Juan J. de Pablo

List of Publications by Year in descending order

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378 papers	23,293 citations	7251 80 h-index	14012 133 g-index
385 all docs	385 docs citations	385 times ranked	17319 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	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
5	Endotoxin-Induced Structural Transformations in Liquid Crystalline Droplets. Science, 2011, 332, 1297-1300.	6.0	339
6	New frontiers for the materials genome initiative. Npj Computational Materials, 2019, 5, .	3.5	312
7	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
8	A coarse grain model for DNA. Journal of Chemical Physics, 2007, 126, 084901.	1.2	271
9	Stochastic simulations of DNA in flow: Dynamics and the effects of hydrodynamic interactions. Journal of Chemical Physics, 2002, 116, 7752-7759.	1.2	252
10	Phase Behavior and Salt Partitioning in Polyelectrolyte Complex Coacervates. Macromolecules, 2018, 51, 2988-2995.	2.2	241
11	Mechanical Heterogeneities in Model Polymer Glasses at Small Length Scales. Physical Review Letters, 2004, 93, 175501.	2.9	214
12	Ultrastable glasses from in silico vapour deposition. Nature Materials, 2013, 12, 139-144.	13.3	213
13	Topological defects in liquid crystals as templates for molecular self-assembly. Nature Materials, 2016, 15, 106-112.	13.3	211
14	Chirality-selected phase behaviour in ionic polypeptide complexes. Nature Communications, 2015, 6, 6052.	5.8	208
15	Thermophysical properties of trehalose and its concentrated aqueous solutions. Pharmaceutical Research, 1997, 14, 578-590.	1.7	201
16	Chemical Patterns for Directed Self-Assembly of Lamellae-Forming Block Copolymers with Density Multiplication of Features. Macromolecules, 2013, 46, 1415-1424.	2.2	201
17	Monte Carlo Simulations of a Coarse Grain Model for Block Copolymers and Nanocomposites. Macromolecules, 2008, 41, 4989-5001.	2.2	198
18	Poly[n]catenanes: Synthesis of molecular interlocked chains. Science, 2017, 358, 1434-1439.	6.0	196

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19	Expanded grand canonical and Gibbs ensemble Monte Carlo simulation of polymers. Journal of Chemical Physics, 1996, 105, 4391-4394.	1.2	194
20	Monte Carlo Simulations of Asymmetric Diblock Copolymer Thin Films Confined between Two Homogeneous Surfaces. Macromolecules, 2001, 34, 3458-3470.	2.2	192
21	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
22	Tunable molecular orientation and elevated thermal stability of vapor-deposited organic semiconductors. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, 4227-4232.	3.3	188
23	Polymer Informatics: Opportunities and Challenges. ACS Macro Letters, 2017, 6, 1078-1082.	2.3	184
24	Monte Carlo simulations of diblock copolymer thin films confined between two homogeneous surfaces. Journal of Chemical Physics, 2000, 112, 450-464.	1.2	167
25	Monte Carlo simulations of Wyoming sodium montmorillonite hydrates. Journal of Chemical Physics, 2001, 114, 1405-1413.	1.2	166
26	Effect of confinement on DNA dynamics in microfluidic devices. Journal of Chemical Physics, 2003, 119, 1165-1173.	1.2	160
27	Density-of-states Monte Carlo method for simulation of fluids. Journal of Chemical Physics, 2002, 116, 8745-8749.	1.2	159
28	A Mesoscale Model of DNA and Its Renaturation. Biophysical Journal, 2009, 96, 1675-1690.	0.2	156
29	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
30	Rapid Directed Assembly of Block Copolymer Films at Elevated Temperatures. Macromolecules, 2008, 41, 2759-2761.	2.2	145
31	Fast Calculation of the Density of States of a Fluid by Monte Carlo Simulations. Physical Review Letters, 2003, 90, 035701.	2.9	143
32	Conformation and dynamics of single DNA molecules in parallel-plate slit microchannels. Physical Review E, 2004, 70, 060901.	0.8	139
33	Multivalent counterions diminish the lubricity of polyelectrolyte brushes. Science, 2018, 360, 1434-1438.	6.0	137
34	Interfacial Tension of Polyelectrolyte Complex Coacervate Phases. ACS Macro Letters, 2014, 3, 565-568.	2.3	135
35	Morphology of multi-component polymer systems: single chain in mean field simulation studies. Soft Matter, 2006, 2, 573-583.	1.2	134
36	Fast Computation of Many-Particle Hydrodynamic and Electrostatic Interactions in a Confined Geometry. Physical Review Letters, 2007, 98, 140602.	2.9	134

