Arun Yethiraj

List of Publications by Year
in descending order

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234 papers	8,159 citations	31902 53 h-index	79541 73 g-index
238 all docs	238 docs citations	238 times ranked	5427 citing authors

#	Article	IF	Citations
1	A New Coarse-Grained Model for Water: The Importance of Electrostatic Interactions. Journal of Physical Chemistry B, 2010, 114, 10524-10529.	1.2	170
2	Self-Diffusion and Viscosity in Electrolyte Solutions. Journal of Physical Chemistry B, 2012, 116, 12007-12013.	1.2	156
3	Monte Carlo density functional theory of nonuniform polymer melts. Journal of Chemical Physics, 1995, 102, 5499-5505.	1.2	147
4	Monte-Carlo simulation of polymers confined between flat plates. Macromolecules, 1990, 23, 1865-1872.	2.2	140
5	Rheology of Confined Polymer Melts. Macromolecules, 1996, 29, 7910-7918.	2.2	125
6	Polymer reference interaction site model theory: New molecular closures for phase separating fluids and alloys. Journal of Chemical Physics, 1993, 98, 9053-9079.	1.2	120
7	Effect of Macromolecular Crowding on Reaction Rates: A Computational and Theoretical Study. Biophysical Journal, 2009, 96, 1333-1340.	0.2	114
8	Low-symmetry sphere packings of simple surfactant micelles induced by ionic sphericity. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, 4072-4077.	3.3	109
9	Why Are Lipid Rafts Not Observed In Vivo?. Biophysical Journal, 2007, 93, 3113-3119.	0.2	100
10	Solvent effects on the collapse dynamics of polymers. Journal of Chemical Physics, 2001, 114, 7688-7699.	1.2	99
11	Short chains at surfaces and interfaces: A quantitative comparison between density-functional theories and Monte Carlo simulations. Journal of Chemical Physics, 2003, 118, 2929.	1.2	99
12	Molecular simulation and continuum mechanics study of simple fluids in non-isothermal planar couette flows. Journal of Chemical Physics, 1997, 107, 2589-2596.	1.2	97
13	Entropy-Based Mechanism of Ribosome-Nucleoid Segregation in E.Âcoli Cells. Biophysical Journal, 2011, 100, 2605-2613.	0.2	96
14	Density functional theory of polymers: A Curtin-Ashcroft type weighted density approximation. Journal of Chemical Physics, 1998, 109, 3269-3275.	1.2	90
15	Phase behavior of semiflexible tangent hard sphere chains. Journal of Chemical Physics, 1998, 108, 1636-1644.	1.2	90
16	Monte Carlo simulation of hard chainâ€“hard sphere mixtures in slitlike pores. Journal of Chemical Physics, 1989, 91, 4827-4837.	1.2	88
17	Monte Carlo simulations and integral equation theory for microscopic correlations in polymeric fluids. Journal of Chemical Physics, 1992, 96, 797-807.	1.2	87
18	Liquidâ€state theory of the density dependent conformation of nonpolar linear polymers. Journal of Chemical Physics, 1994, 100, 6857-6872.	1.2	85

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19	Siteâ€“site correlations in short chain fluids. Journal of Chemical Physics, 1990, 93, 4453-4461.	1.2	84
20	Density functional theory for inhomogeneous polymer solutions. Journal of Chemical Physics, 1994, 100, 3181-3186.	1.2	84
21	Generalized Flory equations of state for squareâ€well chains. Journal of Chemical Physics, 1991, 95, 8494-8506.	1.2	80
22	Structure of Polyelectrolyte Solutions. Physical Review Letters, 1996, 77, 3937-3940.	2.9	80
23	Integral equation theory for the adsorption of chain fluids in slitlike pores. Journal of Chemical Physics, 1991, 95, 3749-3755.	1.2	79
24	Rheological, thermodynamic, and structural studies of linear and branched alkanes under shear. Journal of Chemical Physics, 1997, 107, 6956-6964.	1.2	78
25	Density Functional Theory for the Distribution of Small Ions around Polyions. Journal of Physical Chemistry B, 1999, 103, 6080-6087.	1.2	77
26	Monte Carlo simulation of confined semiflexible polymer melts. Journal of Chemical Physics, 1994, 101, 2489-2497.	1.2	76
27	Ab Initio Force Fields for Imidazolium-Based Ionic Liquids. Journal of Physical Chemistry B, 2016, 120, 7024-7036.	1.2	76
28	A New Coarse-Grained Force Field for Membraneâ€“Peptide Simulations. Journal of Chemical Theory and Computation, 2011, 7, 3793-3802.	2.3	75
29	A Finite Element Framework for Studying the Mechanical Response of Macromolecules: Application to the Gating of the Mechanosensitive Channel MscL. Biophysical Journal, 2006, 91, 1248-1263.	0.2	73
30	Surface segregation in polymer blends due to stiffness disparity. Journal of Chemical Physics, 1994, 100, 4691-4694.	1.2	72
31	Molecular dynamics simulations of heat and momentum transfer at a solidâ€“fluid interface: Relationship between thermal and velocity slip. International Journal of Heat and Mass Transfer, 2006, 49, 3401-3407.	2.5	72
32	Squareâ€well chains: Bulk equation of state using perturbation theory and Monte Carlo simulations of the bulk pressure and of the density profiles near walls. Journal of Chemical Physics, 1991, 95, 1999-2005.	1.2	70
33	Implicit and Explicit Solvent Models for the Simulation of Dilute Polymer Solutions. Macromolecules, 2006, 39, 8536-8542.	2.2	69
34	Conformational Properties and Static Structure Factor of Polyelectrolyte Solutions. Physical Review Letters, 1997, 78, 3789-3792.	2.9	68
35	First-Principles United Atom Force Field for the Ionic Liquid BMIM⁺BF₄^{â€“}: An Alternative to Charge Scaling. Journal of Physical Chemistry B, 2016, 120, 3560-3568.	1.2	68
36	Entropic and Enthalpic Surface Segregation from Blends of Branched and Linear Polymers. Physical Review Letters, 1995, 74, 2018-2021.	2.9	66

