Arun Yethiraj

List of Publications by Citations

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	A new coarse-grained model for water: the importance of electrostatic interactions. *Journal of Physical Chemistry B*, **2010**, 114, 10524-9	3.4	150
232	Monte Carlo density functional theory of nonuniform polymer melts. *Journal of Chemical Physics*, **1995**, 102, 5499-5505	3.9	144
231	Monte-Carlo simulation of polymers confined between flat plates. *Macromolecules*, **1990**, 23, 1865-1872	5.5	130
230	Self-diffusion and viscosity in electrolyte solutions. *Journal of Physical Chemistry B*, **2012**, 116, 12007-13	3.4	117
229	Rheology of Confined Polymer Melts. *Macromolecules*, **1996**, 29, 7910-7918	5.5	115
228	Polymer reference interaction site model theory: New molecular closures for phase separating fluids and alloys. *Journal of Chemical Physics*, **1993**, 98, 9053-9079	3.9	108
227	Effect of macromolecular crowding on reaction rates: a computational and theoretical study. *Biophysical Journal*, **2009**, 96, 1333-40	2.9	96
226	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
225	Solvent effects on the collapse dynamics of polymers. *Journal of Chemical Physics*, **2001**, 114, 7688-7699	3.9	91
224	Density functional theory of polymers: A Curtin-Ashcroft type weighted density approximation. *Journal of Chemical Physics*, **1998**, 109, 3269-3275	3.9	90
223	Why are lipid rafts not observed in vivo?. *Biophysical Journal*, **2007**, 93, 3113-9	2.9	89
222	Phase behavior of semiflexible tangent hard sphere chains. *Journal of Chemical Physics*, **1998**, 108, 1636-1644	3.9	88
221	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
220	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
219	Monte Carlo simulations and integral equation theory for microscopic correlations in polymeric fluids. *Journal of Chemical Physics*, **1992**, 96, 797-807	3.9	82
218	Monte Carlo simulation of hard chain–hard sphere mixtures in slitlike pores. *Journal of Chemical Physics*, **1989**, 91, 4827-4837	3.9	81
217	Density functional theory for inhomogeneous polymer solutions. *Journal of Chemical Physics*, **1994**, 100, 3181-3186	3.9	80

216	Site-Site correlations in short chain fluids. *Journal of Chemical Physics*, **1990**, 93, 4453-4461	3.9	79
215	Density Functional Theory for the Distribution of Small Ions around Polyions. *Journal of Physical Chemistry B*, **1999**, 103, 6080-6087	3.4	77
214	Integral equation theory for the adsorption of chain fluids in slitlike pores. *Journal of Chemical Physics*, **1991**, 95, 3749-3755	3.9	76
213	Structure of Polyelectrolyte Solutions. *Physical Review Letters*, **1996**, 77, 3937-3940	7.4	75
212	Liquid-state theory of the density dependent conformation of nonpolar linear polymers. *Journal of Chemical Physics*, **1994**, 100, 6857-6872	3.9	75
211	Generalized Flory equations of state for square-well chains. *Journal of Chemical Physics*, **1991**, 95, 8494-8506	3.9	75
210	Rheological, thermodynamic, and structural studies of linear and branched alkanes under shear. *Journal of Chemical Physics*, **1997**, 107, 6956-6964	3.9	73
209	Monte Carlo simulation of confined semiflexible polymer melts. *Journal of Chemical Physics*, **1994**, 101, 2489-2497	3.9	72
208	A New Coarse-Grained Force Field for Membrane-Peptide Simulations. *Journal of Chemical Theory and Computation*, **2011**, 7, 3793-802	6.4	70
207	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
206	Entropy-based mechanism of ribosome-nucleoid segregation in E. coli cells. *Biophysical Journal*, **2011**, 100, 2605-13	2.9	65
205	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
204	Conformational Properties and Static Structure Factor of Polyelectrolyte Solutions. *Physical Review Letters*, **1997**, 78, 3789-3792	7.4	64
203	Surface segregation in polymer blends due to stiffness disparity. *Journal of Chemical Physics*, **1994**, 100, 4691-4694	3.9	63
202	Strongly charged flexible polyelectrolytes in poor solvents: Molecular dynamics simulations with explicit solvent. *Journal of Chemical Physics*, **2003**, 118, 6634-6647	3.9	62
201	Square-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	3.9	61
200	Integral equation theory of solutions of rigid polyelectrolytes. *Journal of Chemical Physics*, **1997**, 106, 5706-5719	3.9	60
199	Entropic and enthalpic surface segregation from blends of branched and linear polymers. *Physical Review Letters*, **1995**, 74, 2018-2021	7.4	60

