Carol K Hall

List of Publications by Year in Descending Order

258 papers	9,649 citations	55 h-index	87 g-index
266 ext. papers	10,302 ext. citations	4.5 avg, IF	6.32 L-index

#	Paper	IF	Citations
258	De novo discovery of peptide-based affinity ligands for the fab fragment of human immunoglobulin G.. *Journal of Chromatography A*, **2022**, 1669, 462941	4.5	3
257	Autobiography of Carol K. Hall *Journal of Physical Chemistry B*, **2021**, 125, 11343-11349	3.4	
256	CATCH Peptides Coassemble into Structurally Heterogeneous β-Sheet Nanofibers with Little Preference to β-Strand Alignment. *Journal of Physical Chemistry B*, **2021**, 125, 4004-4015	3.4	2
255	Molecular simulation study of 3,4-dihydroxyphenylalanine in the context of underwater adhesive design. *Journal of Chemical Physics*, **2021**, 154, 144702	3.9	2
254	Membrane morphologies induced by mixtures of arc-shaped particles with opposite curvature. *Soft Matter*, **2021**, 17, 268-275	3.6	1
253	Structural insights into peptide self-assembly using photo-induced crosslinking experiments and discontinuous molecular dynamics. *AICHE Journal*, **2021**, 67, e17101	3.6	2
252	On the liquid demixing of water + elastin-like polypeptide mixtures: bimodal re-entrant phase behaviour. *Physical Chemistry Chemical Physics*, **2021**, 23, 5936-5944	3.6	0
251	Amyloid Oligomers: A Joint Experimental/Computational Perspective on Alzheimer's Disease, Parkinson's Disease, Type II Diabetes, and Amyotrophic Lateral Sclerosis. *Chemical Reviews*, **2021**, 121, 2545-2647	68.1	128
250	Keith E. Gubbins: A retrospective. *AICHE Journal*, **2021**, 67, e17191	3.6	
249	De novo design of peptides that coassemble into β-sheet-based nanofibrils. *Science Advances*, **2021**, 7, eabf7668	14.3	3
248	Engineering β-Sheet Peptide Coassemblies for Biomaterial Applications.. *Journal of Physical Chemistry B*, **2021**, 125, 13599-13609	3.4	2
247	Dynamical self-assembly of dipolar active Brownian particles in two dimensions. *Soft Matter*, **2020**, 16, 2208-2223	3.6	16
246	Molecular complementarity and structural heterogeneity within co-assembled peptide β-sheet nanofibers. *Nanoscale*, **2020**, 12, 4506-4518	7.7	14
245	Anatomy of a selectively coassembled β-sheet peptide nanofiber. *Proceedings of the National Academy of Sciences of the United States of America*, **2020**, 117, 4710-4717	11.5	21
244	Clustering and phase separation in mixtures of dipolar and active particles. *Soft Matter*, **2020**, 16, 3779-3791	3.6	4
243	Novel peptide ligands for antibody purification provide superior clearance of host cell protein impurities. *Journal of Chromatography A*, **2020**, 1625, 461237	4.5	9
242	Clustering and Phase Separation in Mixtures of Dipolar and Active Particles in an External Field. *Langmuir*, **2020**, 36, 6378-6387	4	5

241	In Silico Discovery and Validation of Neuropeptide-Y-Binding Peptides for Sensors. *Journal of Physical Chemistry B*, **2020**, 124, 61-68	3.4	6
240	Development of a coarse-grained lipid model, LIME 2.0, for DSPE using multistate iterative Boltzmann inversion and discontinuous molecular dynamics simulations. *Fluid Phase Equilibria*, **2020**, 521, 112704	2.5	1
239	Charge guides pathway selection in β-sheet fibrillizing peptide co-assembly. *Communications Chemistry*, **2020**, 3,	6.3	11
238	A multiscale coarse-grained model to predict the molecular architecture and drug transport properties of modified chitosan hydrogels. *Soft Matter*, **2020**, 16, 10591-10610	3.6	7
237	A ChemE Grows in Brooklyn. *Annual Review of Chemical and Biomolecular Engineering*, **2020**, 11, 1-22	8.9	2
