Carol K Hall

List of Publications by Citations

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	Polymer-induced phase separations in nonaqueous colloidal suspensions. *Journal of Colloid and Interface Science*, **1983**, 96, 251-267	9.3	543
257	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
256	High density Monte Carlo simulations of chain molecules: Bulk equation of state and density profile near walls. *Journal of Chemical Physics*, **1988**, 89, 3168-3174	3.9	274
255	Equation of state for chain molecules: Continuous-space analog of Flory theory. *Journal of Chemical Physics*, **1986**, 85, 4108-4115	3.9	229
254	A new equation of state for athermal chains. *Journal of Chemical Physics*, **1989**, 90, 1841-1855	3.9	227
253	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
252	Conformational state relaxation in polymers: Time-correlation functions. *Journal of Chemical Physics*, **1982**, 77, 3275-3282	3.9	180
251	First-Order Disorder-to-Order Transition in an Isolated Homopolymer Model. *Physical Review Letters*, **1996**, 77, 2822-2825	7.4	167
250	An experimental and theoretical study of phase transitions in the polystyrene latex and hydroxyethylcellulose system. *Journal of Colloid and Interface Science*, **1986**, 109, 161-171	9.3	167
249	alpha-helix formation: discontinuous molecular dynamics on an intermediate-resolution protein model. *Proteins: Structure, Function and Bioinformatics*, **2001**, 44, 344-60	4.2	156
248	Monte Carlo Simulation of Off-Lattice Polymer Chains: Effective Pair Potentials in Dilute Solution. *Macromolecules*, **1994**, 27, 5399-5412	5.5	151
247	Wrapping of nanoparticles by membranes. *Advances in Colloid and Interface Science*, **2014**, 208, 214-24	14.3	146
246	Prediction of gas adsorption in 5a zeolites using Monte Carlo simulation. *AICHE Journal*, **1991**, 37, 769-779	3.6	131
245	Monte-Carlo simulation of polymers confined between flat plates. *Macromolecules*, **1990**, 23, 1865-1872	5.5	130
244	Computer Simulation of Block Copolymer/Nanoparticle Composites. *Macromolecules*, **2005**, 38, 3007-3016	5.5	129
243	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
242	Molecular Dynamics for Polymeric Fluids Using Discontinuous Potentials. *Journal of Computational Physics*, **1997**, 134, 16-30	4.1	116

241	Molecular description of the LCST behavior of an elastin-like polypeptide. *Biomacromolecules*, **2014**, 15, 3522-30	6.9	109
240	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
239	Protein refolding versus aggregation: computer simulations on an intermediate-resolution protein model. *Journal of Molecular Biology*, **2001**, 312, 187-202	6.5	108
238	Extending the PRIME model for protein aggregation to all 20 amino acids. *Proteins: Structure, Function and Bioinformatics*, **2010**, 78, 2950-60	4.2	98
237	The calorimetric criterion for a two-state process revisited. *Protein Science*, **1999**, 8, 1064-74	6.3	90
236	Phase separations induced in aqueous colloidal suspensions by dissolved polymer. *Faraday Discussions of the Chemical Society*, **1983**, 76, 189		90
235	Influence of polymer molecular weight and temperature on phase composition in aqueous two-phase systems. *Fluid Phase Equilibria*, **1991**, 61, 243-262	2.5	89
234	Spontaneous fibril formation by polyalanines; discontinuous molecular dynamics simulations. *Journal of the American Chemical Society*, **2006**, 128, 1890-901	16.4	87
233	Effect of denaturant and protein concentrations upon protein refolding and aggregation: a simple lattice model. *Protein Science*, **1998**, 7, 2642-52	6.3	83
232	Solvent effects on the conformational transition of a model polyalanine peptide. *Protein Science*, **2004**, 13, 2909-24	6.3	82
231	Monte Carlo simulations and integral equation theory for microscopic correlations in polymeric fluids. *Journal of Chemical Physics*, **1992**, 96, 797-807	3.9	82
230	Monte Carlo simulation of hard chain□ard sphere mixtures in slitlike pores. *Journal of Chemical Physics*, **1989**, 91, 4827-4837	3.9	81
229	Kinetics of fibril formation by polyalanine peptides. *Journal of Biological Chemistry*, **2005**, 280, 9074-82	5.4	80
228	Interfacial tension of polyethyleneglycol-dextran-water systems: influence of temperature and polymer molecular weight. *Journal of Biotechnology*, **1990**, 16, 279-296	3.7	80
227	Site□ite correlations in short chain fluids. *Journal of Chemical Physics*, **1990**, 93, 4453-4461	3.9	79
226	On the pressure equation for chain molecules. *Journal of Chemical Physics*, **1987**, 87, 664-674	3.9	79
225	Protein partitioning at the isoelectric point: influence of polymer molecular weight and concentration and protein size. *Biotechnology and Bioengineering*, **1991**, 38, 986-94	4.9	77
224	Integral equation theory for the adsorption of chain fluids in slitlike pores. *Journal of Chemical Physics*, **1991**, 95, 3749-3755	3.9	76

