Arun Yethiraj

List of Publications by Year in Descending Order

233 papers	7,240 citations	51 h-index	68 g-index
238 ext. papers	7,695 ext. citations	4.2 avg, IF	6.33 L-index

#	Paper	IF	Citations
233	Fast estimation of ion-pairing for screening electrolytes: A cluster can approximate a bulk liquid.. *Journal of Chemical Physics*, **2022**, 156, 054801	3.9	
232	Chemically realistic coarse-grained models for polyelectrolyte solutions.. *Journal of Chemical Physics*, **2022**, 156, 094902	3.9	
231	The effect of explicit counterion binding on the transference number of polyelectrolyte solutions.. *Journal of Chemical Physics*, **2022**, 156, 104901	3.9	0
230	A Tribute to Carol K. Hall. *Journal of Physical Chemistry B*, **2021**, 125, 11341-11342	3.4	
229	Liquid-Liquid Phase Separation As the Second Step of Complex Coacervation. *Journal of Physical Chemistry B*, **2021**, 125, 3023-3031	3.4	3
228	Why Lithium Ions Stick to Some Anions and Not Others. *Journal of Physical Chemistry B*, **2021**, 125, 4447-4455	3.4	5
227	Deep Eutectic Solvents: Molecular Simulations with a First-Principles Polarizable Force Field. *Journal of Physical Chemistry B*, **2021**, 125, 7177-7186	3.4	4
226	Effect of diffusion constant on the morphology of dendrite growth in lithium metal batteries. *Journal of Chemical Physics*, **2021**, 154, 234705	3.9	0
225	Solvation Induced Ring Puckering Effect in Fluorinated Prolines and Its Inclusion in Classical Force Fields. *Journal of Physical Chemistry B*, **2020**, 124, 5899-5906	3.4	1
224	Nematic ordering of hard rods under strong confinement in a dense array of nanoposts. *Physical Review E*, **2020**, 101, 032705	2.4	3
223	Driving Force for the Complexation of Charged Polypeptides. *Journal of Physical Chemistry B*, **2020**, 124, 1285-1292	3.4	10
222	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	3.4	3
221	A Transferable Polarizable Force Field for Urea Crystals and Aqueous Solutions. *Journal of Physical Chemistry B*, **2020**, 124, 7475-7483	3.4	6
220	Phase behavior of continuous-space systems: A supervised machine learning approach.. *Journal of Chemical Physics*, **2020**, 153, 064904	3.9	1
219	Non-universality of the dynamic exponent in two-dimensional random media. *Scientific Reports*, **2019**, 9, 251	4.9	2
218	Understanding the Properties of Ionic Liquids: Electrostatics, Structure Factors, and Their Sum Rules. *Journal of Physical Chemistry B*, **2019**, 123, 3499-3512	3.4	27
217	Can Polymer Chains Cross Each Other and Still Be Entangled?. *Macromolecules*, **2019**, 52, 2000-2006	5.5	2

