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	Molecular characterization of COVID-19 therapeutics: luteolin as an allosteric modulator of the spike protein of SARS-CoV-2. Molecular Systems Design and Engineering, 2022, 7, 58-66.	1.7	11
2	Strongly Chiral Liquid Crystals in Nanoemulsions. Small, 2022, , 2105835.	5.2	4
3	Toward wide-spectrum antivirals against coronaviruses: Molecular characterization of SARS-CoV-2 NSP13 helicase inhibitors. Science Advances, 2022, 8, eabj4526.	4.7	25
4	Is the â€œBricks-and-Mortarâ€•Mesophase Bicontinuous? Dynamic Simulations of Miktoarm Block Copolymer/Homopolymer Blends. Macromolecules, 2022, 55, 745-758.	2.2	3
5	Active learning of polarizable nanoparticle phase diagrams for the guided design of triggerable self-assembling superlattices. Molecular Systems Design and Engineering, 2022, 7, 350-363.	1.7	3
6	From nematic shells to nematic droplets: energetics and defect transitions. Soft Matter, 2022, , .	1.2	2
7	Characterization of the Interfacial Orientation and Molecular Conformation in a Glass-Forming Organic Semiconductor. ACS Applied Materials & Interfaces, 2022, 14, 3455-3466.	4.0	5
8	Tuning the mechanical impedance of disordered networks for impact mitigation. Soft Matter, 2022, 18, 2039-2045.	1.2	3
9	Logic operations with active topological defects. Science Advances, 2022, 8, eabg9060.	4.7	13
10	Collective Variables for Free Energy Surface Tailoring: Understanding and Modifying Functionality in Systems Dominated by Rare Events. Journal of Physical Chemistry Letters, 2022, 13, 2830-2837.	2.1	5
11	Ionic Transport in Electrostatic Janus Membranes. An Explicit Solvent Molecular Dynamic Simulation. ACS Nano, 2022, 16, 3768-3775.	7.3	9
12	Programming Solitons in Liquid Crystals Using Surface Chemistry. Langmuir, 2022, 38, 3575-3584.	1.6	5
13	Metastable doubly threaded [3]rotaxanes with a large macrocycle. Chemical Science, 2022, 13, 5333-5344.	3.7	4
14	Parameter estimation for X-ray scattering analysis with Hamiltonian Markov Chain Monte Carlo. Journal of Synchrotron Radiation, 2022, 29, 721-731.	1.0	2
15	A Coarse-Grained Molecular Dynamics Study of Strongly Charged Polyelectrolyte Coacervates: Interfacial, Structural, and Dynamical Properties. Macromolecules, 2022, 55, 4146-4158.	2.2	5
16	Stress-activated constraints in dense suspension rheology. Physical Review Fluids, 2022, 7, .	1.0	7
17	Catapulting of topological defects through elasticity bands in active nematics. Soft Matter, 2022, 18, 5271-5281.	1.2	5
18	Nonequilibrium statistical thermodynamics of multicomponent interfaces. Proceedings of the National Academy of Sciences of the United States of America, 2022, 119, .	3.3	10

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19	A Generalizable Approach to Direct the Selfâ€Assembly of Functional Blueâ€Phase Liquid Crystals. Advanced Functional Materials, 2022, 32, .	7.8	5
20	Polyelectrolyte Complex Coacervates: Recent Developments and New Frontiers. Annual Review of Condensed Matter Physics, 2021, 12, 155-176.	5.2	96
21	Active motion of multiphase oil droplets: emergent dynamics of squirmers with evolving internal structure. Soft Matter, 2021, 17, 2985-2993.	1.2	24
22	Directing the far-from-equilibrium assembly of nanoparticles in confined liquid crystals by hydrodynamic fields. Soft Matter, 2021, 17, 3463-3472.	1.2	5
23	Role of solvation site segmental dynamics on ion transport in ethylene-oxide based side-chain polymer electrolytes. Journal of Materials Chemistry A, 2021, 9, 9937-9951.	5.2	21
24	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
25	Nucleation and growth of blue phase liquid crystals on chemically-patterned surfaces: a surface anchoring assisted blue phase correlation length. Molecular Systems Design and Engineering, 2021, 6, 534-544.	1.7	3
26	Complex coacervation of statistical polyelectrolytes: role of monomer sequences and formation of inhomogeneous coacervates. Molecular Systems Design and Engineering, 2021, 6, 790-804.	1.7	10