236	Thermodynamic phase diagram of amyloid-β(16-22) peptide. *Proceedings of the National Academy of Sciences of the United States of America*, **2019**, 116, 2091-2096	11.5	40
235	Molecular insights into the surface-catalyzed secondary nucleation of amyloid-β(A) by the peptide fragment Aβ. *Science Advances*, **2019**, 5, eaav8216	14.3	34
234	Characterising the throat diameter of through-pores in network structures using a percolation criterion. *Molecular Physics*, **2019**, 117, 3614-3622	1.7	1
233	Tailoring the Chemical Modification of Chitosan Hydrogels to Fine-Tune the Release of a Synergistic Combination of Chemotherapeutics. *Biomacromolecules*, **2019**, 20, 3126-3141	6.9	17
232	Differential Misfolding Properties of Glaucoma-Associated Olfactomedin Domains from Humans and Mice. *Biochemistry*, **2019**, 58, 1718-1727	3.2	6
231	Seeding and cross-seeding fibrillation of N-terminal prion protein peptides PrP(120-144). *Protein Science*, **2018**, 27, 1304-1313	6.3	8
230	Selectivity of Glycine for Facets on Gold Nanoparticles. *Journal of Physical Chemistry B*, **2018**, 122, 3491-3499	3.4	9
229	Simulations and Experiments Delineate Amyloid Fibrilization by Peptides Derived from Glaucoma-Associated Myocilin. *Journal of Physical Chemistry B*, **2018**, 122, 5845-5850	3.4	8
228	Advancing Peptide-Based Biorecognition Elements for Biosensors Using in-Silico Evolution. *ACS Sensors*, **2018**, 3, 1024-1031	9.2	31
227	Computational Study of DNA-Cross-Linked Hydrogel Formation for Drug Delivery Applications. *Macromolecules*, **2018**, 51, 9758-9768	5.5	6
226	Phase diagrams of mixtures of dipolar rods and discs. *Soft Matter*, **2018**, 14, 7894-7905	3.6	1
225	Development of a simple coarse-grained DNA model for analysis of oligonucleotide complex formation. *Molecular Simulation*, **2018**, 44, 1004-1015	2	3
224	Nanoparticle-induced assembly of hydrophobically modified chitosan. *Molecular Simulation*, **2017**, 43, 664-674	2	2

223	Formation of limit-periodic structures by quadrupole particles confined to a triangular lattice. *Physical Review E*, **2017**, 95, 012604	2.4	
222	The Impact of Colloidal Surface-Anchoring on the Smectic A Phase. *Langmuir*, **2017**, 33, 2222-2234	4	6
221	Simulation study on the structural properties of colloidal particles with offset dipoles. *Soft Matter*, **2017**, 13, 3134-3146	3.6	8
220	Allosteric effects of gold nanoparticles on human serum albumin. *Nanoscale*, **2017**, 9, 380-390	7.7	40
219	Preface to the Tribute to Keith E. Gubbins, Pioneer in the Theory of Liquids Special Issue. *Langmuir*, **2017**, 33, 11095-11101	4	3
218	Aggregation of A(17-36) in the Presence of Naturally Occurring Phenolic Inhibitors Using Coarse-Grained Simulations. *Journal of Molecular Biology*, **2017**, 429, 3893-3908	6.5	36
217	Extended Concerted Rotation Technique Enhances the Sampling Efficiency of the Computational Peptide-Design Algorithm. *Journal of Chemical Theory and Computation*, **2017**, 13, 5709-5720	6.4	7
216	Predicting the Fluid-Phase Behavior of Aqueous Solutions of ELP (VPGVG) Sequences Using SAFT-VR. *Langmuir*, **2017**, 33, 11733-11745	4	5
215	Navigating in foldonia: Using accelerated molecular dynamics to explore stability, unfolding and self-healing of the solenoid structure formed by a silk-like polypeptide. *PLoS Computational Biology*, **2017**, 13, e1005446	5	12
214	Aggregation of amphipathic peptides at an aqueous-organic interface using coarse-grained simulations. *Molecular Simulation*, **2017**, 43, 1448-1458	2	