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37	Liquid State Theory of Polyelectrolyte Solutions. Journal of Physical Chemistry B, 2009, 113, 1539-1551.	1.2	66
38	Dynamics in Crowded Environments: Is Non-Gaussian Brownian Diffusion Normal?. Journal of Physical Chemistry B, 2014, 118, 8128-8134.	1.2	66
39	Square-well diatomics: Bulk equation of state, density profiles near walls, virial coefficients and coexistence properties. Molecular Physics, 1991, 72, 619-641.	0.8	65
40	Strongly charged flexible polyelectrolytes in poor solvents: Molecular dynamics simulations with explicit solvent. Journal of Chemical Physics, 2003, 118, 6634-6647.	1.2	64
41	Interaction between colloids in solutions containing dissolved polymer. Journal of Colloid and Interface Science, 1992, 151, 102-117.	5.0	63
42	Computer Simulation Study of Two-Dimensional Polymer Solutions. Macromolecules, 2003, 36, 5854-5862.	2.2	63
43	Integral equation theory of solutions of rigid polyelectrolytes. Journal of Chemical Physics, 1997, 106, 5706-5719.	1.2	61
44	Theory for chain conformations and static structure of dilute and semidilute polyelectrolyte solutions. Journal of Chemical Physics, 1998, 108, 1184-1192.	1.2	61
45	A Monte Carlo simulation study of branched polymers. Journal of Chemical Physics, 2006, 125, 204901.	1.2	61
46	Why Do Arginine and Lysine Organize Lipids Differently? Insights from Coarse-Grained and Atomistic Simulations. Journal of Physical Chemistry B, 2013, 117, 12145-12156.	1.2	60
47	Dilute Solutions of Strongly Charged Flexible Polyelectrolytes in Poor Solvents:â€‰ Molecular Dynamics Simulations with Explicit Solvent. Macromolecules, 2006, 39, 821-828.	2.2	59
48	Selfâ€consistent polymer integral equation theory: Comparisons with Monte Carlo simulations and alternative closure approximations. Journal of Chemical Physics, 1992, 97, 1455-1464.	1.2	57
49	First-Principles, Physically Motivated Force Field for the Ionic Liquid [BMIM][BF₄]. Journal of Physical Chemistry Letters, 2014, 5, 2670-2674.	2.1	57
50	Monte Carlo simulation of the equilibrium partitioning of chain fluids between a bulk and a pore. Molecular Physics, 1991, 73, 503-515.	0.8	55
51	Integral equation theory of polymer blends: Numerical investigation of molecular closure approximations. Journal of Chemical Physics, 1993, 98, 9080-9093.	1.2	55
52	Density functional theory for nonuniform polymers: Accurate treatment of the effect of attractive interactions. Journal of Chemical Physics, 2003, 118, 4702-4706.	1.2	55
53	Polymerâ€induced forces between colloidal particles. A Monte Carlo simulation. Journal of Chemical Physics, 1994, 100, 4683-4690.	1.2	54
54	Perturbation density functional theory and Monte Carlo simulations for the structure of hard triatomic fluids in slitlike pores. Journal of Chemical Physics, 1995, 102, 2141-2150.	1.2	54

