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	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
2	Chemically realistic coarse-grained models for polyelectrolyte solutions. Journal of Chemical Physics, 2022, 156, 094902.	1.2	1
3	The effect of explicit counterion binding on the transference number of polyelectrolyte solutions. Journal of Chemical Physics, 2022, 156, 104901.	1.2	1
4	Liquidâ€“Liquid Phase Separation As the Second Step of Complex Coacervation. Journal of Physical Chemistry B, 2021, 125, 3023-3031.	1.2	16
5	Why Lithium Ions Stick to Some Anions and Not Others. Journal of Physical Chemistry B, 2021, 125, 4447-4455.	1.2	8
6	Deep Eutectic Solvents: Molecular Simulations with a First-Principles Polarizable Force Field. Journal of Physical Chemistry B, 2021, 125, 7177-7186.	1.2	13
7	Effect of diffusion constant on the morphology of dendrite growth in lithium metal batteries. Journal of Chemical Physics, 2021, 154, 234705.	1.2	1
8	A Tribute to Carol K. Hall. Journal of Physical Chemistry B, 2021, 125, 11341-11342.	1.2	0
9	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
10	A Transferable Polarizable Force Field for Urea Crystals and Aqueous Solutions. Journal of Physical Chemistry B, 2020, 124, 7475-7483.	1.2	12
11	Phase behavior of continuous-space systems: A supervised machine learning approach. Journal of Chemical Physics, 2020, 153, 064904.	1.2	2
12	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
13	Nematic ordering of hard rods under strong confinement in a dense array of nanoposts. Physical Review E, 2020, 101, 032705.	0.8	4
14	Driving Force for the Complexation of Charged Polypeptides. Journal of Physical Chemistry B, 2020, 124, 1285-1292.	1.2	29
15	The JPC Periodic Table. Journal of Physical Chemistry A, 2019, 123, 5837-5848.	1.1	2
16	The JPC Periodic Table. Journal of Physical Chemistry B, 2019, 123, 5973-5984.	1.2	1
17	The JPC Periodic Table. Journal of Physical Chemistry C, 2019, 123, 17063-17074.	1.5	1
18	The JPC Periodic Table. Journal of Physical Chemistry Letters, 2019, 10, 4051-4062.	2.1	2

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19	Influence of Charge Scaling on the Solvation Properties of Ionic Liquid Solutions. Journal of Physical Chemistry B, 2019, 123, 9222-9229.	1.2	29
20	Non-universality of the dynamic exponent in two-dimensional random media. Scientific Reports, 2019, 9, 251.	1.6	3
21	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
22	Can Polymer Chains Cross Each Other and Still Be Entangled?. Macromolecules, 2019, 52, 2000-2006.	2.2	4
23	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
24	Palit etÂal. Reply:. Physical Review Letters, 2019, 123, 239802.	2.9	1
25	Counterion-Regulated Dynamics of Water Confined in Lyotropic Liquid Crystalline Morphologies. Journal of Physical Chemistry B, 2018, 122, 2408-2413.	1.2	4
26	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
27	Grotthuss Transport of Iodide in EMIM/I₃ Ionic Crystal. Journal of Physical Chemistry B, 2018, 122, 250-257.	1.2	17
28	The Driving Force for the Association of Gemini Surfactants. Journal of Physical Chemistry B, 2018, 122, 3259-3265.	1.2	10
29	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
30	A simulation method for the phase diagram of complex fluid mixtures. Journal of Chemical Physics, 2018, 148, 244903.	1.2	7
31	Influence of Electronic Polarization on the Structure of Ionic Liquids. Journal of Physical Chemistry Letters, 2018, 9, 4765-4770.	2.1	54
32	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
33	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
34	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
35	Coupling between the Dynamics of Water and Surfactants in Lyotropic Liquid Crystals. Journal of Physical Chemistry B, 2017, 121, 5048-5057.	1.2	3
36	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