213	Protein adsorption on nanoparticles: model development using computer simulation. *Journal of Physics Condensed Matter*, **2016**, 28, 414019	1.8	28
212	Binding Preferences of Amino Acids for Gold Nanoparticles: A Molecular Simulation Study. *Langmuir*, **2016**, 32, 7888-96	4	41
211	Simulation study of the ability of a computationally-designed peptide to recognize target tRNA and other decoy tRNAs. *Protein Science*, **2016**, 25, 2243-2255	6.3	8
210	Capillary Bridging as a Tool for Assembling Discrete Clusters of Patchy Particles. *Journal of the American Chemical Society*, **2016**, 138, 14948-14953	16.4	42
209	A Discontinuous Potential Model for Protein-Protein Interactions. *Molecular Modeling and Simulation*, **2016**, 2016, 1-20		
208	Development of a Coarse-Grained Model of Chitosan for Predicting Solution Behavior. *Journal of Physical Chemistry B*, **2016**, 120, 7253-64	3.4	20
207	LCST Behavior is Manifested in a Single Molecule: Elastin-Like polypeptide (VPGVG)n. *Biomacromolecules*, **2016**, 17, 111-8	6.9	50
206	Dock n roll: folding of a silk-inspired polypeptide into an amyloid-like beta solenoid. *Soft Matter*, **2016**, 12, 3721-9	3.6	16

205	George Stell (1933-2014). *Journal of Physics Condensed Matter*, **2016**, 28, 410401	1.8	2
204	Introducing folding stability into the score function for computational design of RNA-binding peptides boosts the probability of success. *Proteins: Structure, Function and Bioinformatics*, **2016**, 84, 700-11	4.2	12
203	Effect of Monomer Sequence and Degree of Acetylation on the Self-Assembly and Porosity of Chitosan Networks in Solution. *Macromolecules*, **2016**, 49, 5281-5290	5.5	7
202	Fifty years of liquid state physics. *Journal of Physics Condensed Matter*, **2016**, 28, 410301	1.8	1
201	A novel model for smectic liquid crystals: Elastic anisotropy and response to a steady-state flow. *Journal of Chemical Physics*, **2016**, 145, 164903	3.9	3
200	The effect of charge separation on the phase behavior of dipolar colloidal rods. *Soft Matter*, **2016**, 12, 4932-43	3.6	8
199	N-terminal Prion Protein Peptides (PrP(120-144)) Form Parallel In-register β Sheets via Multiple Nucleation-dependent Pathways. *Journal of Biological Chemistry*, **2016**, 291, 22093-22105	5.4	22
198	Adding energy minimization strategy to peptide-design algorithm enables better search for RNA-binding peptides: Redesigned λN peptide binds boxB RNA. *Journal of Computational Chemistry*, **2016**, 37, 2423-35	3.5	10
197	Multidirectional colloidal assembly in concurrent electric and magnetic fields. *Soft Matter*, **2016**, 12, 7747-58	3.6	34
196	Modeling nanoparticle wrapping or translocation in bilayer membranes. *Nanoscale*, **2015**, 7, 14505-14	7.7	35
195	Structural Conversion of Aβ17-42 Peptides from Disordered Oligomers to U-Shape Protofilaments via Multiple Kinetic Pathways. *PLoS Computational Biology*, **2015**, 11, e1004258	5	39
194	Effects of hydrophobic macromolecular crowders on amyloid β(16-22) aggregation. *Biophysical Journal*, **2015**, 109, 124-34	2.9	18
193	Proteinlike copolymers as encapsulating agents for small-molecule solutes. *Langmuir*, **2015**, 31, 3518-26	4	9
192	Generic model for tunable colloidal aggregation in multidirectional fields. *Soft Matter*, **2015**, 11, 7356-66	3.6	11
191	Molecular recognition mechanism of peptide chain bound to the tRNALys3 anticodon loop in silico. *Journal of Biomolecular Structure and Dynamics*, **2015**, 33, 14-27	3.6	12