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55	Influence of Electronic Polarization on the Structure of Ionic Liquids. Journal of Physical Chemistry Letters, 2018, 9, 4765-4770.	2.1	54
56	Local density enhancement in dilute supercritical solutions. Chemical Physics Letters, 2000, 317, 558-566.	1.2	53
57	Different states of synaptotagmin regulate evoked versus spontaneous release. Nature Communications, 2016, 7, 10971.	5.8	53
58	Lateral Diffusion and Percolation in Membranes. Physical Review Letters, 2006, 96, 228103.	2.9	52
59	Isotropic to nematic transition in semiflexible polymer melts. Molecular Physics, 1998, 93, 693-701.	0.8	51
60	Atomistic Simulations of Poly(ethylene oxide) in Water and an Ionic Liquid at Room Temperature. Macromolecules, 2014, 47, 438-446.	2.2	50
61	Microscopic equations of state of polyethylene: Hardâ€chain contribution to the pressure. Journal of Chemical Physics, 1993, 98, 1635-1646.	1.2	49
62	Monte Carlo calculation of the osmotic second virial coefficient of off-lattice athermal polymers. Macromolecules, 1992, 25, 3979-3983.	2.2	48
63	Generalized van der Waals density functional theory for nonuniform polymers. Journal of Chemical Physics, 2000, 112, 1579-1584.	1.2	48
64	Understanding the Properties of Ionic Liquids: Electrostatics, Structure Factors, and Their Sum Rules. Journal of Physical Chemistry B, 2019, 123, 3499-3512.	1.2	48
65	Density Functional Theory for the Nonspecific Binding of Salt to Polyelectrolytes: Thermodynamic Properties. Biophysical Journal, 2000, 78, 699-706.	0.2	45
66	Crowding Effects on Association Reactions at Membranes. Biophysical Journal, 2010, 98, 951-958.	0.2	45
67	Anionic Phospholipids Stabilize RecA Filament Bundles in Escherichia coli. Molecular Cell, 2015, 60, 374-384.	4.5	45
68	Ab Initio Force Fields for Organic Anions: Properties of [BMIM][TFSI], [BMIM][FSI], and [BMIM][OTf] Ionic Liquids. Journal of Physical Chemistry B, 2018, 122, 4101-4114.	1.2	45
69	On the scaling of the critical temperature with the degree of polymerization in symmetric polymer blends. Journal of Chemical Physics, 1992, 97, 5927-5930.	1.2	44
70	Brownian dynamics simulations of salt-free polyelectrolyte solutions. Journal of Chemical Physics, 2002, 116, 5284.	1.2	44
71	Diffusion of hard sphere fluids in disordered media: A molecular dynamics simulation study. Physical Review E, 2004, 69, 051101.	0.8	44
72	Gating Mechanisms of Mechanosensitive Channels of Large Conductance, I: A Continuum Mechanics-Based Hierarchical Framework. Biophysical Journal, 2008, 95, 563-580.	0.2	44

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73	Lateral Diffusion of Proteins in the Plasma Membrane:â€‰ Spatial Tessellation and Percolation Theory. Journal of Physical Chemistry B, 2008, 112, 143-149.	1.2	44
74	Self-Assembly of Gemini Surfactants: A Computer Simulation Study. Journal of Physical Chemistry B, 2013, 117, 4254-4262.	1.2	44
75	Polymer Melts at Solid Surfaces. Advances in Chemical Physics, 2002, , 89-139.	0.3	43
76	Characterization of nanofibers formed by self-assembly of Î²-peptide oligomers using small angle x-ray scattering. Journal of Chemical Physics, 2008, 129, 095103.	1.2	43
77	The effect of salt on the melting of ice: A molecular dynamics simulation study. Journal of Chemical Physics, 2008, 129, 124504.	1.2	43
78	Computer simulations and integral equation theory for the structure of salt-free rigid rod polyelectrolyte solutions: Explicit incorporation of counterions. Journal of Chemical Physics, 1999, 110, 11599-11607.	1.2	41
79	Forces between surfaces immersed in polyelectrolyte solutions. Journal of Chemical Physics, 1999, 111, 1797-1800.	1.2	40
80	Fracking: What Can Physical Chemistry Offer?. Journal of Physical Chemistry Letters, 2013, 4, 687-690.	2.1	40
81	Entropic Mechanism for the Lower Critical Solution Temperature of Poly(ethylene oxide) in a Room Temperature Ionic Liquid. ACS Macro Letters, 2015, 4, 799-803.	2.3	40
82	Dynamics of Chain Molecules in Disordered Materials. Physical Review Letters, 2006, 96, 107802.	2.9	38
83	Microfluidic Based Platform for Characterization of Protein Interactions in Hydrogel Nanoenvironments. Analytical Chemistry, 2007, 79, 5322-5327.	3.2	38
84	The effect of matrix structure on the diffusion of fluids in porous media. Journal of Chemical Physics, 2008, 128, 054702.	1.2	38
85	Driving Force for the Association of Hydrophobic Peptides: The Importance of Electrostatic Interactions in Coarse-Grained Water Models. Journal of Physical Chemistry Letters, 2011, 2, 1794-1798.	2.1	38
86	Local structure of fluids containing chainâ€like molecules: Polymer reference interaction site model with a Yukawa closure. Journal of Chemical Physics, 1990, 93, 5315-5321.	1.2	36
87	Structure of Polyelectrolyte Solutions at a Charged Surface. Journal of Physical Chemistry B, 2004, 108, 9126-9132.	1.2	36
88	Solvent effects in polyelectrolyte adsorption: Computer simulations with explicit and implicit solvent. Journal of Chemical Physics, 2010, 132, 074903.	1.2	36
89	Monte Carlo simulations and self-consistent integral equation theory for polyelectrolyte solutions. Journal of Chemical Physics, 1999, 110, 5437-5443.	1.2	35
90	Equations of state for star polymers. Journal of Chemical Physics, 1991, 94, 3943-3948.	1.2	34

