Athanassios Panagiotopoulos

List of Publications by Year
in descending order

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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	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
2	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
3	Phase equilibria by simulation in the Gibbs ensemble. Molecular Physics, 1988, 63, 527-545.	0.8	1,070
4	Anisotropic self-assembly of spherical polymer-grafted nanoparticles. Nature Materials, 2009, 8, 354-359.	13.3	925
5	Water: A Tale of Two Liquids. Chemical Reviews, 2016, 116, 7463-7500.	23.0	627
6	Metastable liquidâ€“liquid transition in a molecular model of water. Nature, 2014, 510, 385-388.	13.7	431
7	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
8	Direct Determination of Fluid Phase Equilibria by Simulation in the Gibbs Ensemble: A Review. Molecular Simulation, 1992, 9, 1-23.	0.9	340
9	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
10	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
11	Monte Carlo methods for phase equilibria of fluids. Journal of Physics Condensed Matter, 2000, 12, R25-R52.	0.7	230
12	Molecular structural order and anomalies in liquid silica. Physical Review E, 2002, 66, 011202.	0.8	215
13	Generalization of the Wang-Landau method for off-lattice simulations. Physical Review E, 2002, 66, 056703.	0.8	209
14	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
15	Reactive canonical Monte Carlo. Molecular Physics, 1994, 81, 717-733.	0.8	191
16	Micellization in Model Surfactant Systems. Langmuir, 1999, 15, 3143-3151.	1.6	190
17	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
18	A New Intermolecular Potential Model for the n-Alkane Homologous Series. Journal of Physical Chemistry B, 1999, 103, 6314-6322.	1.2	171

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19	Universality Class of Criticality in the Restricted Primitive Model Electrolyte. Physical Review Letters, 2002, 88, 185701.	2.9	167
20	Determination of the chemical potentials of polymeric systems from Monte Carlo simulations. Physical Review Letters, 1991, 66, 2935-2938.	2.9	162
21	Composite Block Copolymer Stabilized Nanoparticles:â€‰ Simultaneous Encapsulation of Organic Actives and Inorganic Nanostructures. Langmuir, 2008, 24, 83-90.	1.6	161
22	Phase Equilibria of Lattice Polymers from Histogram Reweighting Monte Carlo Simulations. Macromolecules, 1998, 31, 912-918.	2.2	159
23	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
24	Liquid-liquid transition in ST2 water. Journal of Chemical Physics, 2012, 137, 214505.	1.2	144
25	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
26	Nonlinear dimensionality reduction in molecular simulation: The diffusion map approach. Chemical Physics Letters, 2011, 509, 1-11.	1.2	141
27	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
28	Aggregation Behavior of a Lattice Model for Amphiphiles. Langmuir, 1997, 13, 5022-5031.	1.6	139
29	Low-temperature fluid-phase behavior of ST2 water. Journal of Chemical Physics, 2009, 131, 104508.	1.2	139
30	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
31	Molecular simulation of phase equilibria for mixtures of polar and non-polar components. Molecular Physics, 1999, 97, 1073-1083.	0.8	137
32	New Mixing Rule for Cubic Equations of State for Highly Polar, Asymmetric Systems. ACS Symposium Series, 1986, , 571-582.	0.5	134
33	Solubility and Molecular Conformations of n-Alkane Chains in Water. Journal of Physical Chemistry B, 2009, 113, 6405-6414.	1.2	131
34	An improved Monte Carlo method for direct calculation of the density of states. Journal of Chemical Physics, 2003, 119, 9406-9411.	1.2	128
35	Molecular simulation of phase equilibria: simple, ionic and polymeric fluids. Fluid Phase Equilibria, 1992, 76, 97-112.	1.4	125
36	Self-assembly of coarse-grained ionic surfactants accelerated by graphics processing units. Soft Matter, 2012, 8, 2385-2397.	1.2	125