27	Nanoscale chromatin imaging and analysis platform bridges 4D chromatin organization with molecular function. Science Advances, 2021, 7, .	4.7	37
28	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
29	OpenAWSEM with Open3SPN2: A fast, flexible, and accessible framework for large-scale coarse-grained biomolecular simulations. PLoS Computational Biology, 2021, 17, e1008308.	1.5	31
30	Code interoperability extends the scope of quantum simulations. Npj Computational Materials, 2021, 7, .	3.5	8
31	Autonomous materials systems from active liquid crystals. Nature Reviews Materials, 2021, 6, 437-453.	23.3	53
32	Spatiotemporal control of liquid crystal structure and dynamics through activity patterning. Nature Materials, 2021, 20, 875-882.	13.3	70
33	Role of Molecular Architecture on Ion Transport in Ethylene oxide-Based Polymer Electrolytes. Macromolecules, 2021, 54, 2266-2276.	2.2	33
34	Neural Network Sampling of the Free Energy Landscape for Nitrogen Dissociation on Ruthenium. Journal of Physical Chemistry Letters, 2021, 12, 2954-2962.	2.1	16
35	Scaling Theory of Neutral Sequence-Specific Polyampholytes. Macromolecules, 2021, 54, 3232-3246.	2.2	14
36	Machine learning active-nematic hydrodynamics. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, .	3.3	44

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37	Harnessing Peptide Binding to Capture and Reclaim Phosphate. Journal of the American Chemical Society, 2021, 143, 4440-4450.	6.6	11
38	Anisotropic Coarse-Grained Model for Conjugated Polymers: Investigations into Solution Morphologies. Macromolecules, 2021, 54, 3780-3789.	2.2	23
39	Tetranucleosome Interactions Drive Chromatin Folding. ACS Central Science, 2021, 7, 1019-1027.	5.3	14
40	Molecular Mass Dependence of Interfacial Tension in Complex Coacervation. Physical Review Letters, 2021, 126, 237801.	2.9	11
41	Liquid Crystal Films as Active Substrates for Nanoparticle Control. ACS Applied Nano Materials, 2021, 4, 6700-6708.	2.4	6
42	Transformation between elastic dipoles, quadrupoles, octupoles, and hexadecapoles driven by surfactant self-assembly in nematic emulsion. Science Advances, 2021, 7, .	4.7	9
43	Defect Spirograph: Dynamical Behavior of Defects in Spatially Patterned Active Nematics. Physical Review Letters, 2021, 126, 227801.	2.9	15
44	Sequence Blockiness Controls the Structure of Polyampholyte Necklaces. ACS Macro Letters, 2021, 10, 1048-1054.	2.3	14
45	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
46	Polyelectrolyte Complex Coacervation across a Broad Range of Charge Densities. Macromolecules, 2021, 54, 6878-6890.	2.2	60
47	Sustainable Polymers Square Table. Macromolecules, 2021, 54, 8257-8258.	2.2	2
48	Control of Monodomain Polymer-Stabilized Cuboidal Nanocrystals of Chiral Nematics by Confinement. ACS Nano, 2021, 15, 15972-15981.	7.3	10
49	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
50	Effect of Solvent Quality on the Phase Behavior of Polyelectrolyte Complexes. Macromolecules, 2021, 54, 105-114.	2.2	53
51	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
52	Fluctuating hydrodynamics of chiral active fluids. Nature Physics, 2021, 17, 1260-1269.	6.5	41
53	Stability and molecular pathways to the formation of spin defects in silicon carbide. Nature Communications, 2021, 12, 6325.	5.8	9
54	Efficient Multiscale Optoelectronic Prediction for Conjugated Polymers. Macromolecules, 2020, 53, 482-490.	2.2	22

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55	Hydrodynamic interactions in topologically linked ring polymers. Physical Review E, 2020, 102, 032502.	0.8	11
56	Targeted sequence design within the coarse-grained polymer genome. Science Advances, 2020, 6, .	4.7	84
57	Direct Observation of Liquid Crystal Droplet Configurational Transitions using Optical Tweezers. Langmuir, 2020, 36, 7074-7082.	1.6	17
58	Prolate and oblate chiral liquid crystal spheroids. Science Advances, 2020, 6, eaba6728.	4.7	27