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91	The effects of local stiffness disparity on the surface segregation from binary polymer blends. Journal of Chemical Physics, 1995, 103, 10332-10346.	1.2	34
92	Brownian dynamics simulations of polyelectrolyte solutions with divalent counterions. Journal of Chemical Physics, 2003, 118, 11315-11325.	1.2	34
93	Water Dynamics in Gyroid Phases of Self-Assembled Gemini Surfactants. Journal of the American Chemical Society, 2016, 138, 2472-2475.	6.6	34
94	Phase behavior of the Widomâ€“Rowlinson mixture. Journal of Chemical Physics, 1996, 104, 7665-7670.	1.2	33
95	Establishing Effective Simulation Protocols for Î²- and Î±/Î²-Mixed Peptides. I. QM and QM/MM Models. Journal of Chemical Theory and Computation, 2007, 3, 1538-1549.	2.3	33
96	Crowding Effects on Protein Association: Effect of Interactions between Crowding Agents. Journal of Physical Chemistry B, 2011, 115, 347-353.	1.2	33
97	Cavity hydration dynamics in cytochrome c oxidase and functional implications. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, E8830-E8836.	3.3	33
98	Structure and Dynamics of Conjugated Polymers in Liquid Crystalline Solvents. Annual Review of Physical Chemistry, 2007, 58, 565-584.	4.8	32
99	A Diffusive Anomaly of Water in Aqueous Sodium Chloride Solutions at Low Temperatures. Journal of Physical Chemistry B, 2008, 112, 1729-1735.	1.2	32
100	Sequence-Dependent Interaction of Î²-Peptides with Membranes. Journal of Physical Chemistry B, 2010, 114, 13585-13592.	1.2	31
101	Driving Force for the Association of Amphiphilic Molecules. Journal of Physical Chemistry Letters, 2011, 2, 2391-2395.	2.1	31
102	FRET by FET and Dynamics of Polymer Folding. Journal of Physical Chemistry B, 2001, 105, 2475-2478.	1.2	30
103	Nonexponentiality of time dependent survival probability and the fractional viscosity dependence of the rate in diffusion controlled reactions in a polymer chain. Journal of Chemical Physics, 2001, 114, 9170-9178.	1.2	30
104	Density functional theory for pair correlation functions in polymeric liquids. Journal of Chemical Physics, 2001, 114, 4323-4330.	1.2	30
105	Osmotic Pressure of Salt-Free Polyelectrolyte Solutions:Â A Monte Carlo Simulation Study. Macromolecules, 2005, 38, 607-616.	2.2	30
106	Retardation of Ice Crystallization by Short Peptides. Journal of Physical Chemistry A, 2009, 113, 4403-4407.	1.1	30
107	Liquid state theories for the structure of water. Journal of Chemical Physics, 2003, 119, 13012-13016.	1.2	29
108	Coarse-Grained Models for Aqueous Polyethylene Glycol Solutions. Journal of Physical Chemistry B, 2014, 118, 323-329.	1.2	29

