Athanassios Panagiotopoulos

List of Publications by Year
in descending order

329 papers	21,803 citations	12303 69 h-index	12558 132 g-index
348 all docs	348 docs citations	348 times ranked	10331 citing authors

#	Article	IF	Citations
1	Dissolving salt is not equivalent to applying a pressure on water. Nature Communications, 2022, 13, 822.	5.8	41
2	A deep potential model with long-range electrostatic interactions. Journal of Chemical Physics, 2022, 156, 124107.	1.2	57
3	Transferability of data-driven, many-body models for CO2 simulations in the vapor and liquid phases. Journal of Chemical Physics, 2022, 156, 104503.	1.2	12
4	Activity Coefficients and Solubilities of NaCl in Waterâ€“Methanol Solutions from Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2022, 126, 2891-2898.	1.2	7
5	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, 13, 3652-3658.	2.1	25
6	Liquidâ€“liquid criticality in the WAIL water model. Journal of Chemical Physics, 2022, 157, .	1.2	20
7	Predicting chemical reaction equilibria in molten carbonate fuel cells via molecular simulations. AICHE Journal, 2021, 67, e16988.	1.8	8
8	When do short-range atomistic machine-learning models fall short?. Journal of Chemical Physics, 2021, 154, 034111.	1.2	61
9	First-Principles Modeling of Transport Mechanisms in Carbonateâ€“Hydroxide Electrolytes. Journal of Physical Chemistry C, 2021, 125, 4412-4422.	1.5	3
10	Phase Equilibrium of Water with Hexagonal and Cubic Ice Using the SCAN Functional. Journal of Chemical Theory and Computation, 2021, 17, 3065-3077.	2.3	37
11	Vaporâ€“liquid equilibrium of water with the MB-pol many-body potential. Journal of Chemical Physics, 2021, 154, 211103.	1.2	32
12	Individual Ion Activity Coefficients in Aqueous Electrolytes from Explicit-Water Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2021, 125, 8511-8521.	1.2	21
13	Phase separation vs aggregation behavior for model disordered proteins. Journal of Chemical Physics, 2021, 155, 125101.	1.2	46
14	Activity coefficients of aqueous electrolytes from implicit-water molecular dynamics simulations. Journal of Chemical Physics, 2021, 155, 184501.	1.2	7
15	Activity Coefficients and Solubility of CaCl₂ from Molecular Simulations. Journal of Chemical & Engineering Data, 2020, 65, 337-348.	1.0	13
16	Transport and Interfacial Properties of Mixed Molten Carbonate/Hydroxide Electrolytes by Molecular Dynamics Simulations. Journal of Physical Chemistry C, 2020, 124, 23532-23540.	1.5	7
17	Signatures of a liquidâ€“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.	3.3	112
18	Molecular simulation of liquidâ€“vapor coexistence for NaCl: Full-charge vs scaled-charge interaction models. Journal of Chemical Physics, 2020, 153, 024501.	1.2	10

#	Article	IF	Citations
19	Genetic Algorithm Driven Force Field Parameterization for Molten Alkali-Metal Carbonate and Hydroxide Salts. Journal of Chemical Theory and Computation, 2020, 16, 5736-5746.	2.3	12
20	Shear-induced ordering in systems with competing interactions: A machine learning study. Journal of Chemical Physics, 2020, 152, 204905.	1.2	8
21	Simulations of activities, solubilities, transport properties, and nucleation rates for aqueous electrolyte solutions. Journal of Chemical Physics, 2020, 153, 010903.	1.2	37
22	Model for disordered proteins with strongly sequence-dependent liquid phase behavior. Journal of Chemical Physics, 2020, 152, 075101.	1.2	120
23	Dynamic properties of aqueous electrolyte solutions from non-polarisable, polarisable, and scaled-charge models. Molecular Physics, 2019, 117, 3538-3549.	0.8	30
24	Thermodynamic analysis of the stability of planar interfaces between coexisting phases and its application to supercooled water. Journal of Chemical Physics, 2019, 150, 224503.	1.2	7
25	Self-Organization and Flow of Low-Functionality Telechelic Star Polymers with Varying Attraction. ACS Macro Letters, 2019, 8, 766-772.	2.3	14
26	Quantized bounding volume hierarchies for neighbor search in molecular simulations on graphics processing units. Computational Materials Science, 2019, 164, 139-146.	1.4	12
27	Nucleation in aqueous NaCl solutions shifts from 1-step to 2-step mechanism on crossing the spinodal. Journal of Chemical Physics, 2019, 150, 124502.	1.2	70
28	Self-Assembly of Polymer Blends and Nanoparticles through Rapid Solvent Exchange. Langmuir, 2019, 35, 3780-3789.	1.6	6
29	On the Stability of Polymeric Nanoparticles Fabricated through Rapid Solvent Mixing. Langmuir, 2019, 35, 709-717.	1.6	23
30	Directed assembly of photonic crystals through simple substrate patterning. Journal of Chemical Physics, 2019, 150, 014503.	1.2	5
31	Molecular Modeling of Surfactant Micellization Using Solvent-Accessible Surface Area. Langmuir, 2019, 35, 2443-2450.	1.6	40
32	Unexpected secondary flows in reverse nonequilibrium shear flow simulations. Physical Review Fluids, 2019, 4, .	1.0	7
33	Crystal growth kinetics of triblock Janus colloids. Journal of Chemical Physics, 2018, 148, 124506.	1.2	16
34	Forward flux sampling calculation of homogeneous nucleation rates from aqueous NaCl solutions. Journal of Chemical Physics, 2018, 148, 044505.	1.2	47
35	Comment on â€œThe putative liquid-liquid transition is a liquid-solid transition in atomistic models of waterâ€• [I and II: J. Chem. Phys. 135, 134503 (2011); J. Chem. Phys. 138, 214504 (2013)]. Journal of Chemical Physics, 2018, 148, 137101.	1.2	58
36	Communication: Modeling electrolyte mixtures with concentration dependent dielectric permittivity. Journal of Chemical Physics, 2018, 148, 041102.	1.2	8