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37	Model for disordered proteins with strongly sequence-dependent liquid phase behavior. Journal of Chemical Physics, 2020, 152, 075101.	1.2	120
38	Liquid-Liquid Immiscibility in Pure Fluids: Polyamorphism in Simulations of a Network-Forming Fluid. Physical Review Letters, 1996, 77, 4386-4389.	2.9	117
39	Micellization and Phase Separation of Diblock and Triblock Model Surfactants. Langmuir, 2002, 18, 2940-2948.	1.6	116
40	Molecular Simulation of Phase Equilibria for Waterâ˜Methane and Waterâ˜Ethane Mixtures. Journal of Physical Chemistry B, 1998, 102, 8865-8873.	1.2	115
41	Monte Carlo calculation of phase equilibria for a bead-spring polymeric model. Macromolecules, 1994, 27, 400-406.	2.2	114
42	New intermolecular potential models for benzene and cyclohexane. Journal of Chemical Physics, 1999, 111, 9731-9738.	1.2	113
43	Coexistence and Criticality in Size-Asymmetric Hard-Core Electrolytes. Physical Review Letters, 2000, 85, 4558-4561.	2.9	113
44	Mean ionic activity coefficients in aqueous NaCl solutions from molecular dynamics simulations. Journal of Chemical Physics, 2015, 142, 044507.	1.2	113
45	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
46	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
47	Modeling the anisotropic self-assembly of spherical polymer-grafted nanoparticles. Journal of Chemical Physics, 2009, 131, 221102.	1.2	111
48	Precise simulation of criticality in asymmetric fluids. Physical Review E, 2001, 63, 051507.	0.8	104
49	Preparation of Poly(ethylene glycol) Protected Nanoparticles with Variable Bioconjugate Ligand Density. Biomacromolecules, 2008, 9, 2705-2711.	2.6	104
50	Adsorption of fluids in model zeolite cavities. Molecular Physics, 1988, 63, 49-63.	0.8	103
51	Large Lattice Discretization Effects on the Phase Coexistence of Ionic Fluids. Physical Review Letters, 1999, 83, 2981-2984.	2.9	99
52	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
53	How good is conformal solutions theory for phase equilibrium predictions?. Fluid Phase Equilibria, 1991, 65, 1-18.	1.4	93
54	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

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55	Phase coexistence properties of polarizable water models. Molecular Physics, 1998, 94, 803-808.	0.8	90
56	Machine learning for autonomous crystal structure identification. Soft Matter, 2017, 13, 4733-4745.	1.2	86
57	Critical parameters of the restricted primitive model. Journal of Chemical Physics, 2002, 116, 3007-3011.	1.2	85
58	Coarse-grained kinetic computations for rare events: Application to micelle formation. Journal of Chemical Physics, 2005, 122, 044908.	1.2	84
59	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
60	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
61	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
62	Vapourâ€“liquid phase equilibrium and surface tension of fully flexible Lennardâ€“Jones chains. Molecular Physics, 2017, 115, 320-327.	0.8	79
63	Multiphase high pressure equilibria in ternary aqueous systems. Fluid Phase Equilibria, 1986, 29, 525-534.	1.4	78
64	Efficient pressure estimation in molecular simulations without evaluating the virial. Journal of Chemical Physics, 1996, 105, 8469-8470.	1.2	78
65	On the equivalence of continuum and lattice models for fluids. Journal of Chemical Physics, 2000, 112, 7132-7137.	1.2	77
66	Atomistic Simulations of Micellization of Sodium Hexyl, Heptyl, Octyl, and Nonyl Sulfates. Journal of Physical Chemistry B, 2012, 116, 2430-2437.	1.2	76
67	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
68	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
69	Micellization behavior of coarse grained surfactant models. Journal of Chemical Physics, 2010, 132, 114902.	1.2	72
70	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
71	Self-assembly of polymer-grafted nanoparticles in thin films. Soft Matter, 2014, 10, 786-794.	1.2	72
72	Stratification Dynamics in Drying Colloidal Mixtures. Langmuir, 2017, 33, 3685-3693.	1.6	70