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109	Influence of Charge Scaling on the Solvation Properties of Ionic Liquid Solutions. Journal of Physical Chemistry B, 2019, 123, 9222-9229.	1.2	29
110	Proper Thermal Equilibration of Simulations with Drude Polarizable Models: Temperature-Grouped Dual-NosÃ©â€“Hoover Thermostat. Journal of Physical Chemistry Letters, 2019, 10, 7523-7530.	2.1	29
111	Driving Force for the Complexation of Charged Polypeptides. Journal of Physical Chemistry B, 2020, 124, 1285-1292.	1.2	29
112	Fluctuation phenomena in structurally symmetric polymer blends. Journal of Chemical Physics, 1995, 102, 2187-2208.	1.2	28
113	Molecular simulation and continuum mechanics investigation of viscoelastic properties of fluids confined to molecularly thin films. Journal of Chemical Physics, 2001, 114, 7593-7601.	1.2	28
114	Monte Carlo simulations for the phase behavior of symmetric nonadditive hard sphere mixtures. Journal of Chemical Physics, 2003, 118, 7907-7911.	1.2	28
115	Behavior of starlike polymers between walls. Macromolecules, 1991, 24, 709-713.	2.2	27
116	Microscopic equations-of-state for hydrocarbon fluids: effect of attractions and comparison with polyethylene experiments. Macromolecules, 1993, 26, 2655-2662.	2.2	27
117	On equations of state for hard chain fluids. Molecular Physics, 1993, 80, 469-477.	0.8	27
118	Effect of chain stiffness on the conformational properties, pair correlations, and equation of state of polymer melts. Journal of Chemical Physics, 1994, 101, 9104-9112.	1.2	27
119	Establishing Effective Simulation Protocols for Î²- and Î±/Î²-Peptides. II. Molecular Mechanical (MM) Model for a Cyclic Î²-Residue. Journal of Physical Chemistry B, 2008, 112, 5439-5448.	1.2	27
120	Local structure of model polymeric fluids: Hardâ€sphere chains and the threeâ€dimensional fluctuating bond model. Journal of Chemical Physics, 1992, 97, 4468-4475.	1.2	26
121	Adsorption and Dynamics of a Single Polyelectrolyte Chain near a Planar Charged Surface:Â Molecular Dynamics Simulations with Explicit Solvent. Journal of Chemical Theory and Computation, 2006, 2, 630-636.	2.3	26
122	Gating Mechanisms of Mechanosensitive Channels of Large Conductance, II: Systematic Study of Conformational Transitions. Biophysical Journal, 2008, 95, 581-596.	0.2	26
123	Atomistic Simulations of Dilute Polyelectrolyte Solutions. Journal of Physical Chemistry B, 2012, 116, 4319-4327.	1.2	25
124	Free Energy Calculations for the Peripheral Binding of Proteins/Peptides to an Anionic Membrane. 1. Implicit Membrane Models. Journal of Chemical Theory and Computation, 2014, 10, 2845-2859.	2.3	25
125	Self-consistent integral equation theory for semiflexible chain polyelectrolyte solutions. Journal of Chemical Physics, 2000, 113, 8841-8847.	1.2	24
126	Molecular Dynamics Simulations of a Fluid near Its Critical Point. Physical Review Letters, 2004, 93, 015701.	2.9	24

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127	Conformational Properties of Sodium Polystyrenesulfonate in Water: Insights from a Coarse-Grained Model with Explicit Solvent. Journal of Physical Chemistry B, 2015, 119, 11010-11018.	1.2	24
128	Combining Diffusion NMR and Small-Angle Neutron Scattering Enables Precise Measurements of Polymer Chain Compression in a Crowded Environment. Physical Review Letters, 2017, 118, 097801.	2.9	24
129	Conformational properties of isolated polyelectrolytes in poor solvents. Journal of Chemical Physics, 1999, 110, 676-681.	1.2	23
130	Two- and three-body interactions among nanoparticles in a polymer melt. Journal of Chemical Physics, 2011, 134, 174901.	1.2	23
131	The effect of attractions on the structure of fused sphere chains confined between surfaces. Journal of Chemical Physics, 1999, 111, 1608-1614.	1.2	21
132	Structure of void space in polymer solutions. Physical Review E, 2010, 81, 031801.	0.8	21
133	Effect of Polydispersity on Diffusion in Random Obstacle Matrices. Physical Review Letters, 2012, 109, 155901.	2.9	21
134	Conformational and Dynamic Properties of Poly(ethylene oxide) in an Ionic Liquid: Development and Implementation of a First-Principles Force Field. Journal of Physical Chemistry B, 2016, 120, 231-243.	1.2	21
135	Monte Carlo simulations for the equation of state of athermal linear alkanes. Journal of Chemical Physics, 1995, 102, 6874-6880.	1.2	20
136	Self-consistent mode-coupling theory for the viscosity of rodlike polyelectrolyte solutions. Journal of Chemical Physics, 2004, 121, 8120.	1.2	20
137	Integral Equation Theory of Random Copolymer Melts. Macromolecules, 2005, 38, 2000-2008.	2.2	20
138	Swelling of polymers in porous media. Journal of Chemical Physics, 2009, 130, 124908.	1.2	20
139	Ionic Hydrogen Bonds and Lipid Packing Defects Determine the Binding Orientation and Insertion Depth of RecA on Multicomponent Lipid Bilayers. Journal of Physical Chemistry B, 2016, 120, 8424-8437.	1.2	20
140	Excited state kinetics of neutral transition metal atoms by stimulated emission pumping: V*(3d44s,a4D)+hydrocarbons. Journal of Chemical Physics, 1997, 106, 5509-5525.	1.2	19
141	Generation and sensing of membrane curvature: Where materials science and biophysics meet. Current Opinion in Solid State and Materials Science, 2013, 17, 164-174.	5.6	19
142	Ion binding in tobacco mosaic virus solutions. Journal of Chemical Physics, 1998, 109, 5162-5163.	1.2	18
143	Monte Carlo simulations and integral equation theory for the structure of telechelic polymers. Journal of Chemical Physics, 2003, 119, 6916-6924.	1.2	18
144	Monte Carlo simulation and self-consistent integral equation theory for polymers in quenched random media. Journal of Chemical Physics, 2005, 123, 074909.	1.2	18