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37	Interpolation in the Directed Assembly of Block Copolymers on Nanopatterned Substrates: Simulation and Experiments. Macromolecules, 2010, 43, 3446-3454.	2.2	131
38	Ternary, Tunable Polyelectrolyte Complex Fluids Driven by Complex Coacervation. Macromolecules, 2014, 47, 3076-3085.	2.2	127
39	MonteÂCarlo Simulation of Coarse Grain Polymeric Systems. Physical Review Letters, 2009, 102, 197801.	2.9	126
40	Coarse-Grained Simulations of Macromolecules: From DNA to Nanocomposites. Annual Review of Physical Chemistry, 2011, 62, 555-574.	4.8	126
41	Tunable structure and dynamics of active liquid crystals. Science Advances, 2018, 4, eaat7779.	4.7	125
42	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
43	Influence of Surfactant Tail Branching and Organization on the Orientation of Liquid Crystals at Aqueousâ^'Liquid Crystal Interfaces. Langmuir, 2005, 21, 6805-6814.	1.6	120
44	Directly Observing Micelle Fusion and Growth in Solution by Liquid-Cell Transmission Electron Microscopy. Journal of the American Chemical Society, 2017, 139, 17140-17151.	6.6	118
45	Theoretically informed coarse grain simulations of polymeric systems. Journal of Chemical Physics, 2009, 131, 084903.	1.2	113
46	A pH-Triggered, Self-Assembled, and Bioprintable Hybrid Hydrogel Scaffold for Mesenchymal Stem Cell Based Bone Tissue Engineering. ACS Applied Materials & Interfaces, 2019, 11, 8749-8762.	4.0	112
47	Monte Carlo simulation of the chemical potential of polymers in an expanded ensemble. Journal of Chemical Physics, 1995, 103, 2703-2710.	1.2	110
48	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
49	Recent advances in machine learning towards multiscale soft materials design. Current Opinion in Chemical Engineering, 2019, 23, 106-114.	3.8	110
50	Hyperparallel tempering Monte Carlo simulation of polymeric systems. Journal of Chemical Physics, 2000, 113, 1276-1282.	1.2	107
51	Monte Carlo simulation of proteins through a random walk in energy space. Journal of Chemical Physics, 2002, 116, 7225-7230.	1.2	107
52	Free Energy of Defects in Ordered Assemblies of Block Copolymer Domains. ACS Macro Letters, 2012, 1, 418-422.	2.3	107
53	Coarse-grained modeling of DNA curvature. Journal of Chemical Physics, 2014, 141, 165103.	1.2	106
54	Density of states simulations of proteins. Journal of Chemical Physics, 2003, 118, 4285-4290.	1.2	102

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55	Characterization of Adsorbate-Induced Ordering Transitions of Liquid Crystals within Monodisperse Droplets. Langmuir, 2009, 25, 9016-9024.	1.6	102
56	Directed self-assembly of liquid crystalline blue-phases into ideal single-crystals. Nature Communications, 2017, 8, 15854.	5.8	101
57	Nanoparticle self-assembly at the interface of liquid crystal droplets. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, 5297-5302.	3.3	98
58	Characterizing the Three-Dimensional Structure of Block Copolymers via Sequential Infiltration Synthesis and Scanning Transmission Electron Tomography. ACS Nano, 2015, 9, 5333-5347.	7.3	98
59	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
60	Antiplasticization and the elastic properties of glass-forming polymer liquids. Soft Matter, 2010, 6, 292-304.	1.2	97
61	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
62	Calculation of local mechanical properties of filled polymers. Physical Review E, 2007, 75, 031803.	0.8	96
63	Heterogeneous dynamics during deformation of a polymer glass. Soft Matter, 2010, 6, 287-291.	1.2	96
64	Criticality and Connectivity in Macromolecular Charge Complexation. Macromolecules, 2016, 49, 8789-8800.	2.2	96
65	Polyelectrolyte Complex Coacervates: Recent Developments and New Frontiers. Annual Review of Condensed Matter Physics, 2021, 12, 155-176.	5.2	96
66	SIMULATION OFPHASETRANSITIONS INFLUIDS. Annual Review of Physical Chemistry, 1999, 50, 377-411.	4.8	94
67	Dynamic actuation of glassy polymersomes through isomerization of a single azobenzene unit at the block copolymer interface. Nature Chemistry, 2018, 10, 659-666.	6.6	93
68	Gel phase formation in dilute triblock copolyelectrolyte complexes. Nature Communications, 2017, 8, 14131.	5.8	92
69	Theoretically informed coarse grain simulations of block copolymer melts: method and applications. Soft Matter, 2009, 5, 4858.	1.2	91
70	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
71	Liquid-crystal-mediated self-assembly at nanodroplet interfaces. Nature, 2012, 485, 86-89.	13.7	91
72	Simulation and prediction of vapour-liquid equilibria for chain molecules. Molecular Physics, 1996, 87, 347-366.	0.8	90

