Materials, 2009, 21, 3125-3135.	3.2	13
202	Monte-Carlo simulation of ternary blends of block copolymers and homopolymers. Journal of Chemical Physics, 2011, 135, 114904.	1.2	13
203	Spherical nematic shells with a prolate ellipsoidal core. Soft Matter, 2017, 13, 7465-7472.	1.2	13
204	Optimizing self-consistent field theory block copolymer models with X-ray metrology. Molecular Systems Design and Engineering, 2018, 3, 376-389.	1.7	13
205	Liquid crystal free energy relaxation by a theoretically informed Monte Carlo method using a finite element quadrature approach. Journal of Chemical Physics, 2015, 143, 243157.	1.2	13
206	Homeotropic nano-particle assembly on degenerate planar nematic interfaces: films and droplets. Soft Matter, 2015, 11, 5067-5076.	1.2	12
207	Reconfigurable Multicompartment Emulsion Drops Formed by Nematic Liquid Crystals and Immiscible Perfluorocarbon Oils. Langmuir, 2019, 35, 16312-16323.	1.6	12
208	Sculpting bespoke mountains: Determining free energies with basis expansions. Journal of Chemical Physics, 2015, 143, 044101.	1.2	11
209	Interplay of Surface Energy and Bulk Thermodynamic Forces in Ordered Block Copolymer Droplets. Macromolecules, 2015, 48, 4717-4723.	2.2	11
210	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
211	Combining Particle-Based Simulations and Machine Learning to Understand Defect Kinetics in Thin Films of Symmetric Diblock Copolymers. Macromolecules, 2021, 54, 10074-10085.	2.2	11
212	Mechanism and dynamics of block copolymer directed assembly with density multiplication on chemically patterned surfaces. Journal of Vacuum Science and Technology B:Nanotechnology and Microelectronics, 2010, 28, C6B13-C6B19.	0.6	10
213	Water Flux Induced Reorientation of Liquid Crystals. ACS Central Science, 2017, 3, 1345-1349.	5.3	9
214	Layered nested Markov chain Monte Carlo. Journal of Chemical Physics, 2018, 149, 072326.	1.2	9
215	Transformation between elastic dipoles, quadrupoles, octupoles, and hexadecapoles driven by surfactant self-assembly in nematic emulsion. Science Advances, 2021, 7, .	4.7	9
216	Self-consistent description of electrokinetic phenomena in particle-based simulations. Journal of Chemical Physics, 2015, 143, 014108.	1.2	8

#	Article	IF	Citations
217	Cuboidal liquid crystal phases under multiaxial geometrical frustration. Soft Matter, 2020, 16, 870-880.	1.2	8
218	Shape control and density multiplication of cylinder-forming ternary block copolymer-homopolymer blend thin films on chemical patterns. Journal of Vacuum Science and Technology B:Nanotechnology and Microelectronics, 2010, 28, C6B24-C6B29.	0.6	7
219	Graphoepitaxial assembly of cylinder forming block copolymers in cylindrical holes. Journal of Polymer Science, Part B: Polymer Physics, 2015, 53, 430-441.	2.4	7
220	Phase behavior of polymerâ€“solvent mixtures. Fluid Phase Equilibria, 1998, 150-151, 657-665.	1.4	5
221	Monte Carlo Methods for Polymeric Systems. Advances in Chemical Physics, 0, , 337-367.	0.3	5
222	Comment on â€˜â€˜The effect of charged impurities on a glass transition in a polar mediumâ€™â€™ [J. Chem. Phys. 104, 664 (1996)]. Journal of Chemical Physics, 1996, 105, 8979-8980.	1.2	4
223	Multiple free energy minima in systems of confined tethered polymersâ€”toward soft nanomechanical bistable elements. Soft Matter, 2009, 5, 3694.	1.2	4
224	Surface Adsorption in Nonpolarizable Atomic Models. Journal of Chemical Theory and Computation, 2014, 10, 5616-5624.	2.3	4
225	Mechanisms of Directed Self-Assembly in Cylindrical Hole Confinements. Macromolecules, 2018, 51, 2418-2427.	2.2	4
226	Structure and proton conduction in sulfonated poly(ether ether ketone) semi-permeable membranes: a multi-scale computational approach. Physical Chemistry Chemical Physics, 2019, 21, 9362-9375.	1.3	4
227	Influence of Homopolymer Addition in Templated Assembly of Cylindrical Block Copolymers. ACS Nano, 2019, 13, 4073-4082.	7.3	3
228	Formation, Stability, and Annihilation of the Stitched Morphology in Block Copolymer Thin Films. Macromolecules, 2020, 53, 10446-10456.	2.2	3
229	Simulation of chain molecules for prediction of thermodynamic properties. Fluid Phase Equilibria, 1996, 116, 312-319.	1.4	2
230	Hyperparallel tempering Monte Carlo and its applications. Advances in Chemical Engineering, 2001, 28, 1-20.	0.5	2
231	The effects of geometry and chemistry of nanopatterned substrates on the directed self-assembly of block-copolymer melts. , 2015, , .		2
232	DIAGENESIS AND RHEOLOGY OF A RECENTâ€“PLEISTOCENE VOLCANOGENIC SEDIMENTARY SEQUENCE, MEXICAN BASIN. Clays and Clay Minerals, 2002, 50, 807-823.	0.6	1
233	Scalable simulations for directed self-assembly patterning with the use of GPU parallel computing. , 2012, , .		1
234	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

#	Article	IF	Citations
235	Fluctuations and phase transitions of uniaxial and biaxial liquid crystals using a theoretically informed Monte Carlo and a Landau free energy density. Journal of Physics Condensed Matter, 2019, 31, 175101.	0.7	1