Athanassios Panagiotopoulos

List of Publications by Citations

327 papers	17,792 citations	63 h-index	120 g-index
347 ext. papers	19,090 ext. citations	4.5 avg, IF	7.1 L-index

#	Paper	IF	Citations
327	Direct determination of phase coexistence properties of fluids by Monte Carlo simulation in a new ensemble. *Molecular Physics*, **1987**, 61, 813-826	1.7	1720
326	Phase equilibria by simulation in the Gibbs ensemble. *Molecular Physics*, **1988**, 63, 527-545	1.7	976
325	Anisotropic self-assembly of spherical polymer-grafted nanoparticles. *Nature Materials*, **2009**, 8, 354-9	27	820
324	Water: A Tale of Two Liquids. *Chemical Reviews*, **2016**, 116, 7463-500	68.1	453
323	Metastable liquid-liquid transition in a molecular model of water. *Nature*, **2014**, 510, 385-8	50.4	356
322	Critical point and phase behavior of the pure fluid and a Lennard-Jones mixture. *Journal of Chemical Physics*, **1998**, 109, 10914-10920	3.9	313
321	Direct Determination of Fluid Phase Equilibria by Simulation in the Gibbs Ensemble: A Review. *Molecular Simulation*, **1992**, 9, 1-23	2	309
320	Adsorption and capillary condensation of fluids in cylindrical pores by Monte Carlo simulation in the Gibbs ensemble. *Molecular Physics*, **1987**, 62, 701-719	1.7	268
319	Phase behavior of the restricted primitive model and square-well fluids from Monte Carlo simulations in the grand canonical ensemble. *Journal of Chemical Physics*, **1999**, 110, 1581-1590	3.9	215
318	Monte Carlo methods for phase equilibria of fluids. *Journal of Physics Condensed Matter*, **2000**, 12, R25-R58	2.2	210
317	Molecular structural order and anomalies in liquid silica. *Physical Review E*, **2002**, 66, 011202	2.4	201
316	Generalization of the Wang-Landau method for off-lattice simulations. *Physical Review E*, **2002**, 66, 056703	2.4	200
315	Free energy and phase equilibria for the restricted primitive model of ionic fluids from Monte Carlo simulations. *Journal of Chemical Physics*, **1994**, 101, 1452-1459	3.9	191
314	Micellization in Model Surfactant Systems. *Langmuir*, **1999**, 15, 3143-3151	4	179
313	A Fixed Point Charge Model for Water Optimized to the Vapor−Liquid Coexistence Properties. *Journal of Physical Chemistry B*, **1998**, 102, 7470-7475	3.4	167
312	A New Intermolecular Potential Model for the n-Alkane Homologous Series. *Journal of Physical Chemistry B*, **1999**, 103, 6314-6322	3.4	162
311	Universality class of criticality in the restricted primitive model electrolyte. *Physical Review Letters*, **2002**, 88, 185701	7.4	159

310	Reactive canonical Monte Carlo. *Molecular Physics*, **1994**, 81, 717-733	1.7	156
309	Composite block copolymer stabilized nanoparticles: simultaneous encapsulation of organic actives and inorganic nanostructures. *Langmuir*, **2008**, 24, 83-90	4	150
308	Phase Equilibria of Lattice Polymers from Histogram Reweighting Monte Carlo Simulations. *Macromolecules*, **1998**, 31, 912-918	5.5	146
307	Determination of the chemical potentials of polymeric systems from Monte Carlo simulations. *Physical Review Letters*, **1991**, 66, 2935-2938	7.4	138
306	Aggregation Behavior of a Lattice Model for Amphiphiles. *Langmuir*, **1997**, 13, 5022-5031	4	135
305	Surface tension of the three-dimensional Lennard-Jones fluid from histogram-reweighting Monte Carlo simulations. *Journal of Chemical Physics*, **2000**, 112, 6411-6415	3.9	133
304	Liquid-liquid transition in ST2 water. *Journal of Chemical Physics*, **2012**, 137, 214505	3.9	128
303	Molecular simulation of phase equilibria for mixtures of polar and non-polar components. *Molecular Physics*, **1999**, 97, 1073-1083	1.7	126
302	Vapor+liquid equilibrium of water, carbon dioxide, and the binary system, water+carbon dioxide, from molecular simulation. *Fluid Phase Equilibria*, **2000**, 170, 203-234	2.5	125
301	Low-temperature fluid-phase behavior of ST2 water. *Journal of Chemical Physics*, **2009**, 131, 104508	3.9	124
300	An improved Monte Carlo method for direct calculation of the density of states. *Journal of Chemical Physics*, **2003**, 119, 9406-9411	3.9	121
299	Molecular simulation of phase coexistence: Finite-size effects and determination of critical parameters for two- and three-dimensional Lennard-Jones fluids. *International Journal of Thermophysics*, **1994**, 15, 1057-1072	2.1	120
298	Solubility and molecular conformations of n-alkane chains in water. *Journal of Physical Chemistry B*, **2009**, 113, 6405-14	3.4	116
297	Systematic determination of order parameters for chain dynamics using diffusion maps. *Proceedings of the National Academy of Sciences of the United States of America*, **2010**, 107, 13597-602	11.5	115
296	Molecular simulation of phase equilibria: simple, ionic and polymeric fluids. *Fluid Phase Equilibria*, **1992**, 76, 97-112	2.5	115
295	Micellization and Phase Separation of Diblock and Triblock Model Surfactants. *Langmuir*, **2002**, 18, 2940-2948	4	110
294	New intermolecular potential models for benzene and cyclohexane. *Journal of Chemical Physics*, **1999**, 111, 9731-9738	3.9	110
293	Coexistence and criticality in size-asymmetric hard-core electrolytes. *Physical Review Letters*, **2000**, 85, 4558-61	7.4	108