223	Molecular-dynamics simulation results for the pressure of hard-chain fluids. *Molecular Physics*, **1990**, 71, 541-559	1.7	76
222	Generalized Flory equations of state for square-well chains. *Journal of Chemical Physics*, **1991**, 95, 8494-8506	3.9	75
221	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
220	Computer simulation of copolymer phase behavior. *Journal of Chemical Physics*, **2002**, 117, 10329-10338	3.9	71
219	Solid–liquid phase equilibrium for binary Lennard-Jones mixtures. *Journal of Chemical Physics*, **1999**, 110, 11433-11444	3.9	70
218	Theory and simulation of hard-chain mixtures: Equations of state, mixing properties, and density profiles near hard walls. *Journal of Chemical Physics*, **1991**, 95, 4481-4501	3.9	70
217	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
216	Statistical-mechanical model of protein precipitation by nonionic polymer. *AICHE Journal*, **1990**, 36, 1517-1528	3.6	69
215	Isostructural phase transitions due to core collapse. I. A one-dimensional model. *Journal of Chemical Physics*, **1976**, 65, 2161-2171	3.9	65
214	Side-chain interactions determine amyloid formation by model polyglutamine peptides in molecular dynamics simulations. *Biophysical Journal*, **2006**, 90, 4574-84	2.9	62
213	Phase diagrams describing fibrillization by polyalanine peptides. *Biophysical Journal*, **2004**, 87, 4122-34	2.9	61
212	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
211	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
210	Interaction between colloids in solutions containing dissolved polymer. *Journal of Colloid and Interface Science*, **1992**, 151, 102-117	9.3	60
209	Phase diagram for stimulus-responsive materials containing dipolar colloidal particles. *Physical Review E*, **2008**, 77, 031401	2.4	59
208	Dynamic phase transitions in thin ferromagnetic films. *Physical Review B*, **2003**, 67,	3.3	59
207	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
206	Self-assembly of surfactants in a supercritical solvent from lattice Monte Carlo simulations. *Journal of Chemical Physics*, **2002**, 116, 1171-1184	3.9	58

205	Equation of state for athermal lattice chains. *Journal of Chemical Physics*, **1986**, 85, 3023-3026	3.9	58
204	Spontaneous formation of twisted A(16-22) fibrils in large-scale molecular-dynamics simulations. *Biophysical Journal*, **2011**, 101, 2493-501	2.9	55
203	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
202	Molecular dynamics study of entangled hard-chain fluids. *Journal of Chemical Physics*, **1996**, 104, 5616-5637	3.9	54
201	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
200	Phase Transitions in Two-Dimensional Lattice Gases of Hard-Core Molecules with Long-Range Attractions. *Physical Review A*, **1973**, 7, 1679-1689	2.6	52
199	LCST Behavior is Manifested in a Single Molecule: Elastin-Like polypeptide (VPGVG)n. *Biomacromolecules*, **2016**, 17, 111-8	6.9	50
198	Theory of precipitation of protein mixtures by nonionic polymer. *AICHE Journal*, **1992**, 38, 573-591	3.6	49
197	The phase-change behavior of hydrogen in niobium and in niobium–vanadium alloys. *Journal of Chemical Physics*, **1982**, 77, 6223-6235	3.9	47
196	Monte Carlo calculation of the osmotic second virial coefficient of off-lattice athermal polymers. *Macromolecules*, **1992**, 25, 3979-3983	5.5	44
195	Phase diagram of two-dimensional systems of dipole-like colloids. *Soft Matter*, **2012**, 8, 1521-1531	3.6	43
194	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
193	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
192	Molecular dynamics study of transport coefficients for hard-chain fluids. *Journal of Chemical Physics* , **1995**, 102, 1057-1073	3.9	42
191	Binding Preferences of Amino Acids for Gold Nanoparticles: A Molecular Simulation Study. *Langmuir*, **2016**, 32, 7888-96	4	41
190	Allosteric effects of gold nanoparticles on human serum albumin. *Nanoscale*, **2017**, 9, 380-390	7.7	40
189	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
188	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