59	Formation, Stability, and Annihilation of the Stitched Morphology in Block Copolymer Thin Films. Macromolecules, 2020, 53, 10446-10456.	2.2	3
60	The looks of a million-year-old polymer glass. Nature Materials, 2020, 19, 1041-1042.	13.3	0
61	Molecular characterization of ebselen binding activity to SARS-CoV-2 main protease. Science Advances, 2020, 6, .	4.7	80
62	Crossover from Rouse to Reptation Dynamics in Salt-Free Polyelectrolyte Complex Coacervates. ACS Macro Letters, 2020, 9, 1318-1324.	2.3	21
63	Spatiotemporal Formation and Growth Kinetics of Polyelectrolyte Complex Micelles with Millisecond Resolution. ACS Macro Letters, 2020, 9, 1674-1680.	2.3	17
64	Over What Length Scale Does an Inorganic Substrate Perturb the Structure of a Glassy Organic Semiconductor?. ACS Applied Materials & Interfaces, 2020, 12, 26717-26726.	4.0	22
65	Structure and dynamics of hydrodynamically interacting finite-size Brownian particles in a spherical cavity: Spheres and cylinders. Journal of Chemical Physics, 2020, 152, 204109.	1.2	8
66	Intrinsic Ion Transport Properties of Block Copolymer Electrolytes. ACS Nano, 2020, 14, 8902-8914.	7.3	36
67	Dynamics of poly[n]catenane melts. Journal of Chemical Physics, 2020, 152, 214901.	1.2	39
68	Structural transformations in tetravalent nematic shells induced by a magnetic field. Soft Matter, 2020, 16, 8169-8178.	1.2	5
69	Shear Thickening and Jamming of Dense Suspensions: The â€œRollâ€•of Friction. Physical Review Letters, 2020, 124, 248005.	2.9	80
70	Dissociation of salts in water under pressure. Nature Communications, 2020, 11, 3037.	5.8	21
71	Thermodynamics and Structure of Poly[n]catenane Melts. Macromolecules, 2020, 53, 3390-3408.	2.2	44
72	Vapor-Deposited Glasses Highlight the Role of Density in Photostability. Journal of Physical Chemistry B, 2020, 124, 6112-6120.	1.2	5

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73	Microphase Separation in Polyelectrolyte Blends: Weak Segregation Theory and Relation to Nuclear â€œPastaâ€• Macromolecules, 2020, 53, 1281-1292.	2.2	22
74	An in situ shearing x-ray measurement system for exploring structures and dynamics at the solidâ€“liquid interface. Review of Scientific Instruments, 2020, 91, 013908.	0.6	3
75	Cuboidal liquid crystal phases under multiaxial geometrical frustration. Soft Matter, 2020, 16, 870-880.	1.2	8
76	Combined Force-Frequency Sampling for Simulation of Systems Having Rugged Free Energy Landscapes. Journal of Chemical Theory and Computation, 2020, 16, 1448-1455.	2.3	14
77	Understanding Ion Mobility in P2VP/NMP+Iâ€“ Polymer Electrolytes: A Combined Simulation and Experimental Study. Macromolecules, 2020, 53, 2783-2792.	2.2	12
78	Bottom-Up Meets Top-Down: The Crossroads ofÂMultiscale Chromatin Modeling. Biophysical Journal, 2020, 118, 2057-2065.	0.2	28
79	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
80	Shape induced segregation and anomalous particle transport under spherical confinement. Physics of Fluids, 2020, 32, 053307.	1.6	6
81	Emergence of Radial Tree of Bend Stripes in Active Nematics. Physical Review X, 2019, 9, .	2.8	13
82	Liquid Crystalline and Isotropic Coacervates of Semiflexible Polyanions and Flexible Polycations. Macromolecules, 2019, 52, 5140-5156.	2.2	26
83	Ultrathin initiated chemical vapor deposition polymer interfacial energy control for directed self-assembly hole-shrink applications. Journal of Vacuum Science and Technology B:Nanotechnology and Microelectronics, 2019, 37, 061804.	0.6	3
84	Qresp, a tool for curating, discovering and exploring reproducible scientific papers. Scientific Data, 2019, 6, 190002.	2.4	24
85	Controlling Complex Coacervation via Random Polyelectrolyte Sequences. ACS Macro Letters, 2019, 8, 1296-1302.	2.3	63
86	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
87	Generalised Navier boundary condition for a volume of fluid approach using a finite-volume method. Physics of Fluids, 2019, 31, 021203.	1.6	15
88	Anisotropic Vapor-Deposited Glasses: Hybrid Organic Solids. Accounts of Chemical Research, 2019, 52, 407-414.	7.6	67