#	Article	IF	Citations
37	System-Size Dependence of Electrolyte Activity Coefficients in Molecular Simulations. Journal of Physical Chemistry B, 2018, 122, 3330-3338.	1.2	20
38	Rapid Production of Internally Structured Colloids by Flash Nanoprecipitation of Block Copolymer Blends. ACS Nano, 2018, 12, 4660-4668.	7.3	65
39	Efficient mesoscale hydrodynamics: Multiparticle collision dynamics with massively parallel GPU acceleration. Computer Physics Communications, 2018, 230, 10-20.	3.0	39
40	Differences in free surfactant concentration and aggregation properties for amphiphiles with the same critical micelle concentration. Fluid Phase Equilibria, 2018, 470, 126-133.	1.4	15
41	Communication: Nucleation rates of supersaturated aqueous NaCl using a polarizable force field. Journal of Chemical Physics, 2018, 149, 141102.	1.2	16
42	Evaporation-induced assembly of colloidal crystals. Journal of Chemical Physics, 2018, 149, 094901.	1.2	26
43	Multi-scale simulations of polymeric nanoparticle aggregation during rapid solvent exchange. Journal of Chemical Physics, 2018, 149, 084904.	1.2	11
44	Influence of hydrodynamic interactions on stratification in drying mixtures. Journal of Chemical Physics, 2018, 149, 024902.	1.2	27
45	Automated crystal characterization with a fast neighborhood graph analysis method. Soft Matter, 2018, 14, 6083-6089.	1.2	30
46	Preface: Special Topic on Enhanced Sampling for Molecular Systems. Journal of Chemical Physics, 2018, 149, 072001.	1.2	4
47	Phase Equilibria of Water/CO₂ and Water/n-Alkane Mixtures from Polarizable Models. Journal of Physical Chemistry B, 2017, 121, 1386-1395.	1.2	26
48	Molecular Modeling of Thermodynamic and Transport Properties for CO₂ and Aqueous Brines. Accounts of Chemical Research, 2017, 50, 751-758.	7.6	26
49	Structural and dynamic properties of liquid tin from a new modified embedded-atom method force field. Physical Review B, 2017, 95, .	1.1	22
50	Directionally Interacting Spheres and Rods Form Ordered Phases. ACS Nano, 2017, 11, 4950-4959.	7.3	19
51	Machine learning for autonomous crystal structure identification. Soft Matter, 2017, 13, 4733-4745.	1.2	86
52	Stratification Dynamics in Drying Colloidal Mixtures. Langmuir, 2017, 33, 3685-3693.	1.6	70
53	Structured Nanoparticles from the Self-Assembly of Polymer Blends through Rapid Solvent Exchange. Langmuir, 2017, 33, 6021-6028.	1.6	33
54	Vapourâ€“liquid phase equilibrium and surface tension of fully flexible Lennardâ€“Jones chains. Molecular Physics, 2017, 115, 320-327.	0.8	79

#	Article	IF	Citations
55	Thermodynamic signatures and cluster properties of self-assembly in systems with competing interactions. Soft Matter, 2017, 13, 8055-8063.	1.2	29
56	Controlled production of patchy particles from the combined effects of nanoprecipitation and vitrification. Soft Matter, 2017, 13, 8433-8441.	1.2	17
57	Contact angles from Youngâ€™s equation in molecular dynamics simulations. Journal of Chemical Physics, 2017, 147, 084708.	1.2	48
58	Multi-atom pattern analysis for binary superlattices. Soft Matter, 2017, 13, 6803-6809.	1.2	13
59	Reentrant equilibrium disordering in nanoparticleâ€“polymer mixtures. Npj Computational Materials, 2017, 3, .	3.5	2
60	Characterization of the liquid Li-solid Mo (1â€‰1â€‰0) interface from classical molecular dynamics for plasma-facing applications. Nuclear Fusion, 2017, 57, 116036.	1.6	7
61	Stratification in Drying Polymerâ€“Polymer and Colloidâ€“Polymer Mixtures. Langmuir, 2017, 33, 11390-11398.	1.6	51
62	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.	1.5	9
63	Solvent quality influences surface structure of glassy polymer thin films after evaporation. Journal of Chemical Physics, 2017, 147, 184901.	1.2	11
64	Note: Smooth torsional potentials for degenerate dihedral angles. Journal of Chemical Physics, 2017, 146, 226101.	1.2	8
65	Water: A Tale of Two Liquids. Chemical Reviews, 2016, 116, 7463-7500.	23.0	627
66	Equilibrium crystal phases of triblock Janus colloids. Journal of Chemical Physics, 2016, 145, 094505.	1.2	31
67	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.	1.2	53
68	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.	1.2	80
69	Determination of the critical micelle concentration in simulations of surfactant systems. Journal of Chemical Physics, 2016, 144, 044709.	1.2	44
70	Note: Activity coefficients and solubilities for the NaCl/Ïµ force field. Journal of Chemical Physics, 2016, 145, 046101.	1.2	10
71	Force Fields for Carbohydrateâ€“Divalent Cation Interactions. Journal of Physical Chemistry B, 2016, 120, 5203-5208.	1.2	12
72	Photochemical hydrogen production and cobaloximes: the influence of the cobalt axial N-ligand on the system stability. Dalton Transactions, 2016, 45, 6732-6738.	1.6	84