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73	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
74	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
75	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
76	Simulation of polymer melt intercalation in layered nanocomposites. Journal of Chemical Physics, 1998, 109, 10321-10330.	1.2	67
77	Effective potentials for 1:1 electrolyte solutions incorporating dielectric saturation and repulsive hydration. Journal of Chemical Physics, 2007, 126, 044509.	1.2	67
78	Phase diagrams of nonideal fluid mixtures from Monte Carlo simulation. Industrial & Engineering Chemistry Fundamentals, 1986, 25, 525-535.	0.7	66
79	Thermodynamics of Reversibly Associating Polymer Solutions. Physical Review Letters, 1999, 82, 5060-5063.	2.9	65
80	Rapid Production of Internally Structured Colloids by Flash Nanoprecipitation of Block Copolymer Blends. ACS Nano, 2018, 12, 4660-4668.	7.3	65
81	Finite-size effects and approach to criticality in Gibbs ensemble simulations. Molecular Physics, 1993, 80, 843-852.	0.8	64
82	Phase Transitions in 2:1 and 3:1 Hard-Core Model Electrolytes. Physical Review Letters, 2002, 88, 045701.	2.9	64
83	Integrating diffusion maps with umbrella sampling: Application to alanine dipeptide. Journal of Chemical Physics, 2011, 134, 135103.	1.2	64
84	Monte Carlo simulations of phase equilibria for a lattice homopolymer model. Journal of Chemical Physics, 1995, 102, 1014-1023.	1.2	63
85	Self-assembly of surfactants in a supercritical solvent from lattice Monte Carlo simulations. Journal of Chemical Physics, 2002, 116, 1171-1184.	1.2	63
86	Molecular simulation of thermodynamic and transport properties for the H2O+NaCl system. Journal of Chemical Physics, 2014, 141, 234507.	1.2	63
87	Thermodynamic and Transport Properties of H₂O + NaCl from Polarizable Force Fields. Journal of Chemical Theory and Computation, 2015, 11, 3802-3810.	2.3	63
88	Directed Assembly of Soft Colloids through Rapid Solvent Exchange. ACS Nano, 2016, 10, 1425-1433.	7.3	61
89	When do short-range atomistic machine-learning models fall short?. Journal of Chemical Physics, 2021, 154, 034111.	1.2	61
90	A Monte Carlo study of the structural properties of end-linked polymer networks. Journal of Chemical Physics, 2000, 112, 6910-6916.	1.2	60

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91	An Experimental and Computational Investigation of Spontaneous Lasso Formation in Microcin J25. Biophysical Journal, 2010, 99, 3056-3065.	0.2	58
92	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
93	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
94	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
95	A deep potential model with long-range electrostatic interactions. Journal of Chemical Physics, 2022, 156, 124107.	1.2	57
96	Phase coexistence properties of polarizable Stockmayer fluids. Journal of Chemical Physics, 1997, 106, 3338-3347.	1.2	56
97	Implicit Solvent Models for Micellization of Ionic Surfactants. Journal of Physical Chemistry B, 2008, 112, 13783-13792.	1.2	56
98	Atomistic Molecular Dynamics Simulations of Carbohydrateâ€“Calcite Interactions in Concentrated Brine. Langmuir, 2015, 31, 2407-2413.	1.6	55
99	Phase equilibria of a lattice model for an oilâ€“waterâ€“amphiphile mixture. Journal of Chemical Physics, 1996, 104, 3718-3725.	1.2	54
100	Monte Carlo simulation and molecular theory of tethered polyelectrolytes. Journal of Chemical Physics, 2007, 126, 244902.	1.2	53
101	Structural Transitions of Solvent-Free Oligomer-Grafted Nanoparticles. Physical Review Letters, 2011, 107, 105503.	2.9	53
102	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
103	Efficient neighbor list calculation for molecular simulation of colloidal systems using graphics processing units. Computer Physics Communications, 2016, 203, 45-52.	3.0	53
104	Phase Equilibria of Quadrupolar Fluids by Simulation in the Gibbs Ensemble. Molecular Simulation, 1989, 2, 147-162.	0.9	52
105	Monte Carlo Study of Coulombic Criticality in Polyelectrolytes. Physical Review Letters, 2003, 90, 048303.	2.9	52
106	Molecular Dynamics Simulation of SDS and CTAB Micellization and Prediction of Partition Equilibria with COSMOmic. Langmuir, 2013, 29, 11582-11592.	1.6	52
107	Stratification in Drying Polymerâ€“Polymer and Colloidâ€“Polymer Mixtures. Langmuir, 2017, 33, 11390-11398.	1.6	51
108	Monte Carlo simulation of the collapseâ€coil transition in homopolymers. Journal of Chemical Physics, 1992, 97, 6802-6808.	1.2	50