89	The Free Energy Landscape of Internucleosome Interactions and Its Relation to Chromatin Fiber Structure. ACS Central Science, 2019, 5, 341-348.	5.3	31
90	Role of Defects in Ion Transport in Block Copolymer Electrolytes. Nano Letters, 2019, 19, 4684-4691.	4.5	48

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91	1CPN: A coarse-grained multi-scale model of chromatin. Journal of Chemical Physics, 2019, 150, 215102.	1.2	29
92	Enzyme-Induced Kinetic Control of Peptideâ€“Polymer Micelle Morphology. ACS Macro Letters, 2019, 8, 676-681.	2.3	22
93	Recent advances in machine learning towards multiscale soft materials design. Current Opinion in Chemical Engineering, 2019, 23, 106-114.	3.8	110
94	Electronic structure at coarse-grained resolutions from supervised machine learning. Science Advances, 2019, 5, eaav1190.	4.7	47
95	Free energy of metal-organic framework self-assembly. Journal of Chemical Physics, 2019, 150, 104502.	1.2	18
96	Degenerate conic anchoring and colloidal elastic dipole-hexadecapole transformations. Nature Communications, 2019, 10, 1000.	5.8	18
97	Pair and many-body interactions between ligated Au nanoparticles. Journal of Chemical Physics, 2019, 150, 044904.	1.2	17
98	Influence of Homopolymer Addition in Templated Assembly of Cylindrical Block Copolymers. ACS Nano, 2019, 13, 4073-4082.	7.3	3
99	New frontiers for the materials genome initiative. Npj Computational Materials, 2019, 5, .	3.5	312
100	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
101	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
102	Sculpting stable structures in pure liquids. Science Advances, 2019, 5, eaav4283.	4.7	25
103	Thermally reconfigurable Janus droplets with nematic liquid crystalline and isotropic perfluorocarbon oil compartments. Soft Matter, 2019, 15, 2580-2590.	1.2	19
104	Extracting collective motions underlying nucleosome dynamics via nonlinear manifold learning. Journal of Chemical Physics, 2019, 150, 054902.	1.2	6
105	Perfection in Nucleation and Growth of Blue-Phase Single Crystals: Small Free-Energy Required to Self-Assemble at Specific Lattice Orientation. ACS Applied Materials & Interfaces, 2019, 11, 9487-9495.	4.0	24
106	Reconfigurable Multicompartment Emulsion Drops Formed by Nematic Liquid Crystals and Immiscible Perfluorocarbon Oils. Langmuir, 2019, 35, 16312-16323.	1.6	12
107	Ideal isotropic auxetic networks from random networks. Soft Matter, 2019, 15, 8084-8091.	1.2	18
108	Sculpted grain boundaries in soft crystals. Science Advances, 2019, 5, eaax9112.	4.7	18

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109	Origin of Anisotropic Molecular Packing in Vapor-Deposited Alq3 Glasses. Journal of Physical Chemistry Letters, 2019, 10, 164-170.	2.1	49
110	Graph-Based Approach to Systematic Molecular Coarse-Graining. Journal of Chemical Theory and Computation, 2019, 15, 1199-1208.	2.3	60
111	Drop splashing is independent of substrate wetting. Physics of Fluids, 2018, 30, .	1.6	35
112	SSAGES: Software Suite for Advanced General Ensemble Simulations. Journal of Chemical Physics, 2018, 148, 044104.	1.2	83
113	Role of translational entropy in spatially inhomogeneous, coarse-grained models. Journal of Chemical Physics, 2018, 148, .	1.2	8
114	Ion Distribution in Microphase-Separated Copolymers with Periodic Dielectric Permittivity. Macromolecules, 2018, 51, 1986-1991.	2.2	31
115	In Silico Measurement of Elastic Moduli of Nematic Liquid Crystals. Physical Review Letters, 2018, 120, 107801.	2.9	16
116	Intra-molecular Charge Transfer and Electron Delocalization in Non-fullerene Organic Solar Cells. ACS Applied Materials & Interfaces, 2018, 10, 10043-10052.	4.0	24
117	A Detailed Examination of the Topological Constraints of Lamellae-Forming Block Copolymers. Macromolecules, 2018, 51, 2110-2124.	2.2	19
118	Hierarchical Coupling of First-Principles Molecular Dynamics with Advanced Sampling Methods. Journal of Chemical Theory and Computation, 2018, 14, 2881-2888.	2.3	18