#	Article	IF	Citations
73	Bottom-Up Colloidal Crystal Assembly with a Twist. ACS Nano, 2016, 10, 5459-5467.	7.3	32
74	Hydration Repulsion between Carbohydrate Surfaces Mediated by Temperature and Specific Ions. Scientific Reports, 2016, 6, 28553.	1.6	21
75	Porphyrinâ€Sensitized Evolution of Hydrogen using Dawson and Keplerate Polyoxometalate Photocatalysts. ChemSusChem, 2016, 9, 3213-3219.	3.6	37
76	Hydrogen-Bonding Polarizable Intermolecular Potential Model for Water. Journal of Physical Chemistry B, 2016, 120, 12358-12370.	1.2	40
77	Monte Carlo simulations of H2Oâ€“CaCl2 and H2Oâ€“CaCl2â€“CO2 mixtures. Fluid Phase Equilibria, 2016, 407, 262-268.	1.4	15
78	Gaussian-Charge Polarizable and Nonpolarizable Models for CO₂. Journal of Physical Chemistry B, 2016, 120, 984-994.	1.2	34
79	Palmer et al. reply. Nature, 2016, 531, E2-E3.	13.7	17
80	Efficient neighbor list calculation for molecular simulation of colloidal systems using graphics processing units. Computer Physics Communications, 2016, 203, 45-52.	3.0	53
81	Modeling of CO2 solubility in single and mixed electrolyte solutions using statistical associating fluid theory. Geochimica Et Cosmochimica Acta, 2016, 176, 185-197.	1.6	22
82	Directed Assembly of Soft Colloids through Rapid Solvent Exchange. ACS Nano, 2016, 10, 1425-1433.	7.3	61
83	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.	1.0	45
84	Axial dispersion of Brownian colloids in microfluidic channels. Physical Review Fluids, 2016, 1, .	1.0	13
85	Void-Based Assembly of Colloidal Crystals: Using Structure-Directing Agents to Direct the Assembly of Open Colloidal Crystals. GIT Laboratory Journal Europe, 2016, 5, 1-5.	0.0	0
86	Liquid li structure and dynamics: A comparison between OFDFT and second nearestâ€neighbor embeddedâ€atom method. AICHE Journal, 2015, 61, 2841-2853.	1.8	24
87	Mean ionic activity coefficients in aqueous NaCl solutions from molecular dynamics simulations. Journal of Chemical Physics, 2015, 142, 044507.	1.2	113
88	Grand Canonical Monte Carlo Simulations Guided by an Analytic Equation of Stateâ€”Transferable Anisotropic Mie Potentials for Ethers. Journal of Physical Chemistry B, 2015, 119, 7087-7099.	1.2	34
89	Atomistic Molecular Dynamics Simulations of Carbohydrateâ€“Calcite Interactions in Concentrated Brine. Langmuir, 2015, 31, 2407-2413.	1.6	55
90	Self-assembly of Janus particles under shear. Soft Matter, 2015, 11, 3767-3771.	1.2	39

#	Article	IF	Citations
91	Thermodynamic and Transport Properties of H₂O + NaCl from Polarizable Force Fields. Journal of Chemical Theory and Computation, 2015, 11, 3802-3810.	2.3	63
92	Customizing wormlike mesoscale structures via self-assembly of amphiphilic star polymers. Soft Matter, 2015, 11, 3530-3535.	1.2	21
93	Atomistic molecular dynamics simulations of H₂O diffusivity in liquid and supercritical CO₂. Molecular Physics, 2015, 113, 2805-2814.	0.8	38
94	Coarse-graining and phase behavior of model star polymerâ€“colloid mixtures in solvents of varying quality. Journal of Chemical Physics, 2015, 143, 243108.	1.2	7
95	Tuning polymer architecture to manipulate the relative stability of different colloid crystal morphologies. Soft Matter, 2015, 11, 5146-5153.	1.2	13
96	Inertial and viscoelastic forces on rigid colloids in microfluidic channels. Journal of Chemical Physics, 2015, 142, 224908.	1.2	18
97	Grafted nanoparticles as soft patchy colloids: Self-assembly versus phase separation. Journal of Chemical Physics, 2015, 142, 074901.	1.2	21
98	Temperature-dependent solubilities and mean ionic activity coefficients of alkali halides in water from molecular dynamics simulations. Journal of Chemical Physics, 2015, 143, 044505.	1.2	76
99	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, 8960-8968.	1.2	27
100	Relative stability of the FCC and HCP polymorphs with interacting polymers. Soft Matter, 2015, 11, 280-289.	1.2	22
101	Explicit- and Implicit-Solvent Simulations of Micellization in Surfactant Solutions. Langmuir, 2015, 31, 3283-3292.	1.6	27
102	Molecular Thermodynamic Models for CO2 and Mixtures: Recent Developments and Applications for Process Design. , 2015, , 361-370.		0
103	Atomistic simulation of CO₂ solubility in poly(ethylene oxide) oligomers. Molecular Physics, 2014, 112, 1540-1547.	0.8	4
104	Flory-Huggins parameter Ï‡, from binary mixtures of Lennard-Jones particles to block copolymer melts. Journal of Chemical Physics, 2014, 140, 054909.	1.2	68
105	Flow-induced demixing of polymer-colloid mixtures in microfluidic channels. Journal of Chemical Physics, 2014, 140, 094903.	1.2	17
106	Molecular simulation of thermodynamic and transport properties for the H2O+NaCl system. Journal of Chemical Physics, 2014, 141, 234507.	1.2	63
107	Self-assembly of polymer-grafted nanoparticles in thin films. Soft Matter, 2014, 10, 786-794.	1.2	72
108	Stabilizing colloidal crystals by leveraging void distributions. Nature Communications, 2014, 5, 4472.	5.8	50

#	Article	IF	Citations
109	Communication: Effect of solvophobic block length on critical micelle concentration in model surfactant systems. Journal of Chemical Physics, 2014, 141, 041101.	1.2	6
110	Viscosity of Nafion Oligomers as a Function of Hydration and Counterion Type: A Molecular Dynamics Study. Journal of Physical Chemistry B, 2014, 118, 13981-13991.	1.2	11
111	Atomistic Molecular Dynamics Simulations of CO₂ Diffusivity in H₂O for a Wide Range of Temperatures and Pressures. Journal of Physical Chemistry B, 2014, 118, 5532-5541.	1.2	83
112	Sequential Domain Realignment Driven by Conformational Asymmetry in Block Copolymer Thin Films. Macromolecules, 2014, 47, 1193-1198.	2.2	18
113	Thin Films of Homopolymers and Cylinder-Forming Diblock Copolymers under Shear. ACS Nano, 2014, 8, 8015-8026.	7.3	33
114	Optimization of Intermolecular Potential Parameters for the CO₂/H₂O Mixture. Journal of Physical Chemistry B, 2014, 118, 11504-11511.	1.2	35
115	Molecular Dynamics Simulations of Water Permeation across Nafion Membrane Interfaces. Journal of Physical Chemistry B, 2014, 118, 8798-8807.	1.2	26
116	Metastable liquidâ€“liquid transition in a molecular model of water. Nature, 2014, 510, 385-388.	13.7	431
117	Self-Assembly of Cylinder-Forming Diblock Copolymer Thin Films. Macromolecules, 2013, 46, 6651-6658.	2.2	21
118	Molecular Dynamics Simulation of SDS and CTAB Micellization and Prediction of Partition Equilibria with COSMOmic. Langmuir, 2013, 29, 11582-11592.	1.6	52
119	Simulations of vaporâ€“liquid phase equilibrium and interfacial tension in the CO₂â€“H₂Oâ€“NaCl system. AICHE Journal, 2013, 59, 3514-3522.	1.8	43
120	Simulations of shear-induced morphological transitions in block copolymers. Soft Matter, 2013, 9, 9960.	1.2	32
121	Molecular Dynamics Simulations of Water Sorption in a Perfluorosulfonic Acid Membrane. Journal of Physical Chemistry B, 2013, 117, 12649-12660.	1.2	40
122	Phase behavior of rigid, amphiphilic star polymers. Soft Matter, 2013, 9, 7424.	1.2	11
123	Diffusivities, viscosities, and conductivities of solvent-free ionically grafted nanoparticles. Soft Matter, 2013, 9, 6091.	1.2	10
124	Structure of phase-separated athermal colloid-polymer systems in the protein limit. Physical Review E, 2013, 87, 022309.	0.8	16
125	Phase behavior of athermal colloid-star polymer mixtures. Journal of Chemical Physics, 2013, 139, 024907.	1.2	18
126	Dynamics of solvent-free grafted nanoparticles. Journal of Chemical Physics, 2012, 136, 044902.	1.2	49