216	The Periodic Table. *Journal of Physical Chemistry A*, **2019**, 123, 5837-5848	2.8	1
215	The JPC Periodic Table. *Journal of Physical Chemistry C*, **2019**, 123, 17063-17074	3.8	1
214	The JPC Periodic Table. *Journal of Physical Chemistry Letters*, **2019**, 10, 4051-4062	6.4	1
213	Influence of Charge Scaling on the Solvation Properties of Ionic Liquid Solutions. *Journal of Physical Chemistry B*, **2019**, 123, 9222-9229	3.4	17
212	Proper Thermal Equilibration of Simulations with Drude Polarizable Models: Temperature-Grouped Dual-Nos□Hoover Thermostat. *Journal of Physical Chemistry Letters*, **2019**, 10, 7523-7530	6.4	12
211	Palit et´al. Reply. *Physical Review Letters*, **2019**, 123, 239802	7.4	1
210	Counterion-Regulated Dynamics of Water Confined in Lyotropic Liquid Crystalline Morphologies. *Journal of Physical Chemistry B*, **2018**, 122, 2408-2413	3.4	3
209	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	3.4	29
208	Influence of Electronic Polarization on the Structure of Ionic Liquids. *Journal of Physical Chemistry Letters*, **2018**, 9, 4765-4770	6.4	39
207	Conformational and Dynamic Properties of Poly(ethylene oxide) in BMIM+BF4□A Microsecond Computer Simulation Study Using ab Initio Force Fields. *Macromolecules*, **2018**, 51, 5336-5345	5.5	12
206	Grotthuss Transport of Iodide in EMIM/I Ionic Crystal. *Journal of Physical Chemistry B*, **2018**, 122, 250-257	3.4	13
205	The Driving Force for the Association of Gemini Surfactants. *Journal of Physical Chemistry B*, **2018**, 122, 3259-3265	3.4	7
204	Ion-Specific Confined Water Dynamics in Convex Nanopores of Gemini Surfactant Lyotropic Liquid Crystals. *Journal of Physical Chemistry B*, **2018**, 122, 10031-10043	3.4	2
203	A simulation method for the phase diagram of complex fluid mixtures. *Journal of Chemical Physics*, **2018**, 148, 244903	3.9	6
202	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	7.4	19
201	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	11.5	82
200	Coupling between the Dynamics of Water and Surfactants in Lyotropic Liquid Crystals. *Journal of Physical Chemistry B*, **2017**, 121, 5048-5057	3.4	3
199	Electrostatic Interactions Govern "Odd/Even" Effects in Water-Induced Gemini Surfactant Self-Assembly. *Journal of Physical Chemistry B*, **2017**, 121, 565-576	3.4	12

198	Cavity hydration dynamics in cytochrome oxidase and functional implications. *Proceedings of the National Academy of Sciences of the United States of America*, **2017**, 114, E8830-E8836	11.5	19
197	The effect of crowder charge in a model polymer-colloid system for macromolecular crowding: Polymer structure and dynamics. *Journal of Chemical Physics*, **2017**, 147, 114902	3.9	5
196	Proton Diffusion through Bilayer Pores. *Journal of Physical Chemistry B*, **2017**, 121, 9247-9259	3.4	2
195	More than Virtual Reality: Important New Physical Insights in Simulations of Biomolecules and Synthetic Polymers. *Journal of Physical Chemistry B*, **2017**, 121, 6294	3.4	3
194	Structure of room temperature ionic liquids. *Journal of Physics Condensed Matter*, **2016**, 28, 414020	1.8	8
193	Swing motion as a diffusion mechanism of lipid bilayers in a gel phase. *Physical Review E*, **2016**, 93, 012409	2.4	17
192	Different states of synaptotagmin regulate evoked versus spontaneous release. *Nature Communications*, **2016**, 7, 10971	17.4	32
191	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, 8424-37	3.4	17
190	Water Dynamics in Gyroid Phases of Self-Assembled Gemini Surfactants. *Journal of the American Chemical Society*, **2016**, 138, 2472-5	16.4	31
189	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, 231-43	3.4	20
188	First-Principles United Atom Force Field for the Ionic Liquid BMIM(+)BF4(-): An Alternative to Charge Scaling. *Journal of Physical Chemistry B*, **2016**, 120, 3560-8	3.4	52
187	Importance of hydrophobic traps for proton diffusion in lyotropic liquid crystals. *Journal of Chemical Physics*, **2016**, 144, 094705	3.9	6
186	Comment on "Isolating the non-polar contributions to the intermolecular potential for water-alkane interactions" [J. Chem. Phys. 141, 064905 (2014)]. *Journal of Chemical Physics*, **2016**, 144, 137101	3.9	13
185	Ab Initio Force Fields for Imidazolium-Based Ionic Liquids. *Journal of Physical Chemistry B*, **2016**, 120, 7024-36	3.4	52
184	Dynamics of water confined in lyotropic liquid crystals: Molecular dynamics simulations of the dynamic structure factor. *Journal of Chemical Physics*, **2016**, 144, 084504	3.9	6
183	Dynamics of Water in Gemini Surfactant-Based Lyotropic Liquid Crystals. *Journal of Physical Chemistry B*, **2016**, 120, 10860-10868	3.4	11
182	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	6.6	32
181	Conformational Properties of Sodium Polystyrenesulfonate in Water: Insights from a Coarse-Grained Model with Explicit Solvent. *Journal of Physical Chemistry B*, **2015**, 119, 11010-8	3.4	20