292	Molecular Simulation of Phase Equilibria for Water–Methane and Water–Ethane Mixtures. *Journal of Physical Chemistry B*, **1998**, 102, 8865-8873	3.4	108
291	New Mixing Rule for Cubic Equations of State for Highly Polar, Asymmetric Systems. *ACS Symposium Series*, **1986**, 571-582	0.4	108
290	Liquid-Liquid Immiscibility in Pure Fluids: Polyamorphism in Simulations of a Network-Forming Fluid. *Physical Review Letters*, **1996**, 77, 4386-4389	7.4	106
289	Nonlinear dimensionality reduction in molecular simulation: The diffusion map approach. *Chemical Physics Letters*, **2011**, 509, 1-11	2.5	103
288	Self-assembly of coarse-grained ionic surfactants accelerated by graphics processing units. *Soft Matter*, **2012**, 8, 2385-2397	3.6	102
287	Modeling the anisotropic self-assembly of spherical polymer-grafted nanoparticles. *Journal of Chemical Physics*, **2009**, 131, 221102	3.9	101
286	Precise simulation of criticality in asymmetric fluids. *Physical Review E*, **2001**, 63, 051507	2.4	101
285	Monte Carlo calculation of phase equilibria for a bead-spring polymeric model. *Macromolecules*, **1994**, 27, 400-406	5.5	100
284	Preparation of poly(ethylene glycol) protected nanoparticles with variable bioconjugate ligand density. *Biomacromolecules*, **2008**, 9, 2705-11	6.9	99
283	Large Lattice Discretization Effects on the Phase Coexistence of Ionic Fluids. *Physical Review Letters* , **1999**, 83, 2981-2984	7.4	98
282	Exact calculations of fluid-phase equilibria by Monte Carlo simulation in a new statistical ensemble. *International Journal of Thermophysics*, **1989**, 10, 447-457	2.1	96
281	Mean ionic activity coefficients in aqueous NaCl solutions from molecular dynamics simulations. *Journal of Chemical Physics*, **2015**, 142, 044507	3.9	93
280	Adsorption of fluids in model zeolite cavities. *Molecular Physics*, **1988**, 63, 49-63	1.7	93
279	Phase equilibria of the modified Buckingham exponential-6 potential from Hamiltonian scaling grand canonical Monte Carlo. *Journal of Chemical Physics*, **1998**, 109, 1093-1100	3.9	89
278	Phase coexistence properties of polarizable water models. *Molecular Physics*, **1998**, 94, 803-808	1.7	87
277	Coarse bifurcation analysis of kinetic Monte Carlo simulations: A lattice-gas model with lateral interactions. *Journal of Chemical Physics*, **2002**, 117, 8229-8240	3.9	85
276	Critical parameters of the restricted primitive model. *Journal of Chemical Physics*, **2002**, 116, 3007-3011	3.9	82
275	How good is conformal solutions theory for phase equilibrium predictions?. *Fluid Phase Equilibria*, **1991**, 65, 1-18	2.5	82

274	Coarse-grained kinetic computations for rare events: application to micelle formation. *Journal of Chemical Physics*, **2005**, 122, 44908	3.9	76
273	Efficient pressure estimation in molecular simulations without evaluating the virial. *Journal of Chemical Physics*, **1996**, 105, 8469-8470	3.9	76
272	On the equivalence of continuum and lattice models for fluids. *Journal of Chemical Physics*, **2000**, 112, 7132-7137	3.9	73
271	Multiphase high pressure equilibria in ternary aqueous systems. *Fluid Phase Equilibria*, **1986**, 29, 525-534	2.5	73
270	Monte Carlo simulation of folding transitions of simple model proteins using a chain growth algorithm. *Journal of Chemical Physics*, **1992**, 97, 8644-8652	3.9	69
269	Atomistic simulations of micellization of sodium hexyl, heptyl, octyl, and nonyl sulfates. *Journal of Physical Chemistry B*, **2012**, 116, 2430-7	3.4	68
268	Temperature-dependent solubilities and mean ionic activity coefficients of alkali halides in water from molecular dynamics simulations. *Journal of Chemical Physics*, **2015**, 143, 044505	3.9	66
267	Machine learning for autonomous crystal structure identification. *Soft Matter*, **2017**, 13, 4733-4745	3.6	64
266	Micellization behavior of coarse grained surfactant models. *Journal of Chemical Physics*, **2010**, 132, 114902	3.9	64
265	Atomistic molecular dynamics simulations of CO□diffusivity in H□O for a wide range of temperatures and pressures. *Journal of Physical Chemistry B*, **2014**, 118, 5532-41	3.4	63
264	Phase diagrams of nonideal fluid mixtures from Monte Carlo simulation. *Industrial & Engineering Chemistry Fundamentals*, **1986**, 25, 525-535		63
263	Simulation of polymer melt intercalation in layered nanocomposites. *Journal of Chemical Physics*, **1998**, 109, 10321-10330	3.9	62
262	Application of excluded volume map sampling to phase equilibrium calculations in the Gibbs ensemble. *Journal of Chemical Physics*, **1990**, 92, 1285-1293	3.9	62
261	Self-assembly of polymer-grafted nanoparticles in thin films. *Soft Matter*, **2014**, 10, 786-94	3.6	61
260	Effective potentials for 1:1 electrolyte solutions incorporating dielectric saturation and repulsive hydration. *Journal of Chemical Physics*, **2007**, 126, 044509	3.9	61
259	Phase transitions in 2:1 and 3:1 hard-core model electrolytes. *Physical Review Letters*, **2002**, 88, 045701	7.4	61
258	A comparison of implicit- and explicit-solvent simulations of self-assembly in block copolymer and solute systems. *Journal of Chemical Physics*, **2011**, 134, 164902	3.9	60
257	Monte Carlo simulations of phase equilibria for a lattice homopolymer model. *Journal of Chemical Physics*, **1995**, 102, 1014-1023	3.9	60

256	On the calculation of solubilities via direct coexistence simulations: Investigation of NaCl aqueous solutions and Lennard-Jones binary mixtures. *Journal of Chemical Physics*, **2016**, 145, 154111	3.9	60
255	Thermodynamics of Reversibly Associating Polymer Solutions. *Physical Review Letters*, **1999**, 82, 5060-5063	7.4	59
254	Finite-size effects and approach to criticality in Gibbs ensemble simulations. *Molecular Physics*, **1993**, 80, 843-852	1.7	59
253	Photochemical hydrogen production and cobaloximes: the influence of the cobalt axial N-ligand on the system stability. *Dalton Transactions*, **2016**, 45, 6732-8	4.3	59
252	Self-assembly of surfactants in a supercritical solvent from lattice Monte Carlo simulations. *Journal of Chemical Physics*, **2002**, 116, 1171-1184	3.9	58
251	Stratification Dynamics in Drying Colloidal Mixtures. *Langmuir*, **2017**, 33, 3685-3693	4	56
250	Flory-Huggins parameter □from binary mixtures of Lennard-Jones particles to block copolymer melts. *Journal of Chemical Physics*, **2014**, 140, 054909	3.9	56
249	A Monte Carlo study of the structural properties of end-linked polymer networks. *Journal of Chemical Physics*, **2000**, 112, 6910-6916	3.9	56
248	Integrating diffusion maps with umbrella sampling: application to alanine dipeptide. *Journal of Chemical Physics*, **2011**, 134, 135103	3.9	55
247	Model for disordered proteins with strongly sequence-dependent liquid phase behavior. *Journal of Chemical Physics*, **2020**, 152, 075101	3.9	54
246	Molecular dynamics simulations of silica nanoparticles grafted with poly(ethylene oxide) oligomer chains. *Journal of Physical Chemistry B*, **2012**, 116, 2385-95	3.4	53
245	Phase coexistence properties of polarizable Stockmayer fluids. *Journal of Chemical Physics*, **1997**, 106, 3338-3347	3.9	53
244	Vapour□iquid phase equilibrium and surface tension of fully flexible Lennard□ones chains. *Molecular Physics*, **2017**, 115, 320-327	1.7	52
243	An experimental and computational investigation of spontaneous lasso formation in microcin J25. *Biophysical Journal*, **2010**, 99, 3056-65	2.9	51
242	Implicit solvent models for micellization of ionic surfactants. *Journal of Physical Chemistry B*, **2008**, 112, 13783-92	3.4	51
241	Comment on "The putative liquid-liquid transition is a liquid-solid transition in atomistic models of water" [I and II: J. Chem. Phys. 135, 134503 (2011); J. Chem. Phys. 138, 214504 (2013)]. *Journal of Chemical Physics*, **2018**, 148, 137101	3.9	50
240	Monte carlo simulations of micellization in model ionic surfactants: application to sodium dodecyl sulfate. *Langmuir*, **2006**, 22, 4076-83	4	50
239	Phase equilibria of a lattice model for an oil□water□mphiphile mixture. *Journal of Chemical Physics*, **1996**, 104, 3718-3725	3.9	50