#	Article	IF	Citations
127	A computational investigation of the phase behavior and capillary sublimation of water confined between nanoscale hydrophobic plates. Journal of Chemical Physics, 2012, 137, 144501.	1.2	40
128	Molecular Dynamics Simulations of Silica Nanoparticles Grafted with Poly(ethylene oxide) Oligomer Chains. Journal of Physical Chemistry B, 2012, 116, 2385-2395.	1.2	58
129	Shear-induced alignment of lamellae in thin films of diblock copolymers. Soft Matter, 2012, 8, 7803.	1.2	20
130	Self-assembly of coarse-grained ionic surfactants accelerated by graphics processing units. Soft Matter, 2012, 8, 2385-2397.	1.2	125
131	Massively parallel chemical potential calculation on graphics processing units. Computer Physics Communications, 2012, 183, 2054-2062.	3.0	25
132	Atomistic Simulations of Micellization of Sodium Hexyl, Heptyl, Octyl, and Nonyl Sulfates. Journal of Physical Chemistry B, 2012, 116, 2430-2437.	1.2	76
133	Conformational transitions of weak polyacids grafted to nanoparticles. Journal of Chemical Physics, 2012, 137, 144704.	1.2	19
134	Liquid-liquid transition in ST2 water. Journal of Chemical Physics, 2012, 137, 214505.	1.2	144
135	Simulations of the structure and dynamics of nanoparticle-based ionic liquids. Faraday Discussions, 2012, 154, 29-40.	1.6	25
136	Pressure and density scaling for colloid-polymer systems in the protein limit. Physical Review E, 2012, 85, 051402.	0.8	18
137	Sphere-to-Cylinder Transitions in Thin Films of Diblock Copolymers under Shear: The Role of Wetting Layers. Macromolecules, 2012, 45, 4406-4415.	2.2	23
138	Grand-canonical Monte Carlo method for Donnan equilibria. Physical Review E, 2012, 86, 016703.	0.8	11
139	Dynamics in coarse-grained models for oligomer-grafted silica nanoparticles. Journal of Chemical Physics, 2012, 136, 204904.	1.2	25
140	Coarse-Graining of Chain Models in Dissipative Particle Dynamics Simulations. Industrial & Engineering Chemistry Research, 2011, 50, 69-77.	1.8	26
141	Interactions Between Charged Surfaces with Ionizable Sites. Langmuir, 2011, 27, 8761-8766.	1.6	18
142	Dissipative particle dynamics simulations of polymer-protected nanoparticle self-assembly. Journal of Chemical Physics, 2011, 135, 184903.	1.2	43
143	Lattice model of oligonucleotide hybridization in solution. I. Model and thermodynamics. Journal of Chemical Physics, 2011, 134, 165103.	1.2	20
144	Implicit-Solvent Models for Micellization: Nonionic Surfactants and Temperature-Dependent Properties. Journal of Physical Chemistry B, 2011, 115, 990-1001.	1.2	31

#	Article	IF	Citations
145	Structure of solvent-free grafted nanoparticles: Molecular dynamics and density-functional theory. Journal of Chemical Physics, 2011, 135, 114901.	1.2	49
146	Monte Carlo Simulations of High-Pressure Phase Equilibria of CO₂â€“H₂O Mixtures. Journal of Physical Chemistry B, 2011, 115, 6629-6635.	1.2	45
147	Simulations of Micellization of Sodium Hexyl Sulfate. Journal of Physical Chemistry B, 2011, 115, 1403-1410.	1.2	39
148	Nonlinear dimensionality reduction in molecular simulation: The diffusion map approach. Chemical Physics Letters, 2011, 509, 1-11.	1.2	141
149	Self-assembly scenarios of block copolymer stars. Molecular Physics, 2011, 109, 3049-3060.	0.8	13
150	Structural Transitions of Solvent-Free Oligomer-Grafted Nanoparticles. Physical Review Letters, 2011, 107, 105503.	2.9	53
151	Integrating diffusion maps with umbrella sampling: Application to alanine dipeptide. Journal of Chemical Physics, 2011, 134, 135103.	1.2	64
152	A comparison of implicit- and explicit-solvent simulations of self-assembly in block copolymer and solute systems. Journal of Chemical Physics, 2011, 134, 164902.	1.2	72
153	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, 13597-13602.	3.3	142
154	Micellization behavior of coarse grained surfactant models. Journal of Chemical Physics, 2010, 132, 114902.	1.2	72
155	Diffusivities and Viscosities of Poly(ethylene oxide) Oligomers. Journal of Chemical & Engineering Data, 2010, 55, 4273-4280.	1.0	15
156	An Experimental and Computational Investigation of Spontaneous Lasso Formation in Microcin J25. Biophysical Journal, 2010, 99, 3056-3065.	0.2	58
157	Phase behavior of low-functionality, telechelic star block copolymers. Faraday Discussions, 2010, 144, 143-157.	1.6	14
158	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.	1.2	29
159	Ultra thin films of diblock copolymers under shear. Soft Matter, 2010, 6, 3588.	1.2	21
160	Aggregation phenomena in telechelic star polymer solutions. Physical Review E, 2009, 79, 010401.	0.8	36
161	Micellization and phase separation in binary amphiphile mixtures. Molecular Physics, 2009, 107, 2359-2366.	0.8	14
162	Low-temperature fluid-phase behavior of ST2 water. Journal of Chemical Physics, 2009, 131, 104508.	1.2	139