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37	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
38	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
39	Proton Diffusion through Bilayer Pores. Journal of Physical Chemistry B, 2017, 121, 9247-9259.	1.2	2
40	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
41	Importance of hydrophobic traps for proton diffusion in lyotropic liquid crystals. Journal of Chemical Physics, 2016, 144, 094705.	1.2	6
42	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
43	Ab Initio Force Fields for Imidazolium-Based Ionic Liquids. Journal of Physical Chemistry B, 2016, 120, 7024-7036.	1.2	76
44	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
45	Dynamics of Water in Gemini Surfactant-Based Lyotropic Liquid Crystals. Journal of Physical Chemistry B, 2016, 120, 10860-10868.	1.2	12
46	Structure of room temperature ionic liquids. Journal of Physics Condensed Matter, 2016, 28, 414020.	0.7	8
47	Swing motion as a diffusion mechanism of lipid bilayers in a gel phase. Physical Review E, 2016, 93, 012409.	0.8	17
48	Different states of synaptotagmin regulate evoked versus spontaneous release. Nature Communications, 2016, 7, 10971.	5.8	53
49	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
50	Water Dynamics in Gyroid Phases of Self-Assembled Gemini Surfactants. Journal of the American Chemical Society, 2016, 138, 2472-2475.	6.6	34
51	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
52	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
53	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
54	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

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55	Osmotic Pressure of Polyelectrolyte Solutions with Salt: Grand Canonical Monte Carlo Simulation Studies. Macromolecules, 2015, 48, 7370-7377.	2.2	7
56	Anionic Phospholipids Stabilize RecA Filament Bundles in Escherichia coli. Molecular Cell, 2015, 60, 374-384.	4.5	45
57	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
58	Atomistic Simulations of Poly(ethylene oxide) in Water and an Ionic Liquid at Room Temperature. Macromolecules, 2014, 47, 438-446.	2.2	50
59	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
60	First-Principles, Physically Motivated Force Field for the Ionic Liquid [BMIM][BF₄]. Journal of Physical Chemistry Letters, 2014, 5, 2670-2674.	2.1	57
61	Dynamics in Crowded Environments: Is Non-Gaussian Brownian Diffusion Normal?. Journal of Physical Chemistry B, 2014, 118, 8128-8134.	1.2	66
62	Coarse-Grained Models for Aqueous Polyethylene Glycol Solutions. Journal of Physical Chemistry B, 2014, 118, 323-329.	1.2	29
63	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
64	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
65	Self-Assembly of Gemini Surfactants: A Computer Simulation Study. Journal of Physical Chemistry B, 2013, 117, 4254-4262.	1.2	44
66	Fracking: What Can Physical Chemistry Offer?. Journal of Physical Chemistry Letters, 2013, 4, 687-690.	2.1	40
67	Dynamics of two-dimensional and quasi-two-dimensional polymers. Journal of Chemical Physics, 2013, 138, 234904.	1.2	8
68	Effect of Polydispersity on Diffusion in Random Obstacle Matrices. Physical Review Letters, 2012, 109, 155901.	2.9	21
69	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
70	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
71	Self-Diffusion and Viscosity in Electrolyte Solutions. Journal of Physical Chemistry B, 2012, 116, 12007-12013.	1.2	156
72	Atomistic Simulations of Dilute Polyelectrolyte Solutions. Journal of Physical Chemistry B, 2012, 116, 4319-4327.	1.2	25