238	Phase equilibria of binary Lennard-Jones mixtures: simulation and van der Waals l-fluid theory. *Fluid Phase Equilibria*, **1994**, 100, 153-170	2.5	50
237	Thermodynamic and Transport Properties of H2O + NaCl from Polarizable Force Fields. *Journal of Chemical Theory and Computation*, **2015**, 11, 3802-10	6.4	49
236	Rapid Production of Internally Structured Colloids by Flash Nanoprecipitation of Block Copolymer Blends. *ACS Nano*, **2018**, 12, 4660-4668	16.7	49
235	Directed Assembly of Soft Colloids through Rapid Solvent Exchange. *ACS Nano*, **2016**, 10, 1425-33	16.7	49
234	Molecular simulation of thermodynamic and transport properties for the H2O+NaCl system. *Journal of Chemical Physics*, **2014**, 141, 234507	3.9	49
233	Structural transitions of solvent-free oligomer-grafted nanoparticles. *Physical Review Letters*, **2011**, 107, 105503	7.4	49
232	Atomistic molecular dynamics simulations of carbohydrate-calcite interactions in concentrated brine. *Langmuir*, **2015**, 31, 2407-13	4	48
231	Structure of solvent-free grafted nanoparticles: molecular dynamics and density-functional theory. *Journal of Chemical Physics*, **2011**, 135, 114901	3.9	48
230	Molecular dynamics simulation of SDS and CTAB micellization and prediction of partition equilibria with COSMOmic. *Langmuir*, **2013**, 29, 11582-92	4	47
229	Monte Carlo simulation and molecular theory of tethered polyelectrolytes. *Journal of Chemical Physics*, **2007**, 126, 244902	3.9	47
228	Monte carlo study of coulombic criticality in polyelectrolytes. *Physical Review Letters*, **2003**, 90, 048303	7.4	47
227	Phase Equilibria of Quadrupolar Fluids by Simulation in the Gibbs Ensemble. *Molecular Simulation*, **1989**, 2, 147-162	2	47
226	Electrostatic screening and charge correlation effects in micellization of ionic surfactants. *Journal of Physical Chemistry B*, **2009**, 113, 6314-20	3.4	46
225	Monte Carlo simulation of the collapse-coil transition in homopolymers. *Journal of Chemical Physics*, **1992**, 97, 6802-6808	3.9	45
224	Signatures of a liquid-liquid transition in an ab initio deep neural network model for water. *Proceedings of the National Academy of Sciences of the United States of America*, **2020**, 117, 26040-26046	11.5	45
223	Criticality and crossover in accessible regimes. *Physical Review E*, **2000**, 61, 5930-9	2.4	44
222	Molecular Simulation of Phase Equilibria for Water-Butane and Water-Hexane Mixtures. *Journal of Physical Chemistry B*, **2000**, 104, 4958-4963	3.4	44
221	Liquid-liquid phase transitions in pores. *Molecular Physics*, **1995**, 84, 825-834	1.7	44

220	Dynamics of solvent-free grafted nanoparticles. *Journal of Chemical Physics*, **2012**, 136, 044902	3.9	43
219	Nucleation in aqueous NaCl solutions shifts from 1-step to 2-step mechanism on crossing the spinodal. *Journal of Chemical Physics*, **2019**, 150, 124502	3.9	42
218	Stabilizing colloidal crystals by leveraging void distributions. *Nature Communications*, **2014**, 5, 4472	17.4	42
217	Stratification in Drying Polymer-Polymer and Colloid-Polymer Mixtures. *Langmuir*, **2017**, 33, 11390-11398	4	42
216	Dissipative particle dynamics simulations of polymer-protected nanoparticle self-assembly. *Journal of Chemical Physics*, **2011**, 135, 184903	3.9	41
215	Structure and dynamics of surfactant and hydrocarbon aggregates on graphite: a molecular dynamics simulation study. *Journal of Physical Chemistry B*, **2008**, 112, 2915-21	3.4	41
214	Simulations of micellization of sodium hexyl sulfate. *Journal of Physical Chemistry B*, **2011**, 115, 1403-10	3.4	39
213	Protected peptide nanoparticles: experiments and brownian dynamics simulations of the energetics of assembly. *Nano Letters*, **2009**, 9, 2218-22	11.5	39
212	Coarse-grained simulations of rapid assembly kinetics for polystyrene-b-poly(ethylene oxide) copolymers in aqueous solutions. *Journal of Physical Chemistry B*, **2008**, 112, 16357-66	3.4	39
211	Atomistic Molecular Dynamics Simulations of Carbon Dioxide Diffusivity in n-Hexane, n-Decane, n-Hexadecane, Cyclohexane, and Squalane. *Journal of Physical Chemistry B*, **2016**, 120, 12890-12900	3.4	39
210	The gibbs method for molecular-based computer simulations of phase equilibria. *Fluid Phase Equilibria*, **1989**, 53, 133-141	2.5	38
209	Monte Carlo simulations of high-pressure phase equilibria of CO2-H2O mixtures. *Journal of Physical Chemistry B*, **2011**, 115, 6629-35	3.4	37
208	Contact angles from Young's equation in molecular dynamics simulations. *Journal of Chemical Physics*, **2017**, 147, 084708	3.9	36
207	A computational investigation of the phase behavior and capillary sublimation of water confined between nanoscale hydrophobic plates. *Journal of Chemical Physics*, **2012**, 137, 144501	3.9	36
206	Simulations of phase transitions and free energies for ionic systems. *Molecular Physics*, **2008**, 106, 2039-2051	2.1	36
205	Critical parameters of unrestricted primitive model electrolytes with charge asymmetries up to 10:1. *Journal of Chemical Physics*, **2003**, 119, 8526-8536	3.9	36
204	Thermodynamic scaling Gibbs ensemble Monte Carlo: a new method for determination of phase coexistence properties of fluids. *Molecular Physics*, **1996**, 89, 965-974	1.7	36
203	Determination of the critical micelle concentration in simulations of surfactant systems. *Journal of Chemical Physics*, **2016**, 144, 044709	3.9	36