#	Article	IF	Citations
163	Orientational bonding model for temperature dependent micellization and solubility of diblock surfactants. Journal of Chemical Physics, 2009, 131, 114901.	1.2	5
164	Phase diagrams of charged colloids from thermodynamic integration. Journal of Physics Condensed Matter, 2009, 21, 465104.	0.7	6
165	Anisotropic self-assembly of spherical polymer-grafted nanoparticles. Nature Materials, 2009, 8, 354-359.	13.3	925
166	Electrostatic Screening and Charge Correlation Effects in Micellization of Ionic Surfactants. Journal of Physical Chemistry B, 2009, 113, 6314-6320.	1.2	50
167	Modeling the anisotropic self-assembly of spherical polymer-grafted nanoparticles. Journal of Chemical Physics, 2009, 131, 221102.	1.2	111
168	Charge correlation effects on ionization of weak polyelectrolytes. Journal of Physics Condensed Matter, 2009, 21, 424113.	0.7	29
169	Solubility and Molecular Conformations of n-Alkane Chains in Water. Journal of Physical Chemistry B, 2009, 113, 6405-6414.	1.2	131
170	Protected Peptide Nanoparticles: Experiments and Brownian Dynamics Simulations of the Energetics of Assembly. Nano Letters, 2009, 9, 2218-2222.	4.5	44
171	Structure and Dynamics of Surfactant and Hydrocarbon Aggregates on Graphite: A Molecular Dynamics Simulation Study. Journal of Physical Chemistry B, 2008, 112, 2915-2921.	1.2	44
172	Surfactant and Hydrocarbon Aggregates on Defective Graphite Surface: Structure and Dynamics. Journal of Physical Chemistry B, 2008, 112, 12954-12961.	1.2	31
173	Phase behavior and structure formation in linear multiblock copolymer solutions by Monte Carlo simulation. Journal of Chemical Physics, 2008, 128, 164906.	1.2	31
174	Simulations of phase transitions and free energies for ionic systems. Molecular Physics, 2008, 106, 2039-2051.	0.8	36
175	Implicit Solvent Models for Micellization of Ionic Surfactants. Journal of Physical Chemistry B, 2008, 112, 13783-13792.	1.2	56
176	Coarse-Grained Simulations of Rapid Assembly Kinetics for Polystyrene-b-poly(ethylene oxide) Copolymers in Aqueous Solutions. Journal of Physical Chemistry B, 2008, 112, 16357-16366.	1.2	43
177	Preparation of Poly(ethylene glycol) Protected Nanoparticles with Variable Bioconjugate Ligand Density. Biomacromolecules, 2008, 9, 2705-2711.	2.6	104
178	Composite Block Copolymer Stabilized Nanoparticles:â€‰ Simultaneous Encapsulation of Organic Actives and Inorganic Nanostructures. Langmuir, 2008, 24, 83-90.	1.6	161
179	Monte Carlo simulations of amphiphilic nanoparticle self-assembly. Journal of Chemical Physics, 2008, 129, 194706.	1.2	18
180	Disappearance of the Gas-Liquid Phase Transition for Highly Charged Colloids. Physical Review Letters, 2007, 98, 198301.	2.9	25

#	Article	IF	Citations
181	Effective potentials for 1:1 electrolyte solutions incorporating dielectric saturation and repulsive hydration. Journal of Chemical Physics, 2007, 126, 044509.	1.2	67
182	Monte Carlo simulation and molecular theory of tethered polyelectrolytes. Journal of Chemical Physics, 2007, 126, 244902.	1.2	53
183	Methods for Examining Phase Equilibria. Springer Series in Chemical Physics, 2007, , 353-387.	0.2	4
184	Methods Based on Probability Distributions and Histograms. Springer Series in Chemical Physics, 2007, , 77-118.	0.2	8
185	Monte Carlo Simulations of Micellization in Model Ionic Surfactants:Â Application to Sodium Dodecyl Sulfate. Langmuir, 2006, 22, 4076-4083.	1.6	50
186	Global phase diagram for the honeycomb potential. Journal of Chemical Physics, 2006, 125, 024505.	1.2	10
187	Phase Behavior of Rigid Objects on a Cubic Lattice. Industrial & Engineering Chemistry Research, 2006, 45, 5421-5425.	1.8	2
188	Monte Carlo Simulation of the Phase Behavior of Model Dendrimers. Macromolecules, 2006, 39, 6298-6305.	2.2	16
189	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.	1.8	7
190	Effect of Stiffness on the Micellization Behavior of Model H4T4 Surfactant Chains. Langmuir, 2006, 22, 6514-6522.	1.6	21
191	Tracing the Critical Loci of Binary Fluid Mixtures Using Molecular Simulation. Journal of Physical Chemistry B, 2006, 110, 17200-17206.	1.2	9
192	A conformal solution theory for the energy landscape and glass transition of mixtures. Fluid Phase Equilibria, 2006, 241, 147-154.	1.4	17
193	Computer simulations of phase transitions of bulk and confined colloidâ€“polymer systems. Physica A: Statistical Mechanics and Its Applications, 2006, 369, 275-290.	1.2	26
194	Phase behavior of the lattice restricted primitive model with nearest neighbor exclusion. Journal of Chemical Physics, 2006, 124, 194509.	1.2	4
195	Molecular modeling of shear-induced alignment of cylindrical micelles. Computer Physics Communications, 2005, 169, 262-266.	3.0	12
196	Computational characterization of the sequence landscape in simple protein alphabets. Proteins: Structure, Function and Bioinformatics, 2005, 62, 232-243.	1.5	11
197	Simulations of phase transitions in ionic systems. Journal of Physics Condensed Matter, 2005, 17, S3205-S3213.	0.7	19
198	Critical point of electrolyte mixtures. Journal of Chemical Physics, 2005, 123, 084903.	1.2	28