180	Osmotic Pressure of Polyelectrolyte Solutions with Salt: Grand Canonical Monte Carlo Simulation Studies. *Macromolecules*, **2015**, 48, 7370-7377	5.5	6
179	Anionic Phospholipids Stabilize RecA Filament Bundles in Escherichia coli. *Molecular Cell*, **2015**, 60, 374-84	14.6	36
178	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, 9091-7	3.4	9
177	Atomistic Simulations of Poly(ethylene oxide) in Water and an Ionic Liquid at Room Temperature. *Macromolecules*, **2014**, 47, 438-446	5.5	47
176	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, 2845-59	6.4	19
175	First-Principles, Physically Motivated Force Field for the Ionic Liquid [BMIM][BF4]. *Journal of Physical Chemistry Letters*, **2014**, 5, 2670-4	6.4	52
174	Dynamics in crowded environments: is non-Gaussian Brownian diffusion normal?. *Journal of Physical Chemistry B*, **2014**, 118, 8128-34	3.4	54
173	Coarse-grained models for aqueous polyethylene glycol solutions. *Journal of Physical Chemistry B*, **2014**, 118, 323-9	3.4	25
172	Why do arginine and lysine organize lipids differently? Insights from coarse-grained and atomistic simulations. *Journal of Physical Chemistry B*, **2013**, 117, 12145-56	3.4	52
171	Generation and sensing of membrane curvature: Where materials science and biophysics meet. *Current Opinion in Solid State and Materials Science*, **2013**, 17, 164-174	12	19
170	Self-assembly of gemini surfactants: a computer simulation study. *Journal of Physical Chemistry B*, **2013**, 117, 4254-62	3.4	39
169	Fracking: What Can Physical Chemistry Offer?. *Journal of Physical Chemistry Letters*, **2013**, 4, 687-90	6.4	37
168	Dynamics of two-dimensional and quasi-two-dimensional polymers. *Journal of Chemical Physics*, **2013**, 138, 234904	3.9	7
167	Sequence-dependent pKa shift induced by molecular self-assembly: insights from computer simulation. *Journal of Physical Chemistry B*, **2012**, 116, 491-5	3.4	4
166	Self-diffusion and viscosity in electrolyte solutions. *Journal of Physical Chemistry B*, **2012**, 116, 12007-13	3.4	117
165	Atomistic simulations of dilute polyelectrolyte solutions. *Journal of Physical Chemistry B*, **2012**, 116, 4319-27	3.4	21
164	Effect of polydispersity on diffusion in random obstacle matrices. *Physical Review Letters*, **2012**, 109, 155901	7.4	19
163	Effect of secondary structure on the self-assembly of amphiphilic molecules: a multiscale simulation study. *Journal of Chemical Physics*, **2012**, 136, 084902	3.9	11

162	Entropy-based mechanism of ribosome-nucleoid segregation in E. coli cells. *Biophysical Journal*, **2011**, 100, 2605-13	2.9	65
161	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	6.4	31
160	A New Coarse-Grained Force Field for Membrane-Peptide Simulations. *Journal of Chemical Theory and Computation*, **2011**, 7, 3793-802	6.4	70
159	Two- and three-body interactions among nanoparticles in a polymer melt. *Journal of Chemical Physics*, **2011**, 134, 174901	3.9	22
158	Crowding effects on protein association: effect of interactions between crowding agents. *Journal of Physical Chemistry B*, **2011**, 115, 347-53	3.4	29
157	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	2.6	7
156	Driving Force for the Association of Amphiphilic Molecules. *Journal of Physical Chemistry Letters*, **2011**, 2, 2391-2395	6.4	26
155	Solvent effects in polyelectrolyte adsorption: computer simulations with explicit and implicit solvent. *Journal of Chemical Physics*, **2010**, 132, 074903	3.9	29
154	Sequence dependent self-assembly of beta-peptides: Insights from a coarse-grained model. *Journal of Chemical Physics*, **2010**, 132, 065103	3.9	8
153	Crowding effects on association reactions at membranes. *Biophysical Journal*, **2010**, 98, 951-8	2.9	43
152	A new coarse-grained model for water: the importance of electrostatic interactions. *Journal of Physical Chemistry B*, **2010**, 114, 10524-9	3.4	150
151	Self-Assembly of Peptides: Insight from the Pair and Many-Body Free Energy of Association. *Journal of Physical Chemistry C*, **2010**, 114, 13551-13556	3.8	11
150	Structure of void space in polymer solutions. *Physical Review E*, **2010**, 81, 031801	2.4	16
149	Sequence-dependent interaction of peptides with membranes. *Journal of Physical Chemistry B*, **2010**, 114, 13585-92	3.4	27
148	Establishing effective simulation protocols for beta- and alpha/beta-peptides. III. Molecular mechanical model for acyclic beta-amino acids. *Journal of Computational Chemistry*, **2010**, 31, 2063-77	3.5	14
147	Swelling of polymers in porous media. *Journal of Chemical Physics*, **2009**, 130, 124908	3.9	19
146	NUMERICAL SIMULATION OF NANOINDENTATION AND PATCH CLAMP EXPERIMENTS ON MECHANOSENSITIVE CHANNELS OF LARGE CONDUCTANCE IN ESCHERICHIA COLI. *Experimental Mechanics*, **2009**, 49, 35-46	2.6	10
145	Liquid state theory of polyelectrolyte solutions. *Journal of Physical Chemistry B*, **2009**, 113, 1539-51	3.4	59