202	Efficient neighbor list calculation for molecular simulation of colloidal systems using graphics processing units. *Computer Physics Communications*, **2016**, 203, 45-52	4.2	35
201	Simulations of vapor□liquid phase equilibrium and interfacial tension in the CO2□H2O□NaCl system. *AICHE Journal*, **2013**, 59, 3514-3522	3.6	35
200	Dipolar origin of the gas-liquid coexistence of the hard-core 1:1 electrolyte model. *Physical Review E*, **2002**, 66, 041204	2.4	35
199	Aggregation phenomena in telechelic star polymer solutions. *Physical Review E*, **2009**, 79, 010401	2.4	34
198	The heat capacity of the restricted primitive model electrolyte. *Journal of Chemical Physics*, **2001**, 114, 5468-5471	3.9	34
197	Shear ordering in thin films of spherical block copolymer. *Langmuir*, **2005**, 21, 11518-27	4	33
196	Investigation of the transition to liquid-liquid immiscibilitym for Lennard-Jones (12,6) systems, using Gibbs-ensemble molecular simulations. *Fluid Phase Equilibria*, **1991**, 66, 57-75	2.5	33
195	Thin films of homopolymers and cylinder-forming diblock copolymers under shear. *ACS Nano*, **2014**, 8, 8015-26	16.7	32
194	Flat-Histogram Dynamics and Optimization in Density of States Simulations of Fluids□*Journal of Physical Chemistry B*, **2004**, 108, 19748-19755	3.4	32
193	Self-assembly of Janus particles under shear. *Soft Matter*, **2015**, 11, 3767-71	3.6	31
192	Effect of Chain Stiffness on Polymer Phase Behavior. *Macromolecules*, **1996**, 29, 4444-4446	5.5	31
191	Phase diagram of the two-dimensional Coulomb gas: A thermodynamic scaling Monte Carlo study. *Journal of Chemical Physics*, **1996**, 104, 7205-7209	3.9	31
190	Self-diffusion coefficients of the binary (H 2 O + CO 2) mixture at high temperatures and pressures. *Journal of Chemical Thermodynamics*, **2016**, 93, 424-429	2.9	30
189	Forward flux sampling calculation of homogeneous nucleation rates from aqueous NaCl solutions. *Journal of Chemical Physics*, **2018**, 148, 044505	3.9	30
188	Efficient mesoscale hydrodynamics: Multiparticle collision dynamics with massively parallel GPU acceleration. *Computer Physics Communications*, **2018**, 230, 10-20	4.2	30
187	Grand Canonical Monte Carlo Simulations Guided by an Analytic Equation of State-Transferable Anisotropic Mie Potentials for Ethers. *Journal of Physical Chemistry B*, **2015**, 119, 7087-99	3.4	30
186	Gibbs Ensemble Techniques **1995**, 463-501		30
185	Molecular dynamics simulations of water sorption in a perfluorosulfonic acid membrane. *Journal of Physical Chemistry B*, **2013**, 117, 12649-60	3.4	29

184	Implicit-solvent models for micellization: nonionic surfactants and temperature-dependent properties. *Journal of Physical Chemistry B*, **2011**, 115, 990-1001	3.4	29
183	Coarse-grained computations for a micellar system. *Journal of Chemical Physics*, **2005**, 122, 44907	3.9	29
182	Hydrogen-Bonding Polarizable Intermolecular Potential Model for Water. *Journal of Physical Chemistry B*, **2016**, 120, 12358-12370	3.4	28
181	Simulations of shear-induced morphological transitions in block copolymers. *Soft Matter*, **2013**, 9, 9960	3.6	28
180	Surfactant and hydrocarbon aggregates on defective graphite surface: structure and dynamics. *Journal of Physical Chemistry B*, **2008**, 112, 12954-61	3.4	28
179	Thermodynamic properties of lattice hard-sphere models. *Journal of Chemical Physics*, **2005**, 123, 104504	3.9	28
178	Ternary oil–water–amphiphile systems: self-assembly and phase equilibria. *Molecular Physics*, **2002**, 100, 2213-2220	1.7	28
177	Phase equilibria in ternary Lennard-Jones systems. *Fluid Phase Equilibria*, **1995**, 107, 31-43	2.5	28
176	Bottom-Up Colloidal Crystal Assembly with a Twist. *ACS Nano*, **2016**, 10, 5459-67	16.7	28
175	Atomistic molecular dynamics simulations of H2O diffusivity in liquid and supercritical CO2. *Molecular Physics*, **2015**, 113, 2805-2814	1.7	27
174	Optimization of intermolecular potential parameters for the CO2/H2O mixture. *Journal of Physical Chemistry B*, **2014**, 118, 11504-11	3.4	27
173	Critical point of electrolyte mixtures. *Journal of Chemical Physics*, **2005**, 123, 084903	3.9	27
172	Current advances in Monte Carlo methods. *Fluid Phase Equilibria*, **1996**, 116, 257-266	2.5	27
171	Phase behavior and structure formation in linear multiblock copolymer solutions by Monte Carlo simulation. *Journal of Chemical Physics*, **2008**, 128, 164906	3.9	26
170	Competing Ranges of Attractive and Repulsive Interactions in the Micellization of Model Surfactants. *Langmuir*, **2003**, 19, 5164-5168	4	26
169	Equilibrium crystal phases of triblock Janus colloids. *Journal of Chemical Physics*, **2016**, 145, 094505	3.9	26
168	When do short-range atomistic machine-learning models fall short?. *Journal of Chemical Physics*, **2021**, 154, 034111	3.9	26
167	Gaussian-Charge Polarizable and Nonpolarizable Models for CO2. *Journal of Physical Chemistry B*, **2016**, 120, 984-94	3.4	25