190	Simulation Study of Hydrophobically Modified Chitosan as an Oil Dispersant Additive. *Journal of Physical Chemistry B*, **2015**, 119, 6979-90	3.4	13
189	Molecular recognition mechanism of peptide chain bound to the tRNA(Lys3) anticodon loop in silico. *Journal of Biomolecular Structure and Dynamics*, **2015**, 33, 14-27	3.6	3
188	Designing peptide sequences in flexible chain conformations to bind RNA: a search algorithm combining Monte Carlo, self-consistent mean field and concerted rotation techniques. *Journal of Chemical Theory and Computation*, **2015**, 11, 740-52	6.4	13

187	Phase separation behavior of mixed lipid systems at neutral and low pH: coarse-grained simulations with DMD/LIME. *Langmuir*, **2015**, 31, 1086-94	4	5
186	Wrapping of nanoparticles by membranes. *Advances in Colloid and Interface Science*, **2014**, 208, 214-24	14.3	146
185	The design of a peptide sequence to inhibit HIV replication: a search algorithm combining Monte Carlo and self-consistent mean field techniques. *Journal of Biomolecular Structure and Dynamics*, **2014**, 32, 1523-36	3.6	18
184	Effects of macromolecular crowding on amyloid beta (16-22) aggregation using coarse-grained simulations. *Journal of Physical Chemistry B*, **2014**, 118, 13513-26	3.4	42
183	Properties of DNA **2014**, 1125-1157		5
182	Impact of sequence on the molecular assembly of short amyloid peptides. *Proteins: Structure, Function and Bioinformatics*, **2014**, 82, 1469-83	4.2	13
181	Molecular description of the LCST behavior of an elastin-like polypeptide. *Biomacromolecules*, **2014**, 15, 3522-30	6.9	109
180	Gelation and Cross-Linking in Multifunctional Thiol and Multifunctional Acrylate Systems Involving an in Situ Comonomer Catalyst. *Macromolecules*, **2014**, 47, 821-829	5.5	32
179	Amino acid signature enables proteins to recognize modified tRNA. *Biochemistry*, **2014**, 53, 1125-33	3.2	21
178	Disclination lines at homogeneous and heterogeneous colloids immersed in a chiral liquid crystal. *Soft Matter*, **2014**, 10, 5489-502	3.6	8
177	Two-dimensional colloidal networks induced by a uni-axial external field. *Soft Matter*, **2013**, 9, 2518	3.6	26
176	Molecular dynamics simulations of DPPC bilayers using "LIME", a new coarse-grained model. *Journal of Physical Chemistry B*, **2013**, 117, 5019-30	3.4	40
175	Effect of Protein-like Copolymers Composition on the Phase Separation Dynamics of a Polymer Blend: A Monte Carlo Simulation. *Macromolecules*, **2013**, 46, 4207-4214	5.5	5
174	Nanoconfinement-induced structures in chiral liquid crystals. *International Journal of Molecular Sciences*, **2013**, 14, 17584-607	6.3	14
173	Determining the Polydispersity in Chemical Composition and Monomer Sequence Distribution in Random Copolymers Prepared by Postpolymerization Modification of Homopolymers. *ACS Macro Letters*, **2012**, 1, 1128-1133	6.6	5
172	Fibrillization propensity for short designed hexapeptides predicted by computer simulation. *Journal of Molecular Biology*, **2012**, 416, 598-609	6.5	20
171	Influence of temperature on formation of perfect tau fragment fibrils using PRIME20/DMD simulations. *Protein Science*, **2012**, 21, 1514-27	6.3	29
170	Structural transitions and oligomerization along polyalanine fibril formation pathways from computer simulations. *Proteins: Structure, Function and Bioinformatics*, **2012**, 80, 1582-97	4.2	10

169	Phase diagram of two-dimensional systems of dipole-like colloids. *Soft Matter*, **2012**, 8, 1521-1531	3.6	43
168	Spontaneous formation of twisted A(16-22) fibrils in large-scale molecular-dynamics simulations. *Biophysical Journal*, **2011**, 101, 2493-501	2.9	55