198	Interaction between colloids in solutions containing dissolved polymer. *Journal of Colloid and Interface Science*, **1992**, 151, 102-117	9.3	60
197	Liquid state theory of polyelectrolyte solutions. *Journal of Physical Chemistry B*, **2009**, 113, 1539-51	3.4	59
196	Square-well diatomics: Bulk equation of state, density profiles near walls, virial coefficients and coexistence properties. *Molecular Physics*, **1991**, 72, 619-641	1.7	59
195	Implicit and Explicit Solvent Models for the Simulation of Dilute Polymer Solutions. *Macromolecules* , **2006**, 39, 8536-8542	5.5	57
194	Computer Simulation Study of Two-Dimensional Polymer Solutions. *Macromolecules*, **2003**, 36, 5854-5862	5.5	56
193	Theory for chain conformations and static structure of dilute and semidilute polyelectrolyte solutions. *Journal of Chemical Physics*, **1998**, 108, 1184-1192	3.9	55
192	Dilute Solutions of Strongly Charged Flexible Polyelectrolytes in Poor Solvents: Molecular Dynamics Simulations with Explicit Solvent. *Macromolecules*, **2006**, 39, 821-828	5.5	55
191	Dynamics in crowded environments: is non-Gaussian Brownian diffusion normal?. *Journal of Physical Chemistry B*, **2014**, 118, 8128-34	3.4	54
190	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
189	Integral equation theory of polymer blends: Numerical investigation of molecular closure approximations. *Journal of Chemical Physics*, **1993**, 98, 9080-9093	3.9	54
188	Polymer-induced forces between colloidal particles. A Monte Carlo simulation. *Journal of Chemical Physics*, **1994**, 100, 4683-4690	3.9	54
187	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
186	First-Principles, Physically Motivated Force Field for the Ionic Liquid [BMIM][BF4]. *Journal of Physical Chemistry Letters*, **2014**, 5, 2670-4	6.4	52
185	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
184	Monte Carlo simulation of the equilibrium partitioning of chain fluids between a bulk and a pore. *Molecular Physics*, **1991**, 73, 503-515	1.7	52
183	Ab Initio Force Fields for Imidazolium-Based Ionic Liquids. *Journal of Physical Chemistry B*, **2016**, 120, 7024-36	3.4	52
182	Self-consistent polymer integral equation theory: Comparisons with Monte Carlo simulations and alternative closure approximations. *Journal of Chemical Physics*, **1992**, 97, 1455-1464	3.9	51
181	A Monte Carlo simulation study of branched polymers. *Journal of Chemical Physics*, **2006**, 125, 204901	3.9	50

180	Lateral diffusion and percolation in membranes. *Physical Review Letters*, **2006**, 96, 228103	7.4	50
179	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	3.9	50
178	Local density enhancement in dilute supercritical solutions. *Chemical Physics Letters*, **2000**, 317, 558-566	2.5	49
177	Isotropic to nematic transition in semiflexible polymer melts. *Molecular Physics*, **1998**, 93, 693-701	1.7	49
176	Atomistic Simulations of Poly(ethylene oxide) in Water and an Ionic Liquid at Room Temperature. *Macromolecules*, **2014**, 47, 438-446	5.5	47
175	Microscopic equations of state of polyethylene: Hard-chain contribution to the pressure. *Journal of Chemical Physics*, **1993**, 98, 1635-1646	3.9	46
174	Diffusion of hard sphere fluids in disordered media: a molecular dynamics simulation study. *Physical Review E*, **2004**, 69, 051101	2.4	44
173	Generalized van der Waals density functional theory for nonuniform polymers. *Journal of Chemical Physics*, **2000**, 112, 1579-1584	3.9	44
172	Density functional theory for the nonspecific binding of salt to polyelectrolytes: thermodynamic properties. *Biophysical Journal*, **2000**, 78, 699-706	2.9	44
171	Monte Carlo calculation of the osmotic second virial coefficient of off-lattice athermal polymers. *Macromolecules*, **1992**, 25, 3979-3983	5.5	44
170	Crowding effects on association reactions at membranes. *Biophysical Journal*, **2010**, 98, 951-8	2.9	43
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168	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
167	On the scaling of the critical temperature with the degree of polymerization in symmetric polymer blends. *Journal of Chemical Physics*, **1992**, 97, 5927-5930	3.9	42
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165	Polymer Melts at Solid Surfaces. *Advances in Chemical Physics*, **2002**, 89-139		41
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163	Self-assembly of gemini surfactants: a computer simulation study. *Journal of Physical Chemistry B*, **2013**, 117, 4254-62	3.4	39