187	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
186	Designing pattern-recognition surfaces for selective adsorption of copolymer sequences using lattice monte carlo simulation. *Physical Review Letters*, **2005**, 94, 078103	7.4	40
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184	The molecular structure and intermolecular interactions of 1,3:2,4-dibenzylidene-D-sorbitol. *Molecular Physics*, **2003**, 101, 3017-3027	1.7	39
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181	Nanofibrillar Networks in Poly(ethyl methacrylate) and Its Silica Nanocomposites. *Journal of Physical Chemistry B*, **2003**, 107, 11633-11642	3.4	37
180	Aggregation of A17-36) in the Presence of Naturally Occurring Phenolic Inhibitors Using Coarse-Grained Simulations. *Journal of Molecular Biology*, **2017**, 429, 3893-3908	6.5	36
179	Spontaneous formation of annular structures observed in molecular dynamics simulations of polyglutamine peptides. *Computational Biology and Chemistry*, **2006**, 30, 215-8	3.6	36
178	Monte Carlo simulations of complete phase diagrams for binary Lennard-Jones mixtures. *Fluid Phase Equilibria*, **2001**, 182, 37-46	2.5	36
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176	Molecular simulation of complete phase diagrams for binary mixtures. *AICHE Journal*, **2001**, 47, 1664-1676	3.6	35
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174	Application of a Modified Generalized Flory Dimer Theory to Normal Alkanes. *Industrial & Engineering Chemistry Research*, **1994**, 33, 1290-1298	3.9	35
173	Molecular insights into the surface-catalyzed secondary nucleation of amyloid-A by the peptide fragment A*Science Advances*, **2019**, 5, eaav8216	14.3	34
172	Exchange anisotropy and the dynamic phase transition in thin ferromagnetic Heisenberg films. *Physical Review E*, **2003**, 68, 046115	2.4	34
171	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
170	Self-consistent field model of polymer adsorption: generalized formulation and ground-state solution. *Macromolecules*, **1988**, 21, 1075-1085	5.5	34

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168	Self-assembly in binary mixtures of dipolar colloids: molecular dynamics simulations. *Journal of Chemical Physics*, **2010**, 133, 064511	3.9	33
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165	Equations of state for star polymers. *Journal of Chemical Physics*, **1991**, 94, 3943-3948	3.9	33
164	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
163	Bicontinuous gels formed by self-assembly of dipolar colloid particles. *Soft Matter*, **2010**, 6, 480-484	3.6	32
162	Theory and simulation of the swelling of polymer gels. *Journal of Chemical Physics*, **2000**, 113, 404-418	3.9	32
161	Large-scale molecular dynamics study of entangled hard-chain fluids. *Physical Review Letters*, **1995**, 75, 1316-1319	7.4	32
160	Advancing Peptide-Based Biorecognition Elements for Biosensors Using in-Silico Evolution. *ACS Sensors*, **2018**, 3, 1024-1031	9.2	31
159	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
158	Thermodynamic perturbation theory for fused hard-sphere and hard-disk chain fluids. *Journal of Chemical Physics*, **1995**, 103, 2688-2695	3.9	31
157	Influence of temperature on formation of perfect tau fragment fibrils using PRIME20/DMD simulations. *Protein Science*, **2012**, 21, 1514-27	6.3	29
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144	On equations of state for hard chain fluids. *Molecular Physics*, **1993**, 80, 469-477	1.7	24
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139	N-terminal Prion Protein Peptides (PrP(120-144)) Form Parallel In-register □Sheets via Multiple Nucleation-dependent Pathways. *Journal of Biological Chemistry*, **2016**, 291, 22093-22105	5.4	22
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129	Micellar behavior in supercritical solvent□surfactant systems from lattice Monte Carlo simulations. *Fluid Phase Equilibria*, **2002**, 194-197, 233-247	2.5	18
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126	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
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122	Dynamical self-assembly of dipolar active Brownian particles in two dimensions. *Soft Matter*, **2020**, 16, 2208-2223	3.6	16
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120	Effect of solvent conditions upon refolding pathways and intermediates for a simple lattice protein. *Biopolymers*, **1997**, 42, 399-409	2.2	16
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118	Decorated-lattice model of metamagnetic or host-impurity systems. *Physical Review B*, **1975**, 11, 224-238	3.3	16
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114	Protein folding pathways and kinetics: molecular dynamics simulations of beta-strand motifs. *Biophysical Journal*, **2002**, 83, 819-35	2.9	14
113	Impact of sequence on the molecular assembly of short amyloid peptides. *Proteins: Structure, Function and Bioinformatics*, **2014**, 82, 1469-83	4.2	13
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109	Phase Separation Dynamics for a Polymer Blend Compatibilized by Protein-like Copolymers: A Monte Carlo Simulation. *Macromolecules*, **2011**, 44, 8284-8293	5.5	13
108	Solute excluded-volume effects on the stability of globular proteins: A statistical thermodynamic theory **1998**, 38, 273-284		13
107	Mixtures of polymer tails and loops grafted to an impenetrable interface. *Polymer*, **1998**, 39, 6339-6346	3.9	13
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103	Protein-Like Copolymers (PLCs) as Compatibilizers for Homopolymer Blends. *Macromolecules*, **2010**, 43, 5149-5157	5.5	12
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97	Solute excluded-volume effects on the stability of globular proteins: A statistical thermodynamic theory **1996**, 38, 273		12
96	Generic model for tunable colloidal aggregation in multidirectional fields. *Soft Matter*, **2015**, 11, 7356-66	3.6	11
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91	Computer simulation of protein refolding pathways and intermediates. *AICHE Journal*, **1995**, 41, 985-990	3.6	11
90	Charge guides pathway selection in β-sheet fibrillizing peptide co-assembly. *Communications Chemistry*, **2020**, 3,	6.3	11
89	Structural transitions and oligomerization along polyalanine fibril formation pathways from computer simulations. *Proteins: Structure, Function and Bioinformatics*, **2012**, 80, 1582-97	4.2	10
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