167	Effect of copolymer compatibilizer sequence on the dynamics of phase separation of immiscible binary homopolymer blends. *Soft Matter*, **2011**, 7, 10620	3.6	13
166	Phase Separation Dynamics for a Polymer Blend Compatibilized by Protein-like Copolymers: A Monte Carlo Simulation. *Macromolecules*, **2011**, 44, 8284-8293	5.5	13
165	Computer simulation study of amyloid fibril formation by palindromic sequences in prion peptides. *Proteins: Structure, Function and Bioinformatics*, **2011**, 79, 2132-45	4.2	29
164	Encapsulation Efficiency and Micellar Structure of Solute-Carrying Block Copolymer Nanoparticles. *Macromolecules*, **2011**, 44, 5443-5451	5.5	9
163	Simulation of micelle formation in the presence of solutes. *Langmuir*, **2010**, 26, 15135-41	4	10
162	Simulation of Mechanically-Assembled Monolayers In Poor Solvent Using Discontinuous Molecular Dynamics. *Macromolecules*, **2010**, 43, 3072-3080	5.5	
161	Controlling comonomer distribution in random copolymers by chemical coloring of surface-tethered homopolymers: an insight from discontinuous molecular dynamics simulation. *Langmuir*, **2010**, 26, 8810-20	4	6
160	Protein-Like Copolymers (PLCs) as Compatibilizers for Homopolymer Blends. *Macromolecules*, **2010**, 43, 5149-5157	5.5	12
159	Self-assembly in binary mixtures of dipolar colloids: molecular dynamics simulations. *Journal of Chemical Physics*, **2010**, 133, 064511	3.9	33
158	Bicontinuous gels formed by self-assembly of dipolar colloid particles. *Soft Matter*, **2010**, 6, 480-484	3.6	32
157	Extending the PRIME model for protein aggregation to all 20 amino acids. *Proteins: Structure, Function and Bioinformatics*, **2010**, 78, 2950-60	4.2	98
156	Design of Copolymers with Tunable Randomness Using Discontinuous Molecular Dynamics Simulation. *Macromolecules*, **2009**, 42, 9063-9071	5.5	11
155	Simulation of Mechanically Assembled Monolayers and Polymers in Good Solvent Using Discontinuous Molecular Dynamics. *Macromolecules*, **2008**, 41, 6573-6581	5.5	4
154	Phase diagram for stimulus-responsive materials containing dipolar colloidal particles. *Physical Review E*, **2008**, 77, 031401	2.4	59
153	Solid–liquid phase behavior of ternary mixtures. *AICHE Journal*, **2008**, 54, 1886-1894	3.6	8
152	Thermodynamic and kinetic origins of Alzheimer's and related diseases: A chemical engineer's perspective. *AICHE Journal*, **2008**, 54, 1956-1962	3.6	11

151	Obtaining Concentration Profiles from Computer Simulation Structure Factors. *Macromolecules*, **2007**, 40, 2629-2632	5.5	11
150	Theoretical study of kinetics of zipping phenomena in biomimetic polymers. *Physical Review E*, **2007**, 76, 011915	2.4	1
149	Computer simulation study of probe-target hybridization in model DNA microarrays: effect of probe surface density and target concentration. *Journal of Chemical Physics*, **2007**, 127, 144912	3.9	38
148	Modeling Protein Aggregate Assembly and Structure **2007**, 279-317		3
147	Effects of chain length on the aggregation of model polyglutamine peptides: molecular dynamics simulations. *Proteins: Structure, Function and Bioinformatics*, **2007**, 66, 96-109	4.2	54
146	Computational approaches to fibril structure and formation. *Methods in Enzymology*, **2006**, 412, 338-65	1.7	19
145	Side-chain interactions determine amyloid formation by model polyglutamine peptides in molecular dynamics simulations. *Biophysical Journal*, **2006**, 90, 4574-84	2.9	62