119	Influence of Ion Solvation on the Properties of Electrolyte Solutions. Journal of Physical Chemistry B, 2018, 122, 4029-4034.	1.2	88
120	Phase Behavior and Salt Partitioning in Polyelectrolyte Complex Coacervates. Macromolecules, 2018, 51, 2988-2995.	2.2	241
121	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
122	Adaptive enhanced sampling by force-biasing using neural networks. Journal of Chemical Physics, 2018, 148, 134108.	1.2	39
123	Optimizing self-consistent field theory block copolymer models with X-ray metrology. Molecular Systems Design and Engineering, 2018, 3, 376-389.	1.7	13
124	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
125	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
126	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

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127	Mechanisms of Directed Self-Assembly in Cylindrical Hole Confinements. Macromolecules, 2018, 51, 2418-2427.	2.2	4
128	Nanocrystalline Oligo(ethylene sulfide)-b-poly(ethylene glycol) Micelles: Structure and Stability. Macromolecules, 2018, 51, 9538-9546.	2.2	7
129	Structural Correlations and Percolation in Twisted Perylene Diimides Using a Simple Anisotropic Coarse-Grained Model. Journal of Chemical Theory and Computation, 2018, 14, 6495-6504.	2.3	15
130	Tenfold increase in the photostability of an azobenzene guest in vapor-deposited glass mixtures. Journal of Chemical Physics, 2018, 149, 204503.	1.2	16
131	Towards hybrid human-machine scientific information extraction. , 2018, , .		4
132	Amphiphile-Induced Phase Transition of Liquid Crystals at Aqueous Interfaces. ACS Applied Materials & Interfaces, 2018, 10, 37618-37624.	4.0	23
133	Defect Annihilation Pathways in Directed Assembly of Lamellar Block Copolymer Thin Films. ACS Nano, 2018, 12, 9974-9981.	7.3	38
134	Tunable structure and dynamics of active liquid crystals. Science Advances, 2018, 4, eaat7779.	4.7	125
135	Multivalent counterions diminish the lubricity of polyelectrolyte brushes. Science, 2018, 360, 1434-1438.	6.0	137
136	Evolutionary strategy for inverse charge measurements of dielectric particles. Journal of Chemical Physics, 2018, 148, 234302.	1.2	4
137	Aggregation and Solubility of a Model Conjugated Donorâ€“Acceptor Polymer. Journal of Physical Chemistry Letters, 2018, 9, 4802-4807.	2.1	36
138	Layered nested Markov chain Monte Carlo. Journal of Chemical Physics, 2018, 149, 072326.	1.2	9
139	Simulations of splashing high and low viscosity droplets. Physics of Fluids, 2018, 30, .	1.6	16
140	Oligomers as Triggers for Responsive Liquid Crystals. Langmuir, 2018, 34, 10092-10101.	1.6	20
141	Topological Effects in Isolated Poly[n]catenanes: Molecular Dynamics Simulations and Rouse Mode Analysis. ACS Macro Letters, 2018, 7, 938-943.	2.3	60
142	Early-stage human islet amyloid polypeptide aggregation: Mechanisms behind dimer formation. Journal of Chemical Physics, 2018, 149, 025101.	1.2	22
143	Effect of temperature on the structure and dynamics of triblock polyelectrolyte gels. Journal of Chemical Physics, 2018, 149, 163310.	1.2	9
144	Complex Coacervation in Polyelectrolytes from a Coarse-Grained Model. Macromolecules, 2018, 51, 6717-6723.	2.2	44

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145	Observation of the pressure effect in simulations of droplets splashing on a dry surface. Physical Review Fluids, 2018, 3, .	1.0	8
146	Low-temperature anomalies of a vapor deposited glass. Physical Review Materials, 2018, 2, .	0.9	26
147	Thickness dependence of forming single crystal by liquid-crystalline blue phase on chemically patterned surface. , 2018, , .		2
148	Studying the effects of chemistry and geometry on DSA hole-shrink process in three dimensions. , 2018, , .		1
149	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
150	Comparing Solvophobic and Multivalent Induced Collapse in Polyelectrolyte Brushes. ACS Macro Letters, 2017, 6, 155-160.	2.3	45