166	Finite-size scaling study of the vapor-liquid critical properties of confined fluids: Crossover from three dimensions to two dimensions. *Journal of Chemical Physics*, **2010**, 132, 144107	3.9	25
165	Universality of ionic criticality: size- and charge-asymmetric electrolytes. *Physical Review Letters*, **2005**, 95, 195703	7.4	25
164	Structured Nanoparticles from the Self-Assembly of Polymer Blends through Rapid Solvent Exchange. *Langmuir*, **2017**, 33, 6021-6028	4	24
163	Charge correlation effects on ionization of weak polyelectrolytes. *Journal of Physics Condensed Matter*, **2009**, 21, 424113	1.8	24
162	Phase equilibria of binary Lennard-Jones mixtures with cubic equations of state. *Fluid Phase Equilibria*, **1994**, 94, 1-18	2.5	24
161	Porphyrin-Sensitized Evolution of Hydrogen using Dawson and Keplerate Polyoxometalate Photocatalysts. *ChemSusChem*, **2016**, 9, 3213-3219	8.3	23
160	Molecular dynamics simulations of water permeation across Nafion membrane interfaces. *Journal of Physical Chemistry B*, **2014**, 118, 8798-807	3.4	23
159	Dynamics in coarse-grained models for oligomer-grafted silica nanoparticles. *Journal of Chemical Physics*, **2012**, 136, 204904	3.9	23
158	Coarse-Graining of Chain Models in Dissipative Particle Dynamics Simulations *Industrial & Engineering Chemistry Research*, **2011**, 50, 69-77	3.9	23
157	Computer simulations of phase transitions of bulk and confined colloid polymer systems. *Physica A: Statistical Mechanics and Its Applications*, **2006**, 369, 275-290	3.3	23
156	Saddles in the energy landscape: extensivity and thermodynamic formalism. *Physical Review Letters* , **2004**, 92, 035506	7.4	23
155	Molecular simulation of the solubility of carbon dioxide in aqueous solutions of sodium chloride. *Fluid Phase Equilibria*, **2004**, 226, 237-250	2.5	23
154	Phase equilibria in ternary systems with carbon dioxide, water and carboxylic acids at elevated pressures. *Journal of Chemical & Engineering Data*, **1988**, 33, 321-327	2.8	23
153	Thermodynamic signatures and cluster properties of self-assembly in systems with competing interactions. *Soft Matter*, **2017**, 13, 8055-8063	3.6	22
152	A Comparison of the Predictive Capabilities of the Embedded-Atom Method and Modified Embedded-Atom Method Potentials for Lithium. *Journal of Physical Chemistry B*, **2015**, 119, 8960-8	3.4	22
151	Explicit- and implicit-solvent simulations of micellization in surfactant solutions. *Langmuir*, **2015**, 31, 3283-92	4	22
150	Automated crystal characterization with a fast neighborhood graph analysis method. *Soft Matter*, **2018**, 14, 6083-6089	3.6	22
149	Simulations of the structure and dynamics of nanoparticle-based ionic liquids. *Faraday Discussions*, **2012**, 154, 29-40; discussion 81-96, 465-71	3.6	22

148	Monte Carlo simulation of high-pressure phase equilibria in aqueous systems. *Fluid Phase Equilibria*, **1998**, 150-151, 33-40	2.5	22
147	Impact of Branching on the Phase Behavior of Polymers. *Macromolecules*, **2005**, 38, 10596-10604	5.5	22
146	Monte Carlo study of shear-induced alignment of cylindrical micelles in thin films. *Physical Review E*, **2004**, 70, 031501	2.4	22
145	Effect of sequence and intermolecular interactions on the number and nature of low-energy states for simple model proteins. *Journal of Chemical Physics*, **1993**, 98, 3185-3190	3.9	22
144	High-Pressure Phase Equilibria in Ternary Fluid Mixtures with a Supercritical Component. *ACS Symposium Series*, **1987**, 115-129	0.4	22
143	Molecular Modeling of Surfactant Micellization Using Solvent-Accessible Surface Area. *Langmuir*, **2019**, 35, 2443-2450	4	22
142	Phase Equilibria of Water/CO and Water/n-Alkane Mixtures from Polarizable Models. *Journal of Physical Chemistry B*, **2017**, 121, 1386-1395	3.4	21
141	Influence of hydrodynamic interactions on stratification in drying mixtures. *Journal of Chemical Physics*, **2018**, 149, 024902	3.9	21
140	Disappearance of the gas-liquid phase transition for highly charged colloids. *Physical Review Letters* , **2007**, 98, 198301	7.4	21
139	Phase behaviour of polyampholyte chains from grand canonical Monte Carlo simulations. *Molecular Physics*, **2005**, 103, 3031-3044	1.7	21
138	Gibbs ensemble Monte Carlo simulations of coexistence properties of a polarizable potential model of water. *Journal of Chemical Physics*, **2002**, 117, 3522-3523	3.9	21
137	Chain length and density dependence of the chemical potential of lattice polymers. *Journal of Chemical Physics*, **1992**, 97, 6666-6673	3.9	21
136	On the relationship between pairwise fluctuations and thermodynamic derivatives. *Journal of Chemical Physics*, **1986**, 85, 4650-4653	3.9	21
135	Massively parallel chemical potential calculation on graphics processing units. *Computer Physics Communications*, **2012**, 183, 2054-2062	4.2	20
134	Sphere-to-Cylinder Transitions in Thin Films of Diblock Copolymers under Shear: The Role of Wetting Layers. *Macromolecules*, **2012**, 45, 4406-4415	5.5	20
133	Log-rolling micelles in sheared amphiphilic thin films. *Physical Review Letters*, **2005**, 95, 188301	7.4	20
132	Constant-Pressure Monte Carlo Simulations for Lattice Models. *Europhysics Letters*, **1994**, 27, 549-554	1.6	20
131	Customizing wormlike mesoscale structures via self-assembly of amphiphilic star polymers. *Soft Matter*, **2015**, 11, 3530-5	3.6	19