#	Article	IF	Citations
199	Coarse-grained kinetic computations for rare events: Application to micelle formation. Journal of Chemical Physics, 2005, 122, 044908.	1.2	84
200	Log-Rolling Micelles in Sheared Amphiphilic Thin Films. Physical Review Letters, 2005, 95, 188301.	2.9	22
201	Phase diagrams in the lattice restricted primitive model: From order-disorder to gas-liquid phase transition. Physical Review E, 2005, 71, 046118.	0.8	11
202	Coarse-grained computations for a micellar system. Journal of Chemical Physics, 2005, 122, 044907.	1.2	29
203	Thermodynamic properties of lattice hard-sphere models. Journal of Chemical Physics, 2005, 123, 104504.	1.2	31
204	Effect of Stiffness on the Phase Behavior of Cubic Lattice Chains. Macromolecules, 2005, 38, 2475-2481.	2.2	9
205	Shear Ordering in Thin Films of Spherical Block Copolymer. Langmuir, 2005, 21, 11518-11527.	1.6	35
206	Impact of Branching on the Phase Behavior of Polymers. Macromolecules, 2005, 38, 10596-10604.	2.2	24
207	Phase behaviour of polyampholyte chains from grand canonical Monte Carlo simulations. Molecular Physics, 2005, 103, 3031-3044.	0.8	21
208	Universality of Ionic Criticality: Size- and Charge-Asymmetric Electrolytes. Physical Review Letters, 2005, 95, 195703.	2.9	28
209	Monte Carlo study of shear-induced alignment of cylindrical micelles in thin films. Physical Review E, 2004, 70, 031501.	0.8	24
210	Saddles in the Energy Landscape: Extensivity and Thermodynamic Formalism. Physical Review Letters, 2004, 92, 035506.	2.9	25
211	Flat-Histogram Dynamics and Optimization in Density of States Simulations of Fluidsâ€. Journal of Physical Chemistry B, 2004, 108, 19748-19755.	1.2	34
212	Finely discretized lattice simulations of SPC/E water. Fluid Phase Equilibria, 2004, 222-223, 225-230.	1.4	2
213	Molecular simulation of the solubility of carbon dioxide in aqueous solutions of sodium chloride. Fluid Phase Equilibria, 2004, 226, 237-250.	1.4	29
214	Determination of second virial coefficients by grand canonical Monte Carlo simulations. Fluid Phase Equilibria, 2004, 222-223, 221-224.	1.4	6
215	Phase Transitions of Confined Lattice Homopolymers. Journal of Physical Chemistry B, 2004, 108, 6809-6815.	1.2	15
216	Gibbs Ensemble and Histogram Reweighting Grand Canonical Monte Carlo Methods. , 2004, , .		0

#	Article	IF	Citations
217	Competing Ranges of Attractive and Repulsive Interactions in the Micellization of Model Surfactants. Langmuir, 2003, 19, 5164-5168.	1.6	27
218	Critical parameters of unrestricted primitive model electrolytes with charge asymmetries up to 10:1. Journal of Chemical Physics, 2003, 119, 8526-8536.	1.2	36
219	Formation of Spherical Micelles in a supercritical Solvent: Lattice Monte Carlo Simulation and Multicomponent Solution Model. Molecular Simulation, 2003, 29, 139-157.	0.9	8
220	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.	0.8	6
221	Lattice discretization effects on the critical parameters of model nonpolar and polar fluids. Journal of Chemical Physics, 2003, 118, 7556.	1.2	8
222	Monte Carlo Study of Coulombic Criticality in Polyelectrolytes. Physical Review Letters, 2003, 90, 048303.	2.9	52
223	An improved Monte Carlo method for direct calculation of the density of states. Journal of Chemical Physics, 2003, 119, 9406-9411.	1.2	128
224	Phase transitions and tricriticality in the lattice restricted primitive model supplemented by short-range interactions. Journal of Chemical Physics, 2003, 118, 4993-4998.	1.2	19
225	Thermodynamics of electrolytes on anisotropic lattices. Physical Review E, 2003, 68, 066110.	0.8	6
226	Universality Class of Criticality in the Restricted Primitive Model Electrolyte. Physical Review Letters, 2002, 88, 185701.	2.9	167
227	Generalization of the Wang-Landau method for off-lattice simulations. Physical Review E, 2002, 66, 056703.	0.8	209
228	Coarse bifurcation analysis of kinetic Monte Carlo simulations: A lattice-gas model with lateral interactions. Journal of Chemical Physics, 2002, 117, 8229-8240.	1.2	92
229	Gibbs ensemble Monte Carlo simulations of coexistence properties of a polarizable potential model of water. Journal of Chemical Physics, 2002, 117, 3522-3523.	1.2	22
230	Micellization and Phase Separation of Diblock and Triblock Model Surfactants. Langmuir, 2002, 18, 2940-2948.	1.6	116
231	Ternary oilâ€”waterâ€”amphiphile systems: self-assembly and phase equilibria. Molecular Physics, 2002, 100, 2213-2220.	0.8	29
232	Molecular structural order and anomalies in liquid silica. Physical Review E, 2002, 66, 011202.	0.8	215
233	Phase Transitions in 2:1 and 3:1 Hard-Core Model Electrolytes. Physical Review Letters, 2002, 88, 045701.	2.9	64
234	Critical parameters of the restricted primitive model. Journal of Chemical Physics, 2002, 116, 3007-3011.	1.2	85

#	Article	IF	Citations
235	Self-assembly of surfactants in a supercritical solvent from lattice Monte Carlo simulations. Journal of Chemical Physics, 2002, 116, 1171-1184.	1.2	63
236	Direct determination of phase coexistence properties of fluids by Monte Carlo simulation in a new ensemble. Molecular Physics, 2002, 100, 237-246.	0.8	1,239
237	Dipolar origin of the gas-liquid coexistence of the hard-core 1:1 electrolyte model. Physical Review E, 2002, 66, 041204.	0.8	35
238	Micellar behavior in supercritical solventâ€“surfactant systems from lattice Monte Carlo simulations. Fluid Phase Equilibria, 2002, 194-197, 233-247.	1.4	18
239	Monte Carlo Simulations of Polymer Network Deformation. Macromolecules, 2001, 34, 6090-6096.	2.2	12
240	A SANS Study of the Conformational Behavior of Linear Chains in Compressed and Uncompressed End-Linked Elastomers. Macromolecules, 2001, 34, 7773-7782.	2.2	20
241	Quantitative Lattice Simulations of the Structure and Thermodynamics of Macromolecules. Macromolecules, 2001, 34, 8596-8599.	2.2	12
242	Nanostructure formation and phase separation in surfactant solutions. Advances in Chemical Engineering, 2001, 28, 297-311.	0.5	6
243	Precise simulation of criticality in asymmetric fluids. Physical Review E, 2001, 63, 051507.	0.8	104
244	The heat capacity of the restricted primitive model electrolyte. Journal of Chemical Physics, 2001, 114, 5468-5471.	1.2	34
245	Monte Carlo simulations of free chains in end-linked polymer networks. Journal of Chemical Physics, 2001, 115, 1100-1104.	1.2	16
246	High-Resolution Study of Fluid Criticality. Springer Proceedings in Physics, 2001, , 167-171.	0.1	0
247	Vapor+liquid equilibrium of water, carbon dioxide, and the binary system, water+carbon dioxide, from molecular simulation. Fluid Phase Equilibria, 2000, 170, 203-234.	1.4	140
248	A Monte Carlo study of the structural properties of end-linked polymer networks. Journal of Chemical Physics, 2000, 112, 6910-6916.	1.2	60
249	Coexistence and Criticality in Size-Asymmetric Hard-Core Electrolytes. Physical Review Letters, 2000, 85, 4558-4561.	2.9	113
250	Criticality and crossover in accessible regimes. Physical Review E, 2000, 61, 5930-5939.	0.8	48
251	Monte Carlo methods for phase equilibria of fluids. Journal of Physics Condensed Matter, 2000, 12, R25-R52.	0.7	230
252	Molecular Simulation of Phase Equilibria for Waterâ^'n-Butane and Waterâ^'n-Hexane Mixtures. Journal of Physical Chemistry B, 2000, 104, 4958-4963.	1.2	47