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159	Gating mechanisms of mechanosensitive channels of large conductance, I: a continuum mechanics-based hierarchical framework. *Biophysical Journal*, **2008**, 95, 563-80	2.9	37
158	Dynamics of chain molecules in disordered materials. *Physical Review Letters*, **2006**, 96, 107802	7.4	37
157	Anionic Phospholipids Stabilize RecA Filament Bundles in Escherichia coli. *Molecular Cell*, **2015**, 60, 374-84	17.6	36
156	The effect of salt on the melting of ice: A molecular dynamics simulation study. *Journal of Chemical Physics*, **2008**, 129, 124504	3.9	36
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154	Forces between surfaces immersed in polyelectrolyte solutions. *Journal of Chemical Physics*, **1999**, 111, 1797-1800	3.9	36
153	Microfluidic based platform for characterization of protein interactions in hydrogel nanoenvironments. *Analytical Chemistry*, **2007**, 79, 5322-7	7.8	34
152	Local structure of fluids containing chain-like molecules: Polymer reference interaction site model with a Yukawa closure. *Journal of Chemical Physics*, **1990**, 93, 5315-5321	3.9	34
151	Brownian dynamics simulations of polyelectrolyte solutions with divalent counterions. *Journal of Chemical Physics*, **2003**, 118, 11315-11325	3.9	33
150	Equations of state for star polymers. *Journal of Chemical Physics*, **1991**, 94, 3943-3948	3.9	33
149	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
148	Different states of synaptotagmin regulate evoked versus spontaneous release. *Nature Communications*, **2016**, 7, 10971	17.4	32
147	Monte Carlo simulations and self-consistent integral equation theory for polyelectrolyte solutions. *Journal of Chemical Physics*, **1999**, 110, 5437-5443	3.9	32
146	Water Dynamics in Gyroid Phases of Self-Assembled Gemini Surfactants. *Journal of the American Chemical Society*, **2016**, 138, 2472-5	16.4	31
145	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

144	Establishing Effective Simulation Protocols for □and 丹Mixed Peptides. I. QM and QM/MM Models. *Journal of Chemical Theory and Computation*, **2007**, 3, 1538-49	6.4	31
143	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
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141	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
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136	Monte Carlo simulations for the phase behavior of symmetric nonadditive hard sphere mixtures. *Journal of Chemical Physics*, **2003**, 118, 7907-7911	3.9	28
135	Phase behavior of the WidomRowlinson mixture. *Journal of Chemical Physics*, **1996**, 104, 7665-7670	3.9	28
134	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
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117	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
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114	Self-consistent integral equation theory for semiflexible chain polyelectrolyte solutions. *Journal of Chemical Physics*, **2000**, 113, 8841-8847	3.9	22
113	Atomistic simulations of dilute polyelectrolyte solutions. *Journal of Physical Chemistry B*, **2012**, 116, 4319-27	3.4	21
112	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
111	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
110	Retardation of ice crystallization by short peptides. *Journal of Physical Chemistry A*, **2009**, 113, 4403-7	2.8	20
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99	Monte Carlo simulations and integral equation theory for the structure of telechelic polymers. *Journal of Chemical Physics*, **2003**, 119, 6916-6924	3.9	18
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93	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
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87	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
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80	An Integral Equation Theory for the Widom□Rowlinson Mixture. *Journal of Statistical Physics*, **2000**, 100, 39-47	1.5	13
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