130	Liquid li structure and dynamics: A comparison between OFDFT and second nearest-neighbor embedded-atom method. *AICHE Journal*, **2015**, 61, 2841-2853	3.6	19
129	Ultra thin films of diblock copolymers under shear. *Soft Matter*, **2010**, 6, 3588	3.6	19
128	Effect of stiffness on the micellization behavior of model H4T4 surfactant chains. *Langmuir*, **2006**, 22, 6514-22	4	19
127	Phase transitions and tricriticality in the lattice restricted primitive model supplemented by short-range interactions. *Journal of Chemical Physics*, **2003**, 118, 4993-4998	3.9	19
126	Direct determination of phase coexistence properties of fluids by Monte Carlo simulation in a new ensemble. *Molecular Physics*, **2002**, 100, 237-246	1.7	19
125	Chemical potentials and adsorption isotherms of polymers confined between parallel plates. *Chemical Engineering Science*, **1994**, 49, 2921-2929	4.4	19
124	Self-Assembly of Cylinder-Forming Diblock Copolymer Thin Films. *Macromolecules*, **2013**, 46, 6651-6658	5.5	18
123	Micellar behavior in supercritical solvent–surfactant systems from lattice Monte Carlo simulations. *Fluid Phase Equilibria*, **2002**, 194-197, 233-247	2.5	18
122	Simulations of phase transitions in ionic systems. *Journal of Physics Condensed Matter*, **2005**, 17, S3205-S3213	2.2	18
121	A SANS Study of the Conformational Behavior of Linear Chains in Compressed and Uncompressed End-Linked Elastomers. *Macromolecules*, **2001**, 34, 7773-7782	5.5	18
120	Activity coefficients in nearly athermal model polymer/solvent systems. *AICHE Journal*, **1995**, 41, 2306-2313	3.6	18
119	Evaporation-induced assembly of colloidal crystals. *Journal of Chemical Physics*, **2018**, 149, 094901	3.9	18
118	Directionally Interacting Spheres and Rods Form Ordered Phases. *ACS Nano*, **2017**, 11, 4950-4959	16.7	17
117	Inertial and viscoelastic forces on rigid colloids in microfluidic channels. *Journal of Chemical Physics*, **2015**, 142, 224908	3.9	17
116	Grafted nanoparticles as soft patchy colloids: self-assembly versus phase separation. *Journal of Chemical Physics*, **2015**, 142, 074901	3.9	17
115	Hydration Repulsion between Carbohydrate Surfaces Mediated by Temperature and Specific Ions. *Scientific Reports*, **2016**, 6, 28553	4.9	17
114	Dynamic properties of aqueous electrolyte solutions from non-polarisable, polarisable, and scaled-charge models. *Molecular Physics*, **2019**, 117, 3538-3549	1.7	17
113	Pressure and density scaling for colloid-polymer systems in the protein limit. *Physical Review E*, **2012**, 85, 051402	2.4	17

112	Lattice model of oligonucleotide hybridization in solution. I. Model and thermodynamics. *Journal of Chemical Physics*, **2011**, 134, 165103	3.9	17
111	Monte Carlo simulations of amphiphilic nanoparticle self-assembly. *Journal of Chemical Physics*, **2008**, 129, 194706	3.9	17
110	Molecular Modeling of Thermodynamic and Transport Properties for CO and Aqueous Brines. *Accounts of Chemical Research*, **2017**, 50, 751-758	24.3	16
109	Simulations of activities, solubilities, transport properties, and nucleation rates for aqueous electrolyte solutions. *Journal of Chemical Physics*, **2020**, 153, 010903	3.9	16
108	Shear-induced alignment of lamellae in thin films of diblock copolymers. *Soft Matter*, **2012**, 8, 7803	3.6	16
107	Phase behavior of athermal colloid-star polymer mixtures. *Journal of Chemical Physics*, **2013**, 139, 024907	3.9	16
106	Interactions between charged surfaces with ionizable sites. *Langmuir*, **2011**, 27, 8761-6	4	16
105	Monte Carlo Simulation of the Phase Behavior of Model Dendrimers. *Macromolecules*, **2006**, 39, 6298-6305	3.5	16
104	A conformal solution theory for the energy landscape and glass transition of mixtures. *Fluid Phase Equilibria*, **2006**, 241, 147-154	2.5	16
103	A generalized technique to obtain pure component parameters for two-parameter equations of state. *Fluid Phase Equilibria*, **1985**, 22, 77-88	2.5	16
102	On the Stability of Polymeric Nanoparticles Fabricated through Rapid Solvent Mixing. *Langmuir*, **2019**, 35, 709-717	4	16
101	Controlled production of patchy particles from the combined effects of nanoprecipitation and vitrification. *Soft Matter*, **2017**, 13, 8433-8441	3.6	15
100	Relative stability of the FCC and HCP polymorphs with interacting polymers. *Soft Matter*, **2015**, 11, 280-9	3.6	15
99	Sequential Domain Realignment Driven by Conformational Asymmetry in Block Copolymer Thin Films. *Macromolecules*, **2014**, 47, 1193-1198	5.5	15
98	Structure of phase-separated athermal colloid-polymer systems in the protein limit. *Physical Review E*, **2013**, 87, 022309	2.4	15
97	Diffusivities and Viscosities of Poly(ethylene oxide) Oligomers *Journal of Chemical & Engineering Data*, **2010**, 55, 4273-4280	2.8	15
96	Phase Transitions of Confined Lattice Homopolymers *Journal of Physical Chemistry B*, **2004**, 108, 6809-6815	3.4	15
95	Monte Carlo simulations of free chains in end-linked polymer networks. *Journal of Chemical Physics*, **2001**, 115, 1100-1104	3.9	15

94	Differences in free surfactant concentration and aggregation properties for amphiphiles with the same critical micelle concentration. *Fluid Phase Equilibria*, **2018**, 470, 126-133	2.5	15
93	Palmer et al. reply. *Nature*, **2016**, 531, E2-3	50.4	14
92	Modeling of CO2 solubility in single and mixed electrolyte solutions using statistical associating fluid theory. *Geochimica Et Cosmochimica Acta*, **2016**, 176, 185-197	5.5	14
91	Conformational transitions of weak polyacids grafted to nanoparticles. *Journal of Chemical Physics*, **2012**, 137, 144704	3.9	14
90	Phase Equilibrium of Water with Hexagonal and Cubic Ice Using the SCAN Functional. *Journal of Chemical Theory and Computation*, **2021**, 17, 3065-3077	6.4	14
89	Communication: Nucleation rates of supersaturated aqueous NaCl using a polarizable force field. *Journal of Chemical Physics*, **2018**, 149, 141102	3.9	14
88	Crystal growth kinetics of triblock Janus colloids. *Journal of Chemical Physics*, **2018**, 148, 124506	3.9	13
87	Flow-induced demixing of polymer-colloid mixtures in microfluidic channels. *Journal of Chemical Physics*, **2014**, 140, 094903	3.9	13
86	Phase behavior of low-functionality, telechelic star block copolymers. *Faraday Discussions*, **2010**, 144, 143-57; discussion 203-22, 467-81	3.6	13
85	Molecular simulation of self-assembly in surfactant and protein solutions. *Fluid Phase Equilibria*, **1993**, 82, 251-260	2.5	13
84	Chemical potentials in ionic systems from Monte Carlo simulations with distance-biased test particle insertions. *Fluid Phase Equilibria*, **1993**, 83, 223-231	2.5	13
83	Gibbs-Ensemble Monte Carlo Simulations of Phase Equilibria in Supercritical Fluid Mixtures. *ACS Symposium Series*, **1989**, 39-51	0.4	13
82	Structural and dynamic properties of liquid tin from a new modified embedded-atom method force field. *Physical Review B*, **2017**, 95,	3.3	12
81	Self-Organization and Flow of Low-Functionality Telechelic Star Polymers with Varying Attraction. *ACS Macro Letters*, **2019**, 8, 766-772	6.6	12
80	System-Size Dependence of Electrolyte Activity Coefficients in Molecular Simulations. *Journal of Physical Chemistry B*, **2018**, 122, 3330-3338	3.4	12
79	Self-assembly scenarios of block copolymer stars. *Molecular Physics*, **2011**, 109, 3049-3060	1.7	12
78	Molecular modeling of shear-induced alignment of cylindrical micelles. *Computer Physics Communications*, **2005**, 169, 262-266	4.2	12
77	Monte Carlo Simulations of Polymer Network Deformation. *Macromolecules*, **2001**, 34, 6090-6096	5.5	12