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109	Monte Carlo Simulations of Micellization in Model Ionic Surfactants:Â Application to Sodium Dodecyl Sulfate. Langmuir, 2006, 22, 4076-4083.	1.6	50
110	Electrostatic Screening and Charge Correlation Effects in Micellization of Ionic Surfactants. Journal of Physical Chemistry B, 2009, 113, 6314-6320.	1.2	50
111	Stabilizing colloidal crystals by leveraging void distributions. Nature Communications, 2014, 5, 4472.	5.8	50
112	Structure of solvent-free grafted nanoparticles: Molecular dynamics and density-functional theory. Journal of Chemical Physics, 2011, 135, 114901.	1.2	49
113	Dynamics of solvent-free grafted nanoparticles. Journal of Chemical Physics, 2012, 136, 044902.	1.2	49
114	Criticality and crossover in accessible regimes. Physical Review E, 2000, 61, 5930-5939.	0.8	48
115	Contact angles from Youngâ€™s equation in molecular dynamics simulations. Journal of Chemical Physics, 2017, 147, 084708.	1.2	48
116	Liquid-liquid phase transitions in pores. Molecular Physics, 1995, 84, 825-834.	0.8	47
117	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
118	Forward flux sampling calculation of homogeneous nucleation rates from aqueous NaCl solutions. Journal of Chemical Physics, 2018, 148, 044505.	1.2	47
119	Phase separation vs aggregation behavior for model disordered proteins. Journal of Chemical Physics, 2021, 155, 125101.	1.2	46
120	Monte Carlo Simulations of High-Pressure Phase Equilibria of CO₂â€“H₂O Mixtures. Journal of Physical Chemistry B, 2011, 115, 6629-6635.	1.2	45
121	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
122	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
123	Protected Peptide Nanoparticles: Experiments and Brownian Dynamics Simulations of the Energetics of Assembly. Nano Letters, 2009, 9, 2218-2222.	4.5	44
124	Determination of the critical micelle concentration in simulations of surfactant systems. Journal of Chemical Physics, 2016, 144, 044709.	1.2	44
125	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
126	Dissipative particle dynamics simulations of polymer-protected nanoparticle self-assembly. Journal of Chemical Physics, 2011, 135, 184903.	1.2	43

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127	Simulations of vaporâ€“liquid phase equilibrium and interfacial tension in the CO₂â€“H₂Oâ€“NaCl system. AICHE Journal, 2013, 59, 3514-3522.	1.8	43
128	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
129	Dissolving salt is not equivalent to applying a pressure on water. Nature Communications, 2022, 13, 822.	5.8	41
130	The gibbs method for molecular-based computer simulations of phase equilibria. Fluid Phase Equilibria, 1989, 53, 133-141.	1.4	40
131	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
132	Molecular Dynamics Simulations of Water Sorption in a Perfluorosulfonic Acid Membrane. Journal of Physical Chemistry B, 2013, 117, 12649-12660.	1.2	40
133	Hydrogen-Bonding Polarizable Intermolecular Potential Model for Water. Journal of Physical Chemistry B, 2016, 120, 12358-12370.	1.2	40
134	Molecular Modeling of Surfactant Micellization Using Solvent-Accessible Surface Area. Langmuir, 2019, 35, 2443-2450.	1.6	40
135	Simulations of Micellization of Sodium Hexyl Sulfate. Journal of Physical Chemistry B, 2011, 115, 1403-1410.	1.2	39
136	Self-assembly of Janus particles under shear. Soft Matter, 2015, 11, 3767-3771.	1.2	39
137	Efficient mesoscale hydrodynamics: Multiparticle collision dynamics with massively parallel GPU acceleration. Computer Physics Communications, 2018, 230, 10-20.	3.0	39
138	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
139	Atomistic molecular dynamics simulations of H₂O diffusivity in liquid and supercritical CO₂. Molecular Physics, 2015, 113, 2805-2814.	0.8	38
140	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
141	Porphyrinâ€Sensitized Evolution of Hydrogen using Dawson and Keplerate Polyoxometalate Photocatalysts. ChemSusChem, 2016, 9, 3213-3219.	3.6	37
142	Simulations of activities, solubilities, transport properties, and nucleation rates for aqueous electrolyte solutions. Journal