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145	Local structure of tangent-hard-sphere diatomic fluids. Molecular Physics, 1993, 80, 695-700.	0.8	17
146	Orthogonal Orientations for Solvation of Polymer Molecules in Smectic Solvents. Physical Review Letters, 2006, 96, 017801.	2.9	17
147	Single Molecule Spectroscopy of Conjugated Polymer Chains in an Electric Field-Aligned Liquid Crystal. Journal of Physical Chemistry B, 2008, 112, 448-453.	1.2	17
148	Establishing effective simulation protocols for Î²â€•and Î±/Î²â€•peptides. III. Molecular mechanical model for acyclic Î²â€•amino acids. Journal of Computational Chemistry, 2010, 31, 2063-2077.	1.5	17
149	Swing motion as a diffusion mechanism of lipid bilayers in a gel phase. Physical Review E, 2016, 93, 012409.	0.8	17
150	Grotthuss Transport of Iodide in EMIM/I₃ Ionic Crystal. Journal of Physical Chemistry B, 2018, 122, 250-257.	1.2	17
151	Molecular modeling of polymers at surfaces. Chemical Engineering Journal, 1999, 74, 109-115.	6.6	16
152	Integral equation theory of random copolymer melts: Self-consistent treatment of intramolecular and intermolecular correlations. Journal of Chemical Physics, 2005, 122, 234904.	1.2	16
153	Electrostatic Interactions Govern â€œOdd/Evenâ€•Effects in Water-Induced Gemini Surfactant Self-Assembly. Journal of Physical Chemistry B, 2017, 121, 565-576.	1.2	16
154	Conformational and Dynamic Properties of Poly(ethylene oxide) in BMIM⁺BF₄^{â€“}: A Microsecond Computer Simulation Study Using ab Initio Force Fields. Macromolecules, 2018, 51, 5336-5345.	2.2	16
155	Liquidâ€“Liquid Phase Separation As the Second Step of Complex Coacervation. Journal of Physical Chemistry B, 2021, 125, 3023-3031.	1.2	16
156	Entanglement effects in mode coupling theories of polymers. Journal of Chemical Physics, 2002, 117, 10448-10451.	1.2	15
157	Phase behavior of semiflexible polymer chains. Journal of Chemical Physics, 2008, 128, 124908.	1.2	15
158	A Computational Framework for Mechanical Response of Macromolecules: Application to the Salt Concentration Dependence of DNA Bendability. Biophysical Journal, 2009, 96, 3543-3554.	0.2	15
159	The structure of amorphous polymers near surfaces: athermal systems. Computational and Theoretical Polymer Science, 1998, 8, 159-168.	1.1	14
160	Mechanosensitive Channels: Insights from Continuum-Based Simulations. Cell Biochemistry and Biophysics, 2008, 52, 1-18.	0.9	14
161	Comment on â€œIsolating the non-polar contributions to the intermolecular potential for water-alkane interactionsâ€•[J. Chem. Phys. 141, 064905 (2014)]. Journal of Chemical Physics, 2016, 144, 137101.	1.2	14
162	An Integral Equation Theory for the Widomâ€“Rowlinson Mixture. Journal of Statistical Physics, 2000, 100, 39-47.	0.5	13

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163	Effect of secondary structure on the self-assembly of amphiphilic molecules: A multiscale simulation study. Journal of Chemical Physics, 2012, 136, 084902.	1.2	13
164	Deep Eutectic Solvents: Molecular Simulations with a First-Principles Polarizable Force Field. Journal of Physical Chemistry B, 2021, 125, 7177-7186.	1.2	13
165	Structure and dynamics of short chain molecules in disordered porous materials: A molecular dynamics simulation study. Journal of Chemical Physics, 2007, 126, 174906.	1.2	12
166	Dynamics of Water in Gemini Surfactant-Based Lyotropic Liquid Crystals. Journal of Physical Chemistry B, 2016, 120, 10860-10868.	1.2	12
167	A Transferable Polarizable Force Field for Urea Crystals and Aqueous Solutions. Journal of Physical Chemistry B, 2020, 124, 7475-7483.	1.2	12
168	A Monte Carlo Study of the Self-Assembly of Bacteriorhodopsin. Biophysical Journal, 2002, 83, 1902-1916.	0.2	11
169	Molecular-dynamics simulations for nonclassical kinetics of diffusion-controlled bimolecular reactions. Journal of Chemical Physics, 2005, 123, 114503.	1.2	11
170	Integral Equation Theory for Symmetric Nonadditive Hard Sphere Mixturesâ€. Journal of Physical Chemistry B, 2005, 109, 6764-6768.	1.2	11
171	Numerical Simulation of Nanoindentation and Patch Clamp Experiments on Mechanosensitive Channels of Large Conductance in Escherichia coli. Experimental Mechanics, 2009, 49, 35-46.	1.1	11
172	Sequence dependent self-assembly of Î²-peptides: Insights from a coarse-grained model. Journal of Chemical Physics, 2010, 132, 065103.	1.2	11
173	Self-Assembly of Î²-Peptides: Insight from the Pair and Many-Body Free Energy of Association. Journal of Physical Chemistry C, 2010, 114, 13551-13556.	1.5	11
174	Conformational Properties of a Polymer in an Ionic Liquid: Computer Simulations and Integral Equation Theory of a Coarse-Grained Model. Journal of Physical Chemistry B, 2015, 119, 9091-9097.	1.2	11
175	Local structure and orientational correlations in fluids composed of linear triatomic molecules. Molecular Physics, 1994, 82, 937-955.	0.8	10
176	Integral equation theory for the surface segregation from blends of linear and star polymers. Computational and Theoretical Polymer Science, 2000, 10, 115-123.	1.1	10
177	Integral equations for polymers in quenched random media. Journal of Chemical Physics, 2002, 116, 5910-5911.	1.2	10
178	Computer Simulations of Protein Diffusion in Compartmentalized Cell Membranes. Biophysical Journal, 2009, 97, 472-479.	0.2	10
179	The Driving Force for the Association of Gemini Surfactants. Journal of Physical Chemistry B, 2018, 122, 3259-3265.	1.2	10
180	Monte Carlo simulation of semiflexible hard triatomic fluids. Molecular Physics, 1994, 82, 957-972.	0.8	9