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73	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
74	Influence of Ion Solvation on the Properties of Electrolyte Solutions. Journal of Physical Chemistry B, 2018, 122, 4029-4034.	1.2	88
75	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
76	Nonlinear Creep in a Polymer Glass. Macromolecules, 2008, 41, 4969-4977.	2.2	85
77	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
78	Evidence for size-dependent mechanical properties from simulations of nanoscopic polymeric structures. Journal of Chemical Physics, 2002, 116, 9939-9951.	1.2	84
79	Targeted sequence design within the coarse-grained polymer genome. Science Advances, 2020, 6, .	4.7	84
80	SSAGES: Software Suite for Advanced General Ensemble Simulations. Journal of Chemical Physics, 2018, 148, 044104.	1.2	83
81	Auxetic metamaterials from disordered networks. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, E1384-E1390.	3.3	83
82	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
83	Concentration dependence of shear and extensional rheology of polymer solutions: Brownian dynamics simulations. Journal of Rheology, 2006, 50, 137-167.	1.3	80
84	A molecular view of vapor deposited glasses. Journal of Chemical Physics, 2011, 134, 194903.	1.2	80
85	Molecular characterization of ebselen binding activity to SARS-CoV-2 main protease. Science Advances, 2020, 6, .	4.7	80
86	Shear Thickening and Jamming of Dense Suspensions: The â€œRollâ€•of Friction. Physical Review Letters, 2020, 124, 248005.	2.9	80
87	Study of volume phase transitions in polymeric nanogels by theoretically informed coarse-grained simulations. Soft Matter, 2011, 7, 5965.	1.2	79
88	Model vapor-deposited glasses: Growth front and composition effects. Journal of Chemical Physics, 2013, 139, 144505.	1.2	79
89	Liquid Crystal Enabled Early Stage Detection of Beta Amyloid Formation on Lipid Monolayers. Advanced Functional Materials, 2015, 25, 6050-6060.	7.8	79
90	Simulation of Defect Reduction in Block Copolymer Thin Films by Solvent Annealing. ACS Macro Letters, 2015, 4, 11-15.	2.3	79

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91	Multivalent ions induce lateral structural inhomogeneities in polyelectrolyte brushes. Science Advances, 2017, 3, eaao1497.	4.7	79
92	DNA Shape Dominates Sequence Affinity in Nucleosome Formation. Physical Review Letters, 2014, 113, 168101.	2.9	78
93	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
94	Turning statistical physics models into materials design engines. Proceedings of the National Academy of Sciences of the United States of America, 2016, 113, 34-39.	3.3	71
95	Spatiotemporal control of liquid crystal structure and dynamics through activity patterning. Nature Materials, 2021, 20, 875-882.	13.3	70
96	Monte Carlo simulation of branched and crosslinked polymers. Journal of Chemical Physics, 1996, 104, 4788-4801.	1.2	69
97	Monte Carlo simulation of athermal mesogenic chains: Pure systems, mixtures, and constrained environments. Journal of Chemical Physics, 1997, 106, 9858-9868.	1.2	68
98	Dynamic structure of active nematic shells. Nature Communications, 2016, 7, 13483.	5.8	68
99	Tension-Dependent Free Energies of Nucleosome Unwrapping. ACS Central Science, 2016, 2, 660-666.	5.3	67
100	Anisotropic Vapor-Deposited Glasses: Hybrid Organic Solids. Accounts of Chemical Research, 2019, 52, 407-414.	7.6	67
101	Structural Transitions in Cholesteric Liquid Crystal Droplets. ACS Nano, 2016, 10, 6484-6490.	7.3	66
102	In silico evidence for sequence-dependent nucleosome sliding. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, E9197-E9205.	3.3	65
103	Evolutionary Optimization of Directed Self-Assembly of Triblock Copolymers on Chemically Patterned Substrates. ACS Macro Letters, 2014, 3, 747-752.	2.3	64
104	Anisotropic nanoparticles immersed in a nematic liquid crystal: Defect structures and potentials of mean force. Physical Review E, 2006, 74, 011711.	0.8	63
105	Mechanical properties of antiplasticized polymer nanostructures. Soft Matter, 2010, 6, 2475.	1.2	63
106	Liquid Crystal-Based Emulsions for Synthesis of Spherical and Non-Spherical Particles with Chemical Patches. Journal of the American Chemical Society, 2013, 135, 9972-9975.	6.6	63
107	Controlling Complex Coacervation via Random Polyelectrolyte Sequences. ACS Macro Letters, 2019, 8, 1296-1302.	2.3	63
108	Influence of Molecular Shape on the Thermal Stability and Molecular Orientation of Vapor-Deposited Organic Semiconductors. Journal of Physical Chemistry Letters, 2017, 8, 3380-3386.	2.1	62