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73	Driving Force for the Association of Amphiphilic Molecules. Journal of Physical Chemistry Letters, 2011, 2, 2391-2395.	2.1	31
74	Entropy-Based Mechanism of Ribosome-Nucleoid Segregation in E.Âcoli Cells. Biophysical Journal, 2011, 100, 2605-2613.	0.2	96
75	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
76	A New Coarse-Grained Force Field for Membraneâ€“Peptide Simulations. Journal of Chemical Theory and Computation, 2011, 7, 3793-3802.	2.3	75
77	Two- and three-body interactions among nanoparticles in a polymer melt. Journal of Chemical Physics, 2011, 134, 174901.	1.2	23
78	Crowding Effects on Protein Association: Effect of Interactions between Crowding Agents. Journal of Physical Chemistry B, 2011, 115, 347-353.	1.2	33
79	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
80	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
81	Solvent effects in polyelectrolyte adsorption: Computer simulations with explicit and implicit solvent. Journal of Chemical Physics, 2010, 132, 074903.	1.2	36
82	Sequence dependent self-assembly of Î²-peptides: Insights from a coarse-grained model. Journal of Chemical Physics, 2010, 132, 065103.	1.2	11
83	Crowding Effects on Association Reactions at Membranes. Biophysical Journal, 2010, 98, 951-958.	0.2	45
84	A New Coarse-Grained Model for Water: The Importance of Electrostatic Interactions. Journal of Physical Chemistry B, 2010, 114, 10524-10529.	1.2	170
85	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
86	Structure of void space in polymer solutions. Physical Review E, 2010, 81, 031801.	0.8	21
87	Sequence-Dependent Interaction of Î²-Peptides with Membranes. Journal of Physical Chemistry B, 2010, 114, 13585-13592.	1.2	31
88	Swelling of polymers in porous media. Journal of Chemical Physics, 2009, 130, 124908.	1.2	20
89	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
90	Liquid State Theory of Polyelectrolyte Solutions. Journal of Physical Chemistry B, 2009, 113, 1539-1551.	1.2	66

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91	Effect of Macromolecular Crowding on Reaction Rates: A Computational and Theoretical Study. Biophysical Journal, 2009, 96, 1333-1340.	0.2	114
92	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
93	Computer Simulations of Protein Diffusion in Compartmentalized Cell Membranes. Biophysical Journal, 2009, 97, 472-479.	0.2	10
94	Retardation of Ice Crystallization by Short Peptides. Journal of Physical Chemistry A, 2009, 113, 4403-4407.	1.1	30
95	Sequence-Directed Organization of Î²-Peptides in Self-Assembled Monolayers. Journal of Physical Chemistry B, 2009, 113, 9379-9385.	1.2	9
96	Mechanosensitive Channels: Insights from Continuum-Based Simulations. Cell Biochemistry and Biophysics, 2008, 52, 1-18.	0.9	14
97	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
98	The effect of matrix structure on the diffusion of fluids in porous media. Journal of Chemical Physics, 2008, 128, 054702.	1.2	38
99	Gating Mechanisms of Mechanosensitive Channels of Large Conductance, I: A Continuum Mechanics-Based Hierarchical Framework. Biophysical Journal, 2008, 95, 563-580.	0.2	44
100	Gating Mechanisms of Mechanosensitive Channels of Large Conductance, II: Systematic Study of Conformational Transitions. Biophysical Journal, 2008, 95, 581-596.	0.2	26
101	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
102	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
103	Phase behavior of semiflexible polymer chains. Journal of Chemical Physics, 2008, 128, 124908.	1.2	15
104	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
105	The effect of salt on the melting of ice: A molecular dynamics simulation study. Journal of Chemical Physics, 2008, 129, 124504.	1.2	43
106	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
107	Structure and Dynamics of Conjugated Polymers in Liquid Crystalline Solvents. Annual Review of Physical Chemistry, 2007, 58, 565-584.	4.8	32
108	Permeation of a hard sphere fluid into a quenched matrix. Journal of Chemical Physics, 2007, 126, 034704.	1.2	5