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181	The effect of acid-base equilibria on the fractional charge and conformational properties of polyelectrolyte solutions. Journal of Chemical Physics, 2001, 114, 2830-2838.	1.2	9
182	Integral equation theory for the structure of DNA solutions. Journal of Chemical Physics, 2002, 116, 5308.	1.2	9
183	Density functional theory and Monte Carlo simulations for hard sphere fluids in square and rectangular channels. Journal of Chemical Physics, 2002, 116, 5795-5800.	1.2	9
184	Dynamics of fluids near the consolute critical point: A molecular-dynamics study of the Widomâ€“Rowlinson mixture. Journal of Chemical Physics, 2005, 122, 244506.	1.2	9
185	Sequence-Directed Organization of Î²-Peptides in Self-Assembled Monolayers. Journal of Physical Chemistry B, 2009, 113, 9379-9385.	1.2	9
186	Thermodynamics and local structure of vinyl polymer melts. Journal of Chemical Physics, 1995, 103, 2229-2236.	1.2	8
187	Structural and thermodynamic properties of a freely-jointed Yukawa hard-sphere chain fluid. Journal of Molecular Liquids, 2001, 92, 85-96.	2.3	8
188	Dynamics of Probes in Model Glassy Matrices. Physical Review Letters, 2006, 97, 145503.	2.9	8
189	Anisotropic Diffusion of Elongated and Aligned Polymer Chains In a Nematic Solventâ€. Journal of Physical Chemistry B, 2006, 110, 19799-19803.	1.2	8
190	The influence of the polymer chain stiffness on tracer diffusion in polymeric matrices. Journal of Polymer Science, Part B: Polymer Physics, 2011, 49, 818-825.	2.4	8
191	Dynamics of two-dimensional and quasi-two-dimensional polymers. Journal of Chemical Physics, 2013, 138, 234904.	1.2	8
192	Structure of room temperature ionic liquids. Journal of Physics Condensed Matter, 2016, 28, 414020.	0.7	8
193	Why Lithium Ions Stick to Some Anions and Not Others. Journal of Physical Chemistry B, 2021, 125, 4447-4455.	1.2	8
194	The behavior of fluids near solutes: A density functional theory and computer simulation study. Journal of Chemical Physics, 2004, 121, 4203-4209.	1.2	7
195	Jagannathan and Yethiraj Reply:. Physical Review Letters, 2005, 94, .	2.9	7
196	Integral equation theory for two-dimensional polymer melts. Journal of Chemical Physics, 2005, 122, 094910.	1.2	7
197	Osmotic Pressure of Polyelectrolyte Solutions with Salt: Grand Canonical Monte Carlo Simulation Studies. Macromolecules, 2015, 48, 7370-7377.	2.2	7
198	Dynamics of water confined in lyotropic liquid crystals: Molecular dynamics simulations of the dynamic structure factor. Journal of Chemical Physics, 2016, 144, 084504.	1.2	7