144	Computer simulation study of molecular recognition in model DNA microarrays. *Biophysical Journal*, **2006**, 91, 2227-36	2.9	26
143	Spontaneous fibril formation by polyalanines; discontinuous molecular dynamics simulations. *Journal of the American Chemical Society*, **2006**, 128, 1890-901	16.4	87
142	Commentary on: "Assembly of a tetrameric alpha-helical bundle: computer simulations on an intermediate-resolution protein model" [Proteins 2001;44:376-391]. *Proteins: Structure, Function and Bioinformatics*, **2006**, 63, 709-10	4.2	1
141	Spontaneous formation of annular structures observed in molecular dynamics simulations of polyglutamine peptides. *Computational Biology and Chemistry*, **2006**, 30, 215-8	3.6	36
140	Simulations of Protein Aggregation **2006**, 47-77		2
139	Simulations of Protein Aggregation **2006**, 47-77		
138	Parametric studies of interaction strengths in polymer/CO2 systems: discontinuous molecular dynamics simulations. *Langmuir*, **2005**, 21, 7579-87	4	8
137	Computer Simulation of Block Copolymer/Nanoparticle Composites. *Macromolecules*, **2005**, 38, 3007-3016	5.5	129
136	The dynamics of single chains within a model polymer melt. *Journal of Chemical Physics*, **2005**, 122, 114902	3.9	6
135	Designing pattern-recognition surfaces for selective adsorption of copolymer sequences using lattice monte carlo simulation. *Physical Review Letters*, **2005**, 94, 078103	7.4	40
134	Kinetics of fibril formation by polyalanine peptides. *Journal of Biological Chemistry*, **2005**, 280, 9074-82	5.4	80

133	Solvent effects on the conformational transition of a model polyalanine peptide. *Protein Science*, **2004**, 13, 2909-24	6.3	82
132	Molecular dynamics simulations of spontaneous fibril formation by random-coil peptides. *Proceedings of the National Academy of Sciences of the United States of America*, **2004**, 101, 16180-5	11.5	325
131	Thermodynamics and stability of a beta-sheet complex: molecular dynamics simulations on simplified off-lattice protein models. *Protein Science*, **2004**, 13, 40-53	6.3	31
130	Effect of pressure on the complete phase behavior of binary mixtures. *AICHE Journal*, **2004**, 50, 215-225	3.6	13
129	Effect of the solid phase on the global phase behavior of Lennard□ones mixtures. *AICHE Journal*, **2004**, 50, 1948-1960	3.6	4
128	Phase behavior in model homopolymer/CO2 and surfactant/CO2 systems: discontinuous molecular dynamics simulations. *Langmuir*, **2004**, 20, 8559-68	4	7
127	Lattice Monte Carlo simulations of phase separation and micellization in supercritical CO2/surfactant systems: effect of CO2 density. *Langmuir*, **2004**, 20, 514-23	4	26
126	Phase diagrams describing fibrillization by polyalanine peptides. *Biophysical Journal*, **2004**, 87, 4122-34	2.9	61
125	Assembly and kinetic folding pathways of a tetrameric beta-sheet complex: molecular dynamics simulations on simplified off-lattice protein models. *Biophysical Journal*, **2004**, 86, 31-49	2.9	60
124	Physical organogels composed of amphiphilic block copolymers and 1,3:2,4-dibenzylidene-D-sorbitol. *Journal of Colloid and Interface Science*, **2003**, 267, 509-18	9.3	38
123	Global phase diagram for monomer/dimer mixtures. *Fluid Phase Equilibria*, **2003**, 204, 85-106	2.5	2
122	Effects of Composition and Matrix Polarity on Network Development in Organogels of Poly(ethylene glycol) and Dibenzylidene Sorbitol. *Langmuir*, **2003**, 19, 6004-6013	4	74
121	Nanofibrillar Networks in Poly(ethyl methacrylate) and Its Silica Nanocomposites. *Journal of Physical Chemistry B*, **2003**, 107, 11633-11642	3.4	37