#	Article	IF	Citations
253	On the equivalence of continuum and lattice models for fluids. Journal of Chemical Physics, 2000, 112, 7132-7137.	1.2	77
254	Surface tension of the three-dimensional Lennard-Jones fluid from histogram-reweighting Monte Carlo simulations. Journal of Chemical Physics, 2000, 112, 6411-6415.	1.2	144
255	Monte Carlo Simulations of Model Nonionic Surfactants. Springer Proceedings in Physics, 2000, , 211-222.	0.1	1
256	Thermodynamics of Reversibly Associating Polymer Solutions. Physical Review Letters, 1999, 82, 5060-5063.	2.9	65
257	Large Lattice Discretization Effects on the Phase Coexistence of Ionic Fluids. Physical Review Letters, 1999, 83, 2981-2984.	2.9	99
258	Micellization in Model Surfactant Systems. Langmuir, 1999, 15, 3143-3151.	1.6	190
259	New intermolecular potential models for benzene and cyclohexane. Journal of Chemical Physics, 1999, 111, 9731-9738.	1.2	113
260	A New Intermolecular Potential Model for the n-Alkane Homologous Series. Journal of Physical Chemistry B, 1999, 103, 6314-6322.	1.2	171
261	Molecular simulation of phase equilibria for mixtures of polar and non-polar components. Molecular Physics, 1999, 97, 1073-1083.	0.8	137
262	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.	1.2	231
263	Critical point and phase behavior of the pure fluid and a Lennard-Jones mixture. Journal of Chemical Physics, 1998, 109, 10914-10920.	1.2	347
264	Monte Carlo simulation of high-pressure phase equilibria in aqueous systems. Fluid Phase Equilibria, 1998, 150-151, 33-40.	1.4	25
265	Phase equilibria of the modified Buckingham exponential-6 potential from Hamiltonian scaling grand canonical Monte Carlo. Journal of Chemical Physics, 1998, 109, 1093-1100.	1.2	98
266	A Fixed Point Charge Model for Water Optimized to the Vaporâ^'Liquid Coexistence Properties. Journal of Physical Chemistry B, 1998, 102, 7470-7475.	1.2	178
267	Phase Equilibria of Lattice Polymers from Histogram Reweighting Monte Carlo Simulations. Macromolecules, 1998, 31, 912-918.	2.2	159
268	Molecular Simulation of Phase Equilibria for Waterâ^'Methane and Waterâ^'Ethane Mixtures. Journal of Physical Chemistry B, 1998, 102, 8865-8873.	1.2	115
269	Simulation of polymer melt intercalation in layered nanocomposites. Journal of Chemical Physics, 1998, 109, 10321-10330.	1.2	67
270	Modelling Intercalation Kinetics of Polymer Silicate Nanocomposites. Materials Research Society Symposia Proceedings, 1998, 543, 131.	0.1	1

#	Article	IF	Citations
271	Phase coexistence properties of polarizable water models. Molecular Physics, 1998, 94, 803-808.	0.8	90
272	Phase coexistence properties of polarizable Stockmayer fluids. Journal of Chemical Physics, 1997, 106, 3338-3347.	1.2	56
273	Aggregation Behavior of a Lattice Model for Amphiphiles. Langmuir, 1997, 13, 5022-5031.	1.6	139
274	Liquid-Liquid Immiscibility in Pure Fluids: Polyamorphism in Simulations of a Network-Forming Fluid. Physical Review Letters, 1996, 77, 4386-4389.	2.9	117
275	Effect of Chain Stiffness on Polymer Phase Behavior. Macromolecules, 1996, 29, 4444-4446.	2.2	35
276	Efficient pressure estimation in molecular simulations without evaluating the virial. Journal of Chemical Physics, 1996, 105, 8469-8470.	1.2	78
277	Current advances in Monte Carlo methods. Fluid Phase Equilibria, 1996, 116, 257-266.	1.4	31
278	Phase diagram of the twoâ€dimensional Coulomb gas: A thermodynamic scaling Monte Carlo study. Journal of Chemical Physics, 1996, 104, 7205-7209.	1.2	37
279	Phase equilibria of a lattice model for an oilâ€“waterâ€“amphiphile mixture. Journal of Chemical Physics, 1996, 104, 3718-3725.	1.2	54
280	Thermodynamic scaling Gibbs ensemble Monte Carlo: a new method for determination of phase coexistence properties of fluids. Molecular Physics, 1996, 89, 965-974.	0.8	43
281	Simple lattice model of proteins incorporating directional bonding and structured solvent. AICHE Journal, 1995, 41, 954-958.	1.8	7
282	Activity coefficients in nearly athermal model polymer/solvent systems. AICHE Journal, 1995, 41, 2306-2313.	1.8	18
283	Phase equilibria in ternary Lennard-Jones systems. Fluid Phase Equilibria, 1995, 107, 31-43.	1.4	32
284	Monte carlo simulations of phase coexistence for polymeric and ionic fluids. Fluid Phase Equilibria, 1995, 104, 185-194.	1.4	8
285	Mixing properties of model polymer/solvent systems. Journal of Chemical Physics, 1995, 103, 10315-10324.	1.2	6
286	Liquid-liquid phase transitions in pores. Molecular Physics, 1995, 84, 825-834.	0.8	47
287	Monte Carlo simulations of phase equilibria for a lattice homopolymer model. Journal of Chemical Physics, 1995, 102, 1014-1023.	1.2	63
288	Gibbs Ensemble Techniques. , 1995, , 463-501.		33