144	Effect of macromolecular crowding on reaction rates: a computational and theoretical study. *Biophysical Journal*, **2009**, 96, 1333-40	2.9	96
143	A computational framework for mechanical response of macromolecules: application to the salt concentration dependence of DNA bendability. *Biophysical Journal*, **2009**, 96, 3543-54	2.9	15
142	Computer simulations of protein diffusion in compartmentalized cell membranes. *Biophysical Journal*, **2009**, 97, 472-9	2.9	8
141	Retardation of ice crystallization by short peptides. *Journal of Physical Chemistry A*, **2009**, 113, 4403-7	2.8	20
140	Sequence-directed organization of beta-peptides in self-assembled monolayers. *Journal of Physical Chemistry B*, **2009**, 113, 9379-85	3.4	8
139	The effect of matrix structure on the diffusion of fluids in porous media. *Journal of Chemical Physics* , **2008**, 128, 054702	3.9	37
138	Gating mechanisms of mechanosensitive channels of large conductance, I: a continuum mechanics-based hierarchical framework. *Biophysical Journal*, **2008**, 95, 563-80	2.9	37
137	Gating mechanisms of mechanosensitive channels of large conductance, II: systematic study of conformational transitions. *Biophysical Journal*, **2008**, 95, 581-96	2.9	25
136	Lateral diffusion of proteins in the plasma membrane: spatial tessellation and percolation theory. *Journal of Physical Chemistry B*, **2008**, 112, 143-9	3.4	41
135	Establishing effective simulation protocols for beta- and alpha/beta-peptides. II. Molecular mechanical (MM) model for a cyclic beta-residue. *Journal of Physical Chemistry B*, **2008**, 112, 5439-48	3.4	25
134	Phase behavior of semiflexible polymer chains. *Journal of Chemical Physics*, **2008**, 128, 124908	3.9	14
133	Characterization of nanofibers formed by self-assembly of beta-peptide oligomers using small angle x-ray scattering. *Journal of Chemical Physics*, **2008**, 129, 095103	3.9	42
132	The effect of salt on the melting of ice: A molecular dynamics simulation study. *Journal of Chemical Physics*, **2008**, 129, 124504	3.9	36
131	A diffusive anomaly of water in aqueous sodium chloride solutions at low temperatures. *Journal of Physical Chemistry B*, **2008**, 112, 1729-35	3.4	30
130	Mechanosensitive channels: insights from continuum-based simulations. *Cell Biochemistry and Biophysics*, **2008**, 52, 1-18	3.2	13
129	Single molecule spectroscopy of conjugated polymer chains in an electric field-aligned liquid crystal. *Journal of Physical Chemistry B*, **2008**, 112, 448-53	3.4	15
128	Establishing Effective Simulation Protocols for □and #Mixed Peptides. I. QM and QM/MM Models. *Journal of Chemical Theory and Computation*, **2007**, 3, 1538-49	6.4	31
127	Why are lipid rafts not observed in vivo?. *Biophysical Journal*, **2007**, 93, 3113-9	2.9	89