120	Dynamic phase transitions in thin ferromagnetic films. *Physical Review B*, **2003**, 67,	3.3	59
119	The molecular structure and intermolecular interactions of 1,3:2,4-dibenzylidene-D-sorbitol. *Molecular Physics*, **2003**, 101, 3017-3027	1.7	39
118	Formation of Spherical Micelles in a supercritical Solvent: Lattice Monte Carlo Simulation and Multicomponent Solution Model. *Molecular Simulation*, **2003**, 29, 139-157	2	7
117	Exchange anisotropy and the dynamic phase transition in thin ferromagnetic Heisenberg films. *Physical Review E*, **2003**, 68, 046115	2.4	34
116	Effect of rate of chemical or thermal renaturation on refolding and aggregation of a simple lattice protein. *Biotechnology and Bioengineering*, **2002**, 80, 823-34	4.9	26

115	Equilibria between solid, liquid, and vapor phases in binary Lennard□ones mixtures. *Fluid Phase Equilibria*, **2002**, 194-197, 197-206	2.5	20
114	Micellar behavior in supercritical solvent□urfactant systems from lattice Monte Carlo simulations. *Fluid Phase Equilibria*, **2002**, 194-197, 233-247	2.5	18
113	Phase behavior of PVAC□TAN block copolymer in supercritical carbon dioxide using SAFT. *Fluid Phase Equilibria*, **2002**, 194-197, 553-565	2.5	11
112	The effect of position along the chain on the dynamic properties of hard chain segments. *Journal of Chemical Physics*, **2002**, 117, 944-957	3.9	5
111	Computer simulation of copolymer phase behavior. *Journal of Chemical Physics*, **2002**, 117, 10329-10338	3.9	71
110	Entanglement Relaxation and Release in Hard Chain Fluids during Molecular Dynamics Simulations. *Macromolecules*, **2002**, 35, 6005-6019	5.5	4
109	Self-assembly of surfactants in a supercritical solvent from lattice Monte Carlo simulations. *Journal of Chemical Physics*, **2002**, 116, 1171-1184	3.9	58
108	Protein folding pathways and kinetics: molecular dynamics simulations of beta-strand motifs. *Biophysical Journal*, **2002**, 83, 819-35	2.9	14
107	Folding thermodynamics of model four-strand antiparallel beta-sheet proteins. *Biophysical Journal*, **2002**, 82, 646-59	2.9	23
106	Propane and propylene sorption in solid polymer electrolytes based on poly(ethylene oxide) and silver salts. *Journal of Membrane Science*, **2001**, 182, 1-12	9.6	109
105	Monte Carlo simulations of complete phase diagrams for binary Lennard□ones mixtures. *Fluid Phase Equilibria*, **2001**, 182, 37-46	2.5	36
104	alpha-helix formation: discontinuous molecular dynamics on an intermediate-resolution protein model. *Proteins: Structure, Function and Bioinformatics*, **2001**, 44, 344-60	4.2	156
103	Assembly of a tetrameric alpha-helical bundle: computer simulations on an intermediate-resolution protein model. *Proteins: Structure, Function and Bioinformatics*, **2001**, 44, 376-91	4.2	69
102	Molecular simulation of complete phase diagrams for binary mixtures. *AICHE Journal*, **2001**, 47, 1664-1675	3.6	35
101	Protein refolding versus aggregation: computer simulations on an intermediate-resolution protein model. *Journal of Molecular Biology*, **2001**, 312, 187-202	6.5	108
100	Bridging the gap between homopolymer and protein models: A discontinuous molecular dynamics study. *Journal of Chemical Physics*, **2000**, 113, 9331-9342	3.9	21
99	Theory and simulation of the swelling of polymer gels. *Journal of Chemical Physics*, **2000**, 113, 404-418	3.9	32
98	Grafted polymer tail/loop mixtures differing in chain length. *Polymer*, **1999**, 40, 5207-5211	3.9	6

97	Computer simulation of the competition between protein folding and aggregation. *Fluid Phase Equilibria*, **1999**, 158-160, 87-93	2.5	25