76	Quantitative Lattice Simulations of the Structure and Thermodynamics of Macromolecules. *Macromolecules*, **2001**, 34, 8596-8599	5.5	12
75	Monte Carlo simulations of H2O–CaCl2 and H2O–CaCl2–CO2 mixtures. *Fluid Phase Equilibria*, **2016**, 407, 262-268	2.5	11
74	Viscosity of Nafion oligomers as a function of hydration and counterion type: a molecular dynamics study. *Journal of Physical Chemistry B*, **2014**, 118, 13981-91	3.4	11
73	Multi-atom pattern analysis for binary superlattices. *Soft Matter*, **2017**, 13, 6803-6809	3.6	11
72	Phase diagrams in the lattice restricted primitive model: from order-disorder to gas-liquid phase transition. *Physical Review E*, **2005**, 71, 046118	2.4	11
71	Vapor-liquid equilibrium of water with the MB-pol many-body potential. *Journal of Chemical Physics* , **2021**, 154, 211103	3.9	11
70	Phase separation vs aggregation behavior for model disordered proteins. *Journal of Chemical Physics*, **2021**, 155, 125101	3.9	11
69	Tuning polymer architecture to manipulate the relative stability of different colloid crystal morphologies. *Soft Matter*, **2015**, 11, 5146-53	3.6	10
68	Phase behavior of rigid, amphiphilic star polymers. *Soft Matter*, **2013**, 9, 7424	3.6	10
67	Global phase diagram for the honeycomb potential. *Journal of Chemical Physics*, **2006**, 125, 24505	3.9	10
66	Computational characterization of the sequence landscape in simple protein alphabets. *Proteins: Structure, Function and Bioinformatics*, **2006**, 62, 232-43	4.2	10
65	Dissolving salt is not equivalent to applying a pressure on water.. *Nature Communications*, **2022**, 13, 822	17.4	10
64	Axial dispersion of Brownian colloids in microfluidic channels. *Physical Review Fluids*, **2016**, 1,	2.8	10
63	Note: Activity coefficients and solubilities for the NaCl/? force field. *Journal of Chemical Physics*, **2016**, 145, 046101	3.9	10
62	Micellization and phase separation in binary amphiphile mixtures. *Molecular Physics*, **2009**, 107, 2359-2366	1.7	9
61	Effect of Stiffness on the Phase Behavior of Cubic Lattice Chains. *Macromolecules*, **2005**, 38, 2475-2481	5.5	9
60	Evaluation of a statistical-mechanical virial equation of state, using Gibbs-ensemble molecular simulations. *Fluid Phase Equilibria*, **1991**, 66, 41-55	2.5	9
59	Activity Coefficients and Solubility of CaCl2 from Molecular Simulations. *Journal of Chemical & Engineering Data*, **2020**, 65, 337-348	2.8	9

58	Force Fields for Carbohydrate-Divalent Cation Interactions. *Journal of Physical Chemistry B*, **2016**, 120, 5203-8	3.4	9
57	Diffusivities, viscosities, and conductivities of solvent-free ionically grafted nanoparticles. *Soft Matter*, **2013**, 9, 6091	3.6	8
56	Tracing the critical loci of binary fluid mixtures using molecular simulation. *Journal of Physical Chemistry B*, **2006**, 110, 17200-6	3.4	8
55	Lattice discretization effects on the critical parameters of model nonpolar and polar fluids. *Journal of Chemical Physics*, **2003**, 118, 7556	3.9	8
54	Monte carlo simulations of phase coexistence for polymeric and ionic fluids. *Fluid Phase Equilibria*, **1995**, 104, 185-194	2.5	8
53	Methods Based on Probability Distributions and Histograms. *Springer Series in Chemical Physics*, **2007**, 77-118	0.3	8
52	Genetic Algorithm Driven Force Field Parameterization for Molten Alkali-Metal Carbonate and Hydroxide Salts. *Journal of Chemical Theory and Computation*, **2020**, 16, 5736-5746	6.4	8
51	Polymer Chain Collapse upon Rapid Solvent Exchange: Slip-Spring Dissipative Particle Dynamics Simulations with an Explicit-Solvent Model. *Journal of Physical Chemistry C*, **2017**, 121, 27664-27673	3.8	7
50	Grand-canonical Monte Carlo method for Donnan equilibria. *Physical Review E*, **2012**, 86, 016703	2.4	7
49	Formation of Spherical Micelles in a supercritical Solvent: Lattice Monte Carlo Simulation and Multicomponent Solution Model. *Molecular Simulation*, **2003**, 29, 139-157	2	7
48	Simple lattice model of proteins incorporating directional bonding and structured solvent. *AICHE Journal*, **1995**, 41, 954-958	3.6	7
47	Kumar, Szleifer, and Panagiotopoulos reply. *Physical Review Letters*, **1992**, 68, 3658	7.4	7
46	Molecular simulation of liquid-vapor coexistence for NaCl: Full-charge vs scaled-charge interaction models. *Journal of Chemical Physics*, **2020**, 153, 024501	3.9	7
45	A deep potential model with long-range electrostatic interactions.. *Journal of Chemical Physics*, **2022**, 156, 124107	3.9	7
44	Coarse-graining and phase behavior of model star polymer-colloid mixtures in solvents of varying quality. *Journal of Chemical Physics*, **2015**, 143, 243108	3.9	6
43	Communication: Effect of solvophobic block length on critical micelle concentration in model surfactant systems. *Journal of Chemical Physics*, **2014**, 141, 041101	3.9	6
42	Solvent quality influences surface structure of glassy polymer thin films after evaporation. *Journal of Chemical Physics*, **2017**, 147, 184901	3.9	6
41	Note: Smooth torsional potentials for degenerate dihedral angles. *Journal of Chemical Physics*, **2017**, 146, 226101	3.9	6