126	Structure and dynamics of short chain molecules in disordered porous materials: a molecular dynamics simulation study. *Journal of Chemical Physics*, **2007**, 126, 174906	3.9	12
125	Structure and dynamics of conjugated polymers in liquid crystalline solvents. *Annual Review of Physical Chemistry*, **2007**, 58, 565-84	15.7	30
124	Permeation of a hard sphere fluid into a quenched matrix. *Journal of Chemical Physics*, **2007**, 126, 034704	3.9	5
123	Microfluidic based platform for characterization of protein interactions in hydrogel nanoenvironments. *Analytical Chemistry*, **2007**, 79, 5322-7	7.8	34
122	A Monte Carlo simulation study of branched polymers. *Journal of Chemical Physics*, **2006**, 125, 204901	3.9	50
121	Orthogonal orientations for solvation of polymer molecules in smectic solvents. *Physical Review Letters*, **2006**, 96, 017801	7.4	14
120	Lateral diffusion and percolation in membranes. *Physical Review Letters*, **2006**, 96, 228103	7.4	50
119	Dynamics of chain molecules in disordered materials. *Physical Review Letters*, **2006**, 96, 107802	7.4	37
118	Dynamics of probes in model glassy matrices. *Physical Review Letters*, **2006**, 97, 145503	7.4	8
117	A finite element framework for studying the mechanical response of macromolecules: application to the gating of the mechanosensitive channel MscL. *Biophysical Journal*, **2006**, 91, 1248-63	2.9	68
116	Implicit and Explicit Solvent Models for the Simulation of Dilute Polymer Solutions. *Macromolecules* , **2006**, 39, 8536-8542	5.5	57
115	Dilute Solutions of Strongly Charged Flexible Polyelectrolytes in Poor Solvents: Molecular Dynamics Simulations with Explicit Solvent. *Macromolecules*, **2006**, 39, 821-828	5.5	55
114	Adsorption and Dynamics of a Single Polyelectrolyte Chain near a Planar Charged Surface: Molecular Dynamics Simulations with Explicit Solvent. *Journal of Chemical Theory and Computation*, **2006**, 2, 630-6	6.4	24
113	Anisotropic diffusion of elongated and aligned polymer chains in a nematic solvent. *Journal of Physical Chemistry B*, **2006**, 110, 19799-803	3.4	7
112	Molecular dynamics simulations of heat and momentum transfer at a solid–fluid interface: Relationship between thermal and velocity slip. *International Journal of Heat and Mass Transfer*, **2006**, 49, 3401-3407	4.9	65
111	Osmotic Pressure of Salt-Free Polyelectrolyte Solutions:´A Monte Carlo Simulation Study. *Macromolecules*, **2005**, 38, 607-616	5.5	27
110	Integral Equation Theory of Random Copolymer Melts. *Macromolecules*, **2005**, 38, 2000-2008	5.5	19
109	Integral equation theory for symmetric nonadditive hard sphere mixtures. *Journal of Physical Chemistry B*, **2005**, 109, 6764-8	3.4	11