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109	Microfluidic Based Platform for Characterization of Protein Interactions in Hydrogel Nanoenvironments. Analytical Chemistry, 2007, 79, 5322-5327.	3.2	38
110	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
111	Why Are Lipid Rafts Not Observed In Vivo?. Biophysical Journal, 2007, 93, 3113-3119.	0.2	100
112	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
113	Dynamics of Chain Molecules in Disordered Materials. Physical Review Letters, 2006, 96, 107802.	2.9	38
114	Dynamics of Probes in Model Glassy Matrices. Physical Review Letters, 2006, 97, 145503.	2.9	8
115	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
116	Implicit and Explicit Solvent Models for the Simulation of Dilute Polymer Solutions. Macromolecules, 2006, 39, 8536-8542.	2.2	69
117	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
118	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
119	Anisotropic Diffusion of Elongated and Aligned Polymer Chains In a Nematic Solventâ€. Journal of Physical Chemistry B, 2006, 110, 19799-19803.	1.2	8
120	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
121	A Monte Carlo simulation study of branched polymers. Journal of Chemical Physics, 2006, 125, 204901.	1.2	61
122	Orthogonal Orientations for Solvation of Polymer Molecules in Smectic Solvents. Physical Review Letters, 2006, 96, 017801.	2.9	17
123	Lateral Diffusion and Percolation in Membranes. Physical Review Letters, 2006, 96, 228103.	2.9	52
124	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
125	Molecular-dynamics simulations for nonclassical kinetics of diffusion-controlled bimolecular reactions. Journal of Chemical Physics, 2005, 123, 114503.	1.2	11
126	Jagannathan and Yethiraj Reply:. Physical Review Letters, 2005, 94, .	2.9	7

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127	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
128	Integral equation theory for two-dimensional polymer melts. Journal of Chemical Physics, 2005, 122, 094910.	1.2	7
129	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
130	Osmotic Pressure of Salt-Free Polyelectrolyte Solutions:Â A Monte Carlo Simulation Study. Macromolecules, 2005, 38, 607-616.	2.2	30
131	Integral Equation Theory of Random Copolymer Melts. Macromolecules, 2005, 38, 2000-2008.	2.2	20
132	Integral Equation Theory for Symmetric Nonadditive Hard Sphere Mixturesâ€. Journal of Physical Chemistry B, 2005, 109, 6764-6768.	1.2	11
133	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
134	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
135	Diffusion of hard sphere fluids in disordered media: A molecular dynamics simulation study. Physical Review E, 2004, 69, 051101.	0.8	44
136	Self-consistent mode-coupling theory for the viscosity of rodlike polyelectrolyte solutions. Journal of Chemical Physics, 2004, 121, 8120.	1.2	20
137	Structure of Polyelectrolyte Solutions at a Charged Surface. Journal of Physical Chemistry B, 2004, 108, 9126-9132.	1.2	36
138	Molecular Dynamics Simulations of a Fluid near Its Critical Point. Physical Review Letters, 2004, 93, 015701.	2.9	24
139	The behavior of salt-free polyelectrolyte solutions at charged surfaces. Progress in Organic Coatings, 2003, 47, 331-336.	1.9	6
140	Liquid state theories for the structure of water. Journal of Chemical Physics, 2003, 119, 13012-13016.	1.2	29
141	Computer Simulation Study of Two-Dimensional Polymer Solutions. Macromolecules, 2003, 36, 5854-5862.	2.2	63
142	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
143	Monte Carlo simulations for the phase behavior of symmetric nonadditive hard sphere mixtures. Journal of Chemical Physics, 2003, 118, 7907-7911.	1.2	28
144	Strongly charged flexible polyelectrolytes in poor solvents: Molecular dynamics simulations with explicit solvent. Journal of Chemical Physics, 2003, 118, 6634-6647.	1.2	64