40	Phase diagrams of charged colloids from thermodynamic integration. *Journal of Physics Condensed Matter*, **2009**, 21, 465104	1.8	6
39	Determination of second virial coefficients by grand canonical Monte Carlo simulations. *Fluid Phase Equilibria*, **2004**, 222-223, 221-224	2.5	6
38	Grand canonical Monte Carlo simulations of phase equilibria of pure silicon tetrachloride and its binary mixture with carbon dioxide. *Molecular Physics*, **2003**, 101, 3213-3221	1.7	6
37	Thermodynamics of electrolytes on anisotropic lattices. *Physical Review E*, **2003**, 68, 066110	2.4	6
36	Nanostructure formation and phase separation in surfactant solutions. *Advances in Chemical Engineering*, **2001**, 28, 297-311	0.6	6
35	Mixing properties of model polymer/solvent systems. *Journal of Chemical Physics*, **1995**, 103, 10315-10324	3.9	6
34	Unexpected secondary flows in reverse nonequilibrium shear flow simulations. *Physical Review Fluids*, **2019**, 4,	2.8	6
33	Quantized bounding volume hierarchies for neighbor search in molecular simulations on graphics processing units. *Computational Materials Science*, **2019**, 164, 139-146	3.2	5
32	Shear-induced ordering in systems with competing interactions: A machine learning study. *Journal of Chemical Physics*, **2020**, 152, 204905	3.9	5
31	Orientational bonding model for temperature dependent micellization and solubility of diblock surfactants. *Journal of Chemical Physics*, **2009**, 131, 114901	3.9	5
30	Phase Behavior of Binary Stockmayer and Polarizable Lennard-Jones Fluid Mixtures Using Adiabatic Nuclear and Electronic Sampling. *Industrial & Engineering Chemistry Research*, **2006**, 45, 6929-6938	3.9	5
29	Directed assembly of photonic crystals through simple substrate patterning. *Journal of Chemical Physics*, **2019**, 150, 014503	3.9	5
28	Multi-scale simulations of polymeric nanoparticle aggregation during rapid solvent exchange. *Journal of Chemical Physics*, **2018**, 149, 084904	3.9	5
27	Thermodynamic analysis of the stability of planar interfaces between coexisting phases and its application to supercooled water. *Journal of Chemical Physics*, **2019**, 150, 224503	3.9	4
26	Communication: Modeling electrolyte mixtures with concentration dependent dielectric permittivity. *Journal of Chemical Physics*, **2018**, 148, 041102	3.9	4
25	Characterization of the liquid Li-solid Mo (1 1 0) interface from classical molecular dynamics for plasma-facing applications. *Nuclear Fusion*, **2017**, 57, 116036	3.3	4
24	Atomistic simulation of CO2 solubility in poly(ethylene oxide) oligomers. *Molecular Physics*, **2014**, 112, 1540-1547	1.7	4
23	Phase behavior of the lattice restricted primitive model with nearest neighbor exclusion. *Journal of Chemical Physics*, **2006**, 124, 194509	3.9	4

22	Self-Assembly of Polymer Blends and Nanoparticles through Rapid Solvent Exchange. *Langmuir*, **2019**, 35, 3780-3789	4	4
21	Predicting chemical reaction equilibria in molten carbonate fuel cells via molecular simulations. *AICHE Journal*, **2021**, 67, e16988	3.6	4
20	Anomalies and Local Structure of Liquid Water from Boiling to the Supercooled Regime as Predicted by the Many-Body MB-pol Model.. *Journal of Physical Chemistry Letters*, **2022**, 3652-3658	6.4	4
19	Methods for Examining Phase Equilibria. *Springer Series in Chemical Physics*, **2007**, 353-387	0.3	3
18	Molecular Simulation of Phase Equilibria **1994**, 411-437		3
17	Transport and Interfacial Properties of Mixed Molten Carbonate/Hydroxide Electrolytes by Molecular Dynamics Simulations. *Journal of Physical Chemistry C*, **2020**, 124, 23532-23540	3.8	3
16	Individual Ion Activity Coefficients in Aqueous Electrolytes from Explicit-Water Molecular Dynamics Simulations. *Journal of Physical Chemistry B*, **2021**, 125, 8511-8521	3.4	3
15	Transferability of data-driven, many-body models for CO simulations in the vapor and liquid phases.. *Journal of Chemical Physics*, **2022**, 156, 104503	3.9	3
14	Preface: Special Topic on Enhanced Sampling for Molecular Systems. *Journal of Chemical Physics*, **2018**, 149, 072001	3.9	2
13	Phase Behavior of Rigid Objects on a Cubic Lattice*Industrial & Engineering Chemistry Research*, **2006**, 45, 5421-5425	3.9	2
12	Finely discretized lattice simulations of SPC/E water. *Fluid Phase Equilibria*, **2004**, 222-223, 225-230	2.5	2
11	High-pressure phase equilibria in ternary systems of propionic acid and water with ethane, sulfur hexafluoride or refrigerant 13 (chlorotrifluoromethane), 23 (trifluoromethane), or 116 (hexafluoroethane). *Journal of Chemical & Engineering Data*, **1991**, 36, 290-293	2.8	2
10	Modelling Intercalation Kinetics of Polymer Silicate Nanocomposites. *Materials Research Society Symposia Proceedings*, **1998**, 543, 131		1
9	Monte Carlo Simulations of Model Nonionic Surfactants. *Springer Proceedings in Physics*, **2000**, 211-222	0.2	1
8	Liquid-liquid transition in ST2 water		1
7	Model for disordered proteins with strongly sequence-dependent liquid phase behavior		1
6	Phase separation versus aggregation behavior for model disordered proteins		1
5	Activity coefficients of aqueous electrolytes from implicit-water molecular dynamics simulations. *Journal of Chemical Physics*, **2021**, 155, 184501	3.9	0

4	First-Principles Modeling of Transport Mechanisms in Carbonate Hydroxide Electrolytes. *Journal of Physical Chemistry C*, **2021**, 125, 4412-4422	3.8	0
3	Void-Based Assembly of Colloidal Crystals: Using Structure-Directing Agents to Direct the Assembly of Open Colloidal Crystals **2016**, 5, 1-5		
2	High-Resolution Study of Fluid Criticality. *Springer Proceedings in Physics*, **2001**, 167-171	0.2	
1	Molecular Thermodynamic Models for CO2 and Mixtures: Recent Developments and Applications for Process Design **2015**, 361-370		