#	Article	IF	Citations
289	Constant-Pressure Monte Carlo Simulations for Lattice Models. Europhysics Letters, 1994, 27, 549-554.	0.7	21
290	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.	1.0	137
291	Chemical potentials and adsorption isotherms of polymers confined between parallel plates. Chemical Engineering Science, 1994, 49, 2921-2929.	1.9	20
292	Phase equilibria of binary Lennard-Jones mixtures: simulation and van der Waals l-fluid theory. Fluid Phase Equilibria, 1994, 100, 153-170.	1.4	57
293	Phase equilibria of binary Lennard-Jones mixtures with cubic equations of state. Fluid Phase Equilibria, 1994, 94, 1-18.	1.4	26
294	Reactive canonical Monte Carlo. Molecular Physics, 1994, 81, 717-733.	0.8	191
295	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.	1.2	203
296	Monte Carlo calculation of phase equilibria for a bead-spring polymeric model. Macromolecules, 1994, 27, 400-406.	2.2	114
297	Molecular Simulation of Phase Equilibria. , 1994, , 411-437.		4
298	Molecular simulation of self-assembly in surfactant and protein solutions. Fluid Phase Equilibria, 1993, 82, 251-260.	1.4	13
299	Chemical potentials in ionic systems from Monte Carlo simulations with distance-biased test particle insertions. Fluid Phase Equilibria, 1993, 83, 223-231.	1.4	19
300	Finite-size effects and approach to criticality in Gibbs ensemble simulations. Molecular Physics, 1993, 80, 843-852.	0.8	64
301	Effect of sequence and intermolecular interactions on the number and nature of lowâ€energy states for simple model proteins. Journal of Chemical Physics, 1993, 98, 3185-3190.	1.2	24
302	Chain length and density dependence of the chemical potential of lattice polymers. Journal of Chemical Physics, 1992, 97, 6666-6673.	1.2	22
303	Monte Carlo simulation of folding transitions of simple model proteins using a chain growth algorithm. Journal of Chemical Physics, 1992, 97, 8644-8652.	1.2	73
304	Kumar, Szleifer, and Panagiotopoulos reply. Physical Review Letters, 1992, 68, 3658-3658.	2.9	11
305	Monte Carlo simulation of the collapseâ€coil transition in homopolymers. Journal of Chemical Physics, 1992, 97, 6802-6808.	1.2	50
306	Direct Determination of Fluid Phase Equilibria by Simulation in the Gibbs Ensemble: A Review. Molecular Simulation, 1992, 9, 1-23.	0.9	340

#	Article	IF	Citations
307	Molecular simulation of phase equilibria: simple, ionic and polymeric fluids. Fluid Phase Equilibria, 1992, 76, 97-112.	1.4	125
308	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.	1.0	2
309	Determination of the chemical potentials of polymeric systems from Monte Carlo simulations. Physical Review Letters, 1991, 66, 2935-2938.	2.9	162
310	Evaluation of a statistical-mechanical virial equation of state, using Gibbs-ensemble molecular simulations. Fluid Phase Equilibria, 1991, 66, 41-55.	1.4	9
311	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.	1.4	38
312	How good is conformal solutions theory for phase equilibrium predictions?. Fluid Phase Equilibria, 1991, 65, 1-18.	1.4	93
313	Application of excluded volume map sampling to phase equilibrium calculations in the Gibbs ensemble. Journal of Chemical Physics, 1990, 92, 1285-1293.	1.2	67
314	Phase Equilibria of Quadrupolar Fluids by Simulation in the Gibbs Ensemble. Molecular Simulation, 1989, 2, 147-162.	0.9	52
315	The gibbs method for molecular-based computer simulations of phase equilibria. Fluid Phase Equilibria, 1989, 53, 133-141.	1.4	40
316	Exact calculations of fluid-phase equilibria by Monte Carlo simulation in a new statistical ensemble. International Journal of Thermophysics, 1989, 10, 447-457.	1.0	111
317	Gibbs-Ensemble Monte Carlo Simulations of Phase Equilibria in Supercritical Fluid Mixtures. ACS Symposium Series, 1989, , 39-51.	0.5	14
318	Phase equilibria in ternary systems with carbon dioxide, water and carboxylic acids at elevated pressures. Journal of Chemical & Engineering Data, 1988, 33, 321-327.	1.0	25
319	Phase equilibria by simulation in the Gibbs ensemble. Molecular Physics, 1988, 63, 527-545.	0.8	1,070
320	Adsorption of fluids in model zeolite cavities. Molecular Physics, 1988, 63, 49-63.	0.8	103
321	Adsorption and capillary condensation of fluids in cylindrical pores by Monte Carlo simulation in the Gibbs ensemble. Molecular Physics, 1987, 62, 701-719.	0.8	293
322	High-Pressure Phase Equilibria in Ternary Fluid Mixtures with a Supercritical Component. ACS Symposium Series, 1987, , 115-129.	0.5	28
323	Direct determination of phase coexistence properties of fluids by Monte Carlo simulation in a new ensemble. Molecular Physics, 1987, 61, 813-826.	0.8	1,834
324	Phase diagrams of nonideal fluid mixtures from Monte Carlo simulation. Industrial & Engineering Chemistry Fundamentals, 1986, 25, 525-535.	0.7	66

#	Article	IF	Citations
325	New Mixing Rule for Cubic Equations of State for Highly Polar, Asymmetric Systems. ACS Symposium Series, 1986, , 571-582.	0.5	134
326	Multiphase high pressure equilibria in ternary aqueous systems. Fluid Phase Equilibria, 1986, 29, 525-534.	1.4	78
327	On the relationship between pairwise fluctuations and thermodynamic derivatives. Journal of Chemical Physics, 1986, 85, 4650-4653.	1.2	24
328	A generalized technique to obtain pure component parameters for two-parameter equations of state. Fluid Phase Equilibria, 1985, 22, 77-88.	1.4	18
329	Liquid-liquid transition in ST2 water. , 0, .		1