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109	Cavitation and Crazing in Rod-Containing Nanocomposites. Macromolecules, 2011, 44, 5498-5509.	2.2	61
110	Morphological transitions in liquid crystal nanodroplets. Soft Matter, 2012, 8, 8679.	1.2	61
111	Topological Effects in Isolated Poly[n]catenanes: Molecular Dynamics Simulations and Rouse Mode Analysis. ACS Macro Letters, 2018, 7, 938-943.	2.3	60
112	Graph-Based Approach to Systematic Molecular Coarse-Graining. Journal of Chemical Theory and Computation, 2019, 15, 1199-1208.	2.3	60
113	Polyelectrolyte Complex Coacervation across a Broad Range of Charge Densities. Macromolecules, 2021, 54, 6878-6890.	2.2	60
114	Cross-stream-line migration in confined flowing polymer solutions: Theory and simulation. Physics of Fluids, 2006, 18, 123101.	1.6	59
115	Dynamical Simulations of Coarse Grain Polymeric Systems: Rouse and Entangled Dynamics. Macromolecules, 2013, 46, 6287-6299.	2.2	59
116	Orientational anisotropy in simulated vapor-deposited molecular glasses. Journal of Chemical Physics, 2015, 143, 094502.	1.2	59
117	Transport properties of polymer melts from nonequilibrium molecular dynamics. Journal of Chemical Physics, 1995, 102, 5836-5844.	1.2	58
118	Coarse-grained modeling of DNA oligomer hybridization: Length, sequence, and salt effects. Journal of Chemical Physics, 2014, 141, 035102.	1.2	58
119	Simulation and theory of the swelling of athermal gels. Journal of Chemical Physics, 1997, 106, 793-810.	1.2	57
120	Directed Assembly of a Cylinder-Forming Diblock Copolymer: Topographic and Chemical Patterns. Macromolecules, 2010, 43, 6495-6504.	2.2	57
121	Evolutionary pattern design for copolymer directed self-assembly. Soft Matter, 2013, 9, 11467.	1.2	57
122	Molecular Structure of Canonical Liquid Crystal Interfaces. Journal of the American Chemical Society, 2017, 139, 3841-3850.	6.6	56
123	Density of states of a binary Lennard-Jones glass. Journal of Chemical Physics, 2003, 119, 4405-4408.	1.2	55
124	A molecular view of the role of chirality in charge-driven polypeptide complexation. Soft Matter, 2015, 11, 1525-1538.	1.2	55
125	Molecular Level Differences in Ionic Solvation and Transport Behavior in Ethylene Oxide-Based Homopolymer and Block Copolymer Electrolytes. Journal of the American Chemical Society, 2021, 143, 3180-3190.	6.6	55
126	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