#	Article	IF	Citations
199	The effect of crowder charge in a model polymerâ€“colloid system for macromolecular crowding: Polymer structure and dynamics. Journal of Chemical Physics, 2017, 147, 114902.	1.2	7
200	A simulation method for the phase diagram of complex fluid mixtures. Journal of Chemical Physics, 2018, 148, 244903.	1.2	7
201	The behavior of salt-free polyelectrolyte solutions at charged surfaces. Progress in Organic Coatings, 2003, 47, 331-336.	1.9	6
202	Integral equation theory of randomly coupled multiblock copolymer melts: Effect of block size on the phase behavior. Journal of Chemical Physics, 2005, 123, 214901.	1.2	6
203	Importance of hydrophobic traps for proton diffusion in lyotropic liquid crystals. Journal of Chemical Physics, 2016, 144, 094705.	1.2	6
204	Osmotic pressure of isotropic solutions of rodlike polymers. Journal of Chemical Physics, 2003, 118, 3904-3905.	1.2	5
205	Permeation of a hard sphere fluid into a quenched matrix. Journal of Chemical Physics, 2007, 126, 034704.	1.2	5
206	Phase Behavior of Poly(ethylene oxide) in Room Temperature Ionic Liquids: A Molecular Simulation and Deep Neural Network Study. Journal of Physical Chemistry B, 2020, 124, 9230-9238.	1.2	5
207	Equations of state for square well chain fluids using the generalized flory approach. Fluid Phase Equilibria, 1993, 83, 313-322.	1.4	4
208	Sequence-Dependent pK_aShift Induced by Molecular Self-Assembly: Insights from Computer Simulation. Journal of Physical Chemistry B, 2012, 116, 491-495.	1.2	4
209	Counterion-Regulated Dynamics of Water Confined in Lyotropic Liquid Crystalline Morphologies. Journal of Physical Chemistry B, 2018, 122, 2408-2413.	1.2	4
210	Can Polymer Chains Cross Each Other and Still Be Entangled?. Macromolecules, 2019, 52, 2000-2006.	2.2	4
211	Nematic ordering of hard rods under strong confinement in a dense array of nanoposts. Physical Review E, 2020, 101, 032705.	0.8	4
212	Nonlinear feedback control of a class of nonlinear systems. Electronics Letters, 1987, 23, 18-20.	0.5	3
213	Weighted Density Approximation for Polymer Melts. ACS Symposium Series, 1996, , 274-285.	0.5	3
214	Coupling between the Dynamics of Water and Surfactants in Lyotropic Liquid Crystals. Journal of Physical Chemistry B, 2017, 121, 5048-5057.	1.2	3
215	More than Virtual Reality: Important New Physical Insights in Simulations of Biomolecules and Synthetic Polymers. Journal of Physical Chemistry B, 2017, 121, 6294-6294.	1.2	3
216	Ion-Specific Confined Water Dynamics in Convex Nanopores of Gemini Surfactant Lyotropic Liquid Crystals. Journal of Physical Chemistry B, 2018, 122, 10031-10043.	1.2	3

#	Article	IF	Citations
217	Non-universality of the dynamic exponent in two-dimensional random media. Scientific Reports, 2019, 9, 251.	1.6	3
218	Solvation Induced Ring Puckering Effect in Fluorinated Prolines and Its Inclusion in Classical Force Fields. Journal of Physical Chemistry B, 2020, 124, 5899-5906.	1.2	3
219	Proton Diffusion through Bilayer Pores. Journal of Physical Chemistry B, 2017, 121, 9247-9259.	1.2	2
220	The JPC Periodic Table. Journal of Physical Chemistry A, 2019, 123, 5837-5848.	1.1	2
221	The JPC Periodic Table. Journal of Physical Chemistry Letters, 2019, 10, 4051-4062.	2.1	2
222	Phase behavior of continuous-space systems: A supervised machine learning approach. Journal of Chemical Physics, 2020, 153, 064904.	1.2	2
223	IDENTIFICATION AND FEEDBACK CONTROL OF NONLINEAR SYSTEMS. Chemical Engineering Communications, 1988, 71, 1-22.	1.5	1
224	Response to â€œComment on â€˜Molecular simulation and continuum mechanics study of simple fluids in nonisothermal planar Couette flowsâ€™â€Šâ€•[J. Chem. Phys. 111, 10730 (1999)]. Journal of Chemical Physics, 1999, 111, 10732-10733.	1.2	1
225	The JPC Periodic Table. Journal of Physical Chemistry B, 2019, 123, 5973-5984.	1.2	1
226	The JPC Periodic Table. Journal of Physical Chemistry C, 2019, 123, 17063-17074.	1.5	1
227	Palit etÂal. Reply:. Physical Review Letters, 2019, 123, 239802.	2.9	1
228	Effect of diffusion constant on the morphology of dendrite growth in lithium metal batteries. Journal of Chemical Physics, 2021, 154, 234705.	1.2	1
229	Chemically realistic coarse-grained models for polyelectrolyte solutions. Journal of Chemical Physics, 2022, 156, 094902.	1.2	1
230	The effect of explicit counterion binding on the transference number of polyelectrolyte solutions. Journal of Chemical Physics, 2022, 156, 104901.	1.2	1
231	A Tribute to Carol K. Hall. Journal of Physical Chemistry B, 2021, 125, 11341-11342.	1.2	0
232	Static Structure and Chain Conformations in Polyelectrolyte Solutions. , 1999, , 393-405.		0
233	Theory and Simulations of Polymers at Surfaces. , 1999, , 379-392.		0
234	Fast estimation of ion-pairing for screening electrolytes: A cluster can approximate a bulk liquid. Journal of Chemical Physics, 2022, 156, 054801.	1.2	0