96	The calorimetric criterion for a two-state process revisited. *Protein Science*, **1999**, 8, 1064-74	6.3	90
95	Solid–liquid phase equilibrium for binary Lennard-Jones mixtures. *Journal of Chemical Physics*, **1999**, 110, 11433-11444	3.9	70
94	Solute excluded-volume effects on the stability of globular proteins: A statistical thermodynamic theory **1998**, 38, 273-284		13
93	Mixtures of polymer tails and loops grafted to an impenetrable interface. *Polymer*, **1998**, 39, 6339-6346	3.9	13
92	Effect of denaturant and protein concentrations upon protein refolding and aggregation: a simple lattice model. *Protein Science*, **1998**, 7, 2642-52	6.3	83
91	Discontinuous Molecular Dynamics Studies of End-Linked Polymer Networks. *Macromolecules*, **1998**, 31, 5861-5879	5.5	33
90	Generalized Flory equations of state for copolymers modeled as square-well chain fluids. *Journal of Chemical Physics*, **1998**, 108, 7478-7492	3.9	22
89	Self Diffusion Coefficients and Atomic Mean-Squared Displacements in Entangled Hard Chain Fluids. *The IMA Volumes in Mathematics and Its Applications*, **1998**, 203-215	0.5	1
88	Equilibrium thermodynamics of homopolymers and clusters: Molecular dynamics and Monte Carlo simulations of systems with square-well interactions. *Journal of Chemical Physics*, **1997**, 107, 10691-10708	3.9	181
87	Pressure-Dependent Photon Correlation Spectroscopic Investigation of Poly(propylene oxide) near the Glass Transition. *Macromolecules*, **1997**, 30, 2052-2057	5.5	17
86	Chemical potential gradient driven permeation of small molecules through polymeric media. *Journal of Chemical Physics*, **1997**, 107, 10714-10722	3.9	7
85	Fluids and fluid mixtures containing square-well diatomics: Equations of state and canonical molecular dynamics simulation. *Journal of Chemical Physics*, **1997**, 107, 3930-3946	3.9	40
84	Effect of solvent conditions upon refolding pathways and intermediates for a simple lattice protein. *Biopolymers*, **1997**, 42, 399-409	2.2	16
83	Molecular Dynamics for Polymeric Fluids Using Discontinuous Potentials. *Journal of Computational Physics*, **1997**, 134, 16-30	4.1	116
82	Modeling of phase separation in PEG–salt aqueous two-phase systems. *AICHE Journal*, **1996**, 42, 3508-3522	3.6	24
81	The Effects of Salts on the Lower Consolute Boundary of a Nonionic Micellar Solution. *Journal of Colloid and Interface Science*, **1996**, 184, 456-68	9.3	18
80	Binary hard chain mixtures. I. Generalized Flory equations of state. *Journal of Chemical Physics*, **1996**, 105, 7669-7682	3.9	35

79	First-Order Disorder-to-Order Transition in an Isolated Homopolymer Model. *Physical Review Letters*, **1996**, 77, 2822-2825	7.4	167
78	Estimation of mutual diffusion coefficients in polymer/penetrant systems using nonequilibrium molecular dynamics simulations. *Journal of Chemical Physics*, **1996**, 105, 1621-1632	3.9	33
77	Equilibrium conformations and dynamic relaxation of double-tethered chain molecules at an impenetrable interface. *Journal of Chemical Physics*, **1996**, 105, 7712-7722	3.9	15
76	Molecular dynamics study of entangled hard-chain fluids. *Journal of Chemical Physics*, **1996**, 104, 5616-5627	3.9	54
75	Computer simulation study of the approximations associated with the generalized Flory theories. *Journal of Chemical Physics*, **1996**, 104, 9100-9110	3.9	9
74	Smith, Hall, and Freeman Reply. *Physical Review Letters*, **1996**, 76, 4449	7.4	3
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