108	Integral equation theory of random copolymer melts: self-consistent treatment of intramolecular and intermolecular correlations. *Journal of Chemical Physics*, **2005**, 122, 234904	3.9	16
107	Integral equation theory of randomly coupled multiblock copolymer melts: effect of block size on the phase behavior. *Journal of Chemical Physics*, **2005**, 123, 214901	3.9	6
106	Molecular-dynamics simulations for nonclassical kinetics of diffusion-controlled bimolecular reactions. *Journal of Chemical Physics*, **2005**, 123, 114503	3.9	11
105	Jagannathan and Yethiraj Reply:. *Physical Review Letters*, **2005**, 94,	7.4	7
104	Monte Carlo simulation and self-consistent integral equation theory for polymers in quenched random media. *Journal of Chemical Physics*, **2005**, 123, 074909	3.9	18
103	Integral equation theory for two-dimensional polymer melts. *Journal of Chemical Physics*, **2005**, 122, 094910	3.9	7
102	Dynamics of fluids near the consolute critical point: a molecular-dynamics study of the Widom-Rowlinson mixture. *Journal of Chemical Physics*, **2005**, 122, 244506	3.9	8
101	The behavior of fluids near solutes: a density functional theory and computer simulation study. *Journal of Chemical Physics*, **2004**, 121, 4203-9	3.9	7
100	Diffusion of hard sphere fluids in disordered media: a molecular dynamics simulation study. *Physical Review E*, **2004**, 69, 051101	2.4	44
99	Self-consistent mode-coupling theory for the viscosity of rodlike polyelectrolyte solutions. *Journal of Chemical Physics*, **2004**, 121, 8120-7	3.9	20
98	Structure of Polyelectrolyte Solutions at a Charged Surface. *Journal of Physical Chemistry B*, **2004**, 108, 9126-9132	3.4	36
97	Molecular dynamics simulations of a fluid near its critical point. *Physical Review Letters*, **2004**, 93, 015701	7.4	22
96	The behavior of salt-free polyelectrolyte solutions at charged surfaces. *Progress in Organic Coatings* , **2003**, 47, 331-336	4.8	6
95	Liquid state theories for the structure of water. *Journal of Chemical Physics*, **2003**, 119, 13012-13016	3.9	26
94	Computer Simulation Study of Two-Dimensional Polymer Solutions. *Macromolecules*, **2003**, 36, 5854-5862	3.5	56
93	Short chains at surfaces and interfaces: A quantitative comparison between density-functional theories and Monte Carlo simulations. *Journal of Chemical Physics*, **2003**, 118, 2929	3.9	96
92	Monte Carlo simulations for the phase behavior of symmetric nonadditive hard sphere mixtures. *Journal of Chemical Physics*, **2003**, 118, 7907-7911	3.9	28
91	Strongly charged flexible polyelectrolytes in poor solvents: Molecular dynamics simulations with explicit solvent. *Journal of Chemical Physics*, **2003**, 118, 6634-6647	3.9	62

90	Density functional theory for nonuniform polymers: Accurate treatment of the effect of attractive interactions. *Journal of Chemical Physics*, **2003**, 118, 4702-4706	3.9	54
89	Osmotic pressure of isotropic solutions of rodlike polymers. *Journal of Chemical Physics*, **2003**, 118, 3904-3905	3.9	4
88	Monte Carlo simulations and integral equation theory for the structure of telechelic polymers. *Journal of Chemical Physics*, **2003**, 119, 6916-6924	3.9	18
87	Brownian dynamics simulations of polyelectrolyte solutions with divalent counterions. *Journal of Chemical Physics*, **2003**, 118, 11315-11325	3.9	33
86	Integral equations for polymers in quenched random media. *Journal of Chemical Physics*, **2002**, 116, 5910-5911	3.9	10
85	Polymer Melts at Solid Surfaces. *Advances in Chemical Physics*, **2002**, 89-139		41
84	Entanglement effects in mode coupling theories of polymers. *Journal of Chemical Physics*, **2002**, 117, 10448-10451	3.9	14
83	Integral equation theory for the structure of DNA solutions. *Journal of Chemical Physics*, **2002**, 116, 5308	3.9	8
82	Brownian dynamics simulations of salt-free polyelectrolyte solutions. *Journal of Chemical Physics*, **2002**, 116, 5284	3.9	43
81	Density functional theory and Monte Carlo simulations for hard sphere fluids in square and rectangular channels. *Journal of Chemical Physics*, **2002**, 116, 5795-5800	3.9	9
80	A Monte Carlo study of the self-assembly of bacteriorhodopsin. *Biophysical Journal*, **2002**, 83, 1902-16	2.9	11
79	Structural and thermodynamic properties of a freely-jointed Yukawa hard-sphere chain fluid. *Journal of Molecular Liquids*, **2001**, 92, 85-96	6	8
78	Solvent effects on the collapse dynamics of polymers. *Journal of Chemical Physics*, **2001**, 114, 7688-7699	3.9	91
77	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	3.9	29
76	Molecular simulation and continuum mechanics investigation of viscoelastic properties of fluids confined to molecularly thin films. *Journal of Chemical Physics*, **2001**, 114, 7593-7601	3.9	23
75	Density functional theory for pair correlation functions in polymeric liquids. *Journal of Chemical Physics*, **2001**, 114, 4323-4330	3.9	27
74	The effect of acid-base equilibria on the fractional charge and conformational properties of polyelectrolyte solutions. *Journal of Chemical Physics*, **2001**, 114, 2830-2838	3.9	8
73	FRET by FET and Dynamics of Polymer Folding. *Journal of Physical Chemistry B*, **2001**, 105, 2475-2478	3.4	26