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127	A new double-rebridging technique for linear polyethylene. Journal of Chemical Physics, 2003, 119, 2456-2462.	1.2	54
128	Behavior of single nanoparticle/homopolymer chain in ordered structures of diblock copolymers. Journal of Chemical Physics, 2003, 118, 11278-11285.	1.2	54
129	Simulations of theoretically informed coarse grain models of polymeric systems. Faraday Discussions, 2010, 144, 111-125.	1.6	53
130	Autonomous materials systems from active liquid crystals. Nature Reviews Materials, 2021, 6, 437-453.	23.3	53
131	Effect of Solvent Quality on the Phase Behavior of Polyelectrolyte Complexes. Macromolecules, 2021, 54, 105-114.	2.2	53
132	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
133	Liquid Crystal Mediated Interactions Between Nanoparticles in a Nematic Phase. Langmuir, 2012, 28, 6124-6131.	1.6	52
134	Topcoat Approaches for Directed Self-Assembly of Strongly Segregating Block Copolymer Thin Films. Journal of Photopolymer Science and Technology = [Fotoporima Konwakai Shi], 2013, 26, 55-58.	0.1	52
135	Block Copolymer Assembly on Nanoscale Patterns of Polymer Brushes Formed by Electrohydrodynamic Jet Printing. ACS Nano, 2014, 8, 6606-6613.	7.3	52
136	Density functional theory of molecular structure for thin diblock copolymer films on chemically heterogeneous surfaces. Journal of Chemical Physics, 1999, 110, 7483-7490.	1.2	51
137	Morphologies of Linear Triblock Copolymers from Monte Carlo Simulations. Macromolecules, 2011, 44, 5490-5497.	2.2	51
138	Effect of Proline Mutations on the Monomer Conformations of Amylin. Biophysical Journal, 2013, 105, 1227-1235.	0.2	51
139	Nematic-Field-Driven Positioning of Particles in Liquid Crystal Droplets. Physical Review Letters, 2013, 111, 227801.	2.9	50
140	Membrane Permeation versus Amyloidogenicity: A Multitechnique Study of Islet Amyloid Polypeptide Interaction with Model Membranes. Journal of the American Chemical Society, 2017, 139, 137-148.	6.6	49
141	Coarse-Grained Model of the Dynamics of Electrolyte Solutions. Journal of Physical Chemistry B, 2017, 121, 8195-8202.	1.2	49
142	Origin of Anisotropic Molecular Packing in Vapor-Deposited Alq3 Glasses. Journal of Physical Chemistry Letters, 2019, 10, 164-170.	2.1	49
143	Chemical potential and equations of state of hard core chain molecules. Journal of Chemical Physics, 1995, 103, 1946-1956.	1.2	48
144	Blue-phase liquid crystal droplets. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, 13195-13200.	3.3	48

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145	Role of Defects in Ion Transport in Block Copolymer Electrolytes. Nano Letters, 2019, 19, 4684-4691.	4.5	48
146	Molecular and multiscale modeling in chemical engineering - current view and future perspectives. AICHE Journal, 2005, 51, 2371-2376.	1.8	47
147	Electronic structure at coarse-grained resolutions from supervised machine learning. Science Advances, 2019, 5, eaav1190.	4.7	47
148	Secondary Structure of Rat and Human Amylin across Force Fields. PLoS ONE, 2015, 10, e0134091.	1.1	47
149	Evolution of fivefold local symmetry during crystal nucleation and growth in dense hard-sphere packings. Soft Matter, 2012, 8, 844-858.	1.2	46
150	Modeling the Binding Mechanism of Remdesivir, Favilavir, and Ribavirin to SARS-CoV-2 RNA-Dependent RNA Polymerase. ACS Central Science, 2021, 7, 164-174.	5.3	46
151	Broadband Liquid Crystal Tunable Metasurfaces in the Visible: Liquid Crystal Inhomogeneities Across the Metasurface Parameter Space. ACS Photonics, 2021, 8, 567-575.	3.2	46
152	Comparing Solvophobic and Multivalent Induced Collapse in Polyelectrolyte Brushes. ACS Macro Letters, 2017, 6, 155-160.	2.3	45
153	Statistical calculation of elastic moduli for atomistic models. Physical Review B, 2005, 71, .	1.1	44
154	Stimuliâ€Responsive Cubosomes Formed from Blue Phase Liquid Crystals. Advanced Materials, 2015, 27, 6892-6898.	11.1	44
155	Complex Coacervation in Polyelectrolytes from a Coarse-Grained Model. Macromolecules, 2018, 51, 6717-6723.	2.2	44
156	Thermodynamics and Structure of Poly[n]catenane Melts. Macromolecules, 2020, 53, 3390-3408.	2.2	44
157	Machine learning active-nematic hydrodynamics. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, .	3.3	44
158	Phase equilibria and clustering in size-asymmetric primitive model electrolytes. Journal of Chemical Physics, 2001, 114, 1727-1731.	1.2	43
159	Theoretically informed entangled polymer simulations: linear and non-linear rheology of melts. Soft Matter, 2013, 9, 2030.	1.2	43
160	Quantitative Three-Dimensional Characterization of Block Copolymer Directed Self-Assembly on Combined Chemical and Topographical Prepatterned Templates. ACS Nano, 2017, 11, 1307-1319.	7.3	43
161	Advanced Materials for Energy-Water Systems: The Central Role of Water/Solid Interfaces in Adsorption, Reactivity, and Transport. Chemical Reviews, 2021, 121, 9450-9501.	23.0	43
162	Bondâ€bias simulation of phase equilibria for strongly associating fluids. Journal of Chemical Physics, 1994, 101, 1477-1489.	1.2	42