151	Gel phase formation in dilute triblock copolyelectrolyte complexes. Nature Communications, 2017, 8, 14131.	5.8	92
152	Molecular Structure of Canonical Liquid Crystal Interfaces. Journal of the American Chemical Society, 2017, 139, 3841-3850.	6.6	56
153	A Molecular View of the Dynamics of dsDNA Packing Inside Viral Capsids in the Presence of Ions. Biophysical Journal, 2017, 112, 1302-1315.	0.2	20
154	Gelatin-Derived Grapheneâ€“Silicate Hybrid Materials Are Biocompatible and Synergistically Promote BMP9-Induced Osteogenic Differentiation of Mesenchymal Stem Cells. ACS Applied Materials & Interfaces, 2017, 9, 15922-15932.	4.0	30
155	Influence of Vapor Deposition on Structural and Charge Transport Properties of Ethylbenzene Films. ACS Central Science, 2017, 3, 415-424.	5.3	21
156	Segregation of liquid crystal mixtures in topological defects. Nature Communications, 2017, 8, 15064.	5.8	25
157	Directed self-assembly of liquid crystalline blue-phases into ideal single-crystals. Nature Communications, 2017, 8, 15854.	5.8	101
158	Directed Self-Assembly of Colloidal Particles onto Nematic Liquid Crystalline Defects Engineered by Chemically Patterned Surfaces. ACS Nano, 2017, 11, 6492-6501.	7.3	22
159	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
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	Strain-induced alignment and phase behavior of blue phase liquid crystals confined to thin films. Soft Matter, 2017, 13, 8999-9006.	1.2	18
162	Sharp Morphological Transitions from Nanoscale Mixed-Anchoring Patterns in Confined Nematic Liquid Crystals. Langmuir, 2017, 33, 12516-12524.	1.6	14

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163	Spherical nematic shells with a prolate ellipsoidal core. Soft Matter, 2017, 13, 7465-7472.	1.2	13
164	Derivation of Multiple Covarying Material and Process Parameters Using Physics-Based Modeling of X-ray Data. Macromolecules, 2017, 50, 7783-7793.	2.2	26
165	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
166	Polymer Informatics: Opportunities and Challenges. ACS Macro Letters, 2017, 6, 1078-1082.	2.3	184
167	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
168	Coarse-Grained Model of the Dynamics of Electrolyte Solutions. Journal of Physical Chemistry B, 2017, 121, 8195-8202.	1.2	49
169	Water Flux Induced Reorientation of Liquid Crystals. ACS Central Science, 2017, 3, 1345-1349.	5.3	9
170	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
171	Poly[n]catenanes: Synthesis of molecular interlocked chains. Science, 2017, 358, 1434-1439.	6.0	196
172	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
173	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
174	Patterned surface anchoring of nematic droplets at miscible liquidâ€“liquid interfaces. Soft Matter, 2017, 13, 5714-5723.	1.2	23
175	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
176	Visualization and simulation of the transfer process of indexâ€matched silica microparticle inks for gravure printing. AIChE Journal, 2017, 63, 1419-1429.	1.8	5
177	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
178	Understanding Atomic-Scale Behavior of Liquid Crystals at Aqueous Interfaces. Journal of Chemical Theory and Computation, 2017, 13, 237-244.	2.3	31
179	Towards a Hybrid Human-Computer Scientific Information Extraction Pipeline. , 2017, , .		18
180	Multivalent ions induce lateral structural inhomogeneities in polyelectrolyte brushes. Science Advances, 2017, 3, eaao1497.	4.7	79

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181	Demixing by a Nematic Mean Field: Coarse-Grained Simulations of Liquid Crystalline Polymers. Polymers, 2017, 9, 88.	2.0	18
182	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
183	Tension-Dependent Free Energies of Nucleosome Unwrapping. ACS Central Science, 2016, 2, 660-666.	5.3	67
184	Controlled deformation of vesicles by flexible structured media. Science Advances, 2016, 2, e1600978.	4.7	16
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