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145	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
146	Osmotic pressure of isotropic solutions of rodlike polymers. Journal of Chemical Physics, 2003, 118, 3904-3905.	1.2	5
147	Monte Carlo simulations and integral equation theory for the structure of telechelic polymers. Journal of Chemical Physics, 2003, 119, 6916-6924.	1.2	18
148	Brownian dynamics simulations of polyelectrolyte solutions with divalent counterions. Journal of Chemical Physics, 2003, 118, 11315-11325.	1.2	34
149	Integral equations for polymers in quenched random media. Journal of Chemical Physics, 2002, 116, 5910-5911.	1.2	10
150	Polymer Melts at Solid Surfaces. Advances in Chemical Physics, 2002, , 89-139.	0.3	43
151	Entanglement effects in mode coupling theories of polymers. Journal of Chemical Physics, 2002, 117, 10448-10451.	1.2	15
152	Integral equation theory for the structure of DNA solutions. Journal of Chemical Physics, 2002, 116, 5308.	1.2	9
153	Brownian dynamics simulations of salt-free polyelectrolyte solutions. Journal of Chemical Physics, 2002, 116, 5284.	1.2	44
154	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
155	A Monte Carlo Study of the Self-Assembly of Bacteriorhodopsin. Biophysical Journal, 2002, 83, 1902-1916.	0.2	11
156	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
157	FRET by FET and Dynamics of Polymer Folding. Journal of Physical Chemistry B, 2001, 105, 2475-2478.	1.2	30
158	Structural and thermodynamic properties of a freely-jointed Yukawa hard-sphere chain fluid. Journal of Molecular Liquids, 2001, 92, 85-96.	2.3	8
159	Solvent effects on the collapse dynamics of polymers. Journal of Chemical Physics, 2001, 114, 7688-7699.	1.2	99
160	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
161	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
162	Density functional theory for pair correlation functions in polymeric liquids. Journal of Chemical Physics, 2001, 114, 4323-4330.	1.2	30

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163	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
164	Local density enhancement in dilute supercritical solutions. Chemical Physics Letters, 2000, 317, 558-566.	1.2	53
165	An Integral Equation Theory for the Widomâ€“Rowlinson Mixture. Journal of Statistical Physics, 2000, 100, 39-47.	0.5	13
166	Generalized van der Waals density functional theory for nonuniform polymers. Journal of Chemical Physics, 2000, 112, 1579-1584.	1.2	48
167	Density Functional Theory for the Nonspecific Binding of Salt to Polyelectrolytes: Thermodynamic Properties. Biophysical Journal, 2000, 78, 699-706.	0.2	45
168	Self-consistent integral equation theory for semiflexible chain polyelectrolyte solutions. Journal of Chemical Physics, 2000, 113, 8841-8847.	1.2	24
169	Monte Carlo simulations and self-consistent integral equation theory for polyelectrolyte solutions. Journal of Chemical Physics, 1999, 110, 5437-5443.	1.2	35
170	Conformational properties of isolated polyelectrolytes in poor solvents. Journal of Chemical Physics, 1999, 110, 676-681.	1.2	23
171	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
172	Forces between surfaces immersed in polyelectrolyte solutions. Journal of Chemical Physics, 1999, 111, 1797-1800.	1.2	40
173	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
174	Molecular modeling of polymers at surfaces. Chemical Engineering Journal, 1999, 74, 109-115.	6.6	16
175	Density Functional Theory for the Distribution of Small Ions around Polyions. Journal of Physical Chemistry B, 1999, 103, 6080-6087.	1.2	77
176	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
177	Static Structure and Chain Conformations in Polyelectrolyte Solutions. , 1999, , 393-405.		0
178	Theory and Simulations of Polymers at Surfaces. , 1999, , 379-392.		0
179	The structure of amorphous polymers near surfaces: athermal systems. Computational and Theoretical Polymer Science, 1998, 8, 159-168.	1.1	14
180	Theory for chain conformations and static structure of dilute and semidilute polyelectrolyte solutions. Journal of Chemical Physics, 1998, 108, 1184-1192.	1.2	61

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181	Density functional theory of polymers: A Curtin-Ashcroft type weighted density approximation. Journal of Chemical Physics, 1998, 109, 3269-3275.	1.2	90
182	Phase behavior of semiflexible tangent hard sphere chains. Journal of Chemical Physics, 1998, 108, 1636-1644.	1.2	90
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