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163	Solubility of Small Molecules and Their Mixtures in Polyethylene. Journal of Physical Chemistry B, 1999, 103, 3539-3544.	1.2	42
164	Dynamics and Deformation Response of Rod-Containing Nanocomposites. Macromolecules, 2012, 45, 543-554.	2.2	42
165	A multichain polymer slip-spring model with fluctuating number of entanglements for linear and nonlinear rheology. Journal of Chemical Physics, 2015, 143, 243147.	1.2	42
166	Mesoscale martensitic transformation in single crystals of topological defects. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, 10011-10016.	3.3	42
167	Photostability Can Be Significantly Modulated by Molecular Packing in Glasses. Journal of the American Chemical Society, 2016, 138, 11282-11289.	6.6	41
168	Fluctuating hydrodynamics of chiral active fluids. Nature Physics, 2021, 17, 1260-1269.	6.5	41
169	An Analysis of Biomolecular Force Fields for Simulations of Polyglutamine in Solution. Biophysical Journal, 2015, 109, 1009-1018.	0.2	40
170	Presentation of Large DNA Molecules for Analysis as Nanoconfined Dumbbells. Macromolecules, 2013, 46, 8356-8368.	2.2	39
171	Age and structure of a model vapour-deposited glass. Nature Communications, 2016, 7, 13062.	5.8	39
172	Adaptive enhanced sampling by force-biasing using neural networks. Journal of Chemical Physics, 2018, 148, 134108.	1.2	39
173	Dynamics of poly[n]catenane melts. Journal of Chemical Physics, 2020, 152, 214901.	1.2	39
174	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
175	Defect Annihilation Pathways in Directed Assembly of Lamellar Block Copolymer Thin Films. ACS Nano, 2018, 12, 9974-9981.	7.3	38
176	Pseudo-ensemble simulations and Gibbsâ€“Duhem integrations for polymers. Journal of Chemical Physics, 1997, 106, 2911-2923.	1.2	37
177	Effects of anchoring strength on the diffusivity of nanoparticles in model liquid-crystalline fluids. Soft Matter, 2011, 7, 6828.	1.2	37
178	Nanoscale chromatin imaging and analysis platform bridges 4D chromatin organization with molecular function. Science Advances, 2021, 7, .	4.7	37
179	Aggregation and Solubility of a Model Conjugated Donorâ€“Acceptor Polymer. Journal of Physical Chemistry Letters, 2018, 9, 4802-4807.	2.1	36
180	Intrinsic Ion Transport Properties of Block Copolymer Electrolytes. ACS Nano, 2020, 14, 8902-8914.	7.3	36

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181	Critical behavior of lattice polymers studied by Monte Carlo simulations. Journal of Chemical Physics, 2000, 113, 5954-5957.	1.2	35
182	Thermodynamic and transport properties of nitrogen and butane mixtures. Molecular Physics, 2000, 98, 43-55.	0.8	35
183	Flow induced deformation of defects around nanoparticles and nanodroplets suspended in liquid crystals. Soft Matter, 2010, 6, 896.	1.2	35
184	Drop splashing is independent of substrate wetting. Physics of Fluids, 2018, 30, .	1.6	35
185	Morphology of Lamellae-Forming Block Copolymer Films between Two Orthogonal Chemically Nanopatterned Striped Surfaces. Physical Review Letters, 2012, 108, 065502.	2.9	34
186	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.	1.2	34
187	Perspective: Evolutionary design of granular media and block copolymer patterns. APL Materials, 2016, 4, .	2.2	33
188	A theory of interactions between polarizable dielectric spheres. Journal of Colloid and Interface Science, 2016, 469, 237-241.	5.0	33
189	Role of Molecular Architecture on Ion Transport in Ethylene oxide-Based Polymer Electrolytes. Macromolecules, 2021, 54, 2266-2276.	2.2	33
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