72	Integral equation theory for the surface segregation from blends of linear and star polymers. *Computational and Theoretical Polymer Science*, **2000**, 10, 115-123		8
71	Local density enhancement in dilute supercritical solutions. *Chemical Physics Letters*, **2000**, 317, 558-566	2.5	49
70	An Integral Equation Theory for the Widom□Rowlinson Mixture. *Journal of Statistical Physics*, **2000**, 100, 39-47	1.5	13
69	Generalized van der Waals density functional theory for nonuniform polymers. *Journal of Chemical Physics*, **2000**, 112, 1579-1584	3.9	44
68	Density functional theory for the nonspecific binding of salt to polyelectrolytes: thermodynamic properties. *Biophysical Journal*, **2000**, 78, 699-706	2.9	44
67	Self-consistent integral equation theory for semiflexible chain polyelectrolyte solutions. *Journal of Chemical Physics*, **2000**, 113, 8841-8847	3.9	22
66	Monte Carlo simulations and self-consistent integral equation theory for polyelectrolyte solutions. *Journal of Chemical Physics*, **1999**, 110, 5437-5443	3.9	32
65	Conformational properties of isolated polyelectrolytes in poor solvents. *Journal of Chemical Physics* , **1999**, 110, 676-681	3.9	20
64	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	3.9	39
63	Forces between surfaces immersed in polyelectrolyte solutions. *Journal of Chemical Physics*, **1999**, 111, 1797-1800	3.9	36
62	The effect of attractions on the structure of fused sphere chains confined between surfaces. *Journal of Chemical Physics*, **1999**, 111, 1608-1614	3.9	20
61	Molecular modeling of polymers at surfaces. *Chemical Engineering Journal*, **1999**, 74, 109-115	14.7	16
60	Density Functional Theory for the Distribution of Small Ions around Polyions. *Journal of Physical Chemistry B*, **1999**, 103, 6080-6087	3.4	77
59	Response to □Comment on □Molecular simulation and continuum mechanics study of simple fluids in nonisothermal planar Couette flows□[J. Chem. Phys. 111, 10730 (1999)]. *Journal of Chemical Physics*, **1999**, 111, 10732-10733	3.9	1
58	Static Structure and Chain Conformations in Polyelectrolyte Solutions **1999**, 393-405		
57	Theory and Simulations of Polymers at Surfaces **1999**, 379-392		
56	The structure of amorphous polymers near surfaces: athermal systems. *Computational and Theoretical Polymer Science*, **1998**, 8, 159-168		12
55	Theory for chain conformations and static structure of dilute and semidilute polyelectrolyte solutions. *Journal of Chemical Physics*, **1998**, 108, 1184-1192	3.9	55

54	Density functional theory of polymers: A Curtin-Ashcroft type weighted density approximation. *Journal of Chemical Physics*, **1998**, 109, 3269-3275	3.9	90
53	Phase behavior of semiflexible tangent hard sphere chains. *Journal of Chemical Physics*, **1998**, 108, 1636-1644	3.9	88
52	Ion binding in tobacco mosaic virus solutions. *Journal of Chemical Physics*, **1998**, 109, 5162-5163	3.9	18
51	Isotropic to nematic transition in semiflexible polymer melts. *Molecular Physics*, **1998**, 93, 693-701	1.7	49
50	Excited state kinetics of neutral transition metal atoms by stimulated emission pumping: V*(3d44s,a4D)+hydrocarbons. *Journal of Chemical Physics*, **1997**, 106, 5509-5525	3.9	17
49	Conformational Properties and Static Structure Factor of Polyelectrolyte Solutions. *Physical Review Letters*, **1997**, 78, 3789-3792	7.4	64
48	Rheological, thermodynamic, and structural studies of linear and branched alkanes under shear. *Journal of Chemical Physics*, **1997**, 107, 6956-6964	3.9	73
47	Molecular simulation and continuum mechanics study of simple fluids in non-isothermal planar couette flows. *Journal of Chemical Physics*, **1997**, 107, 2589-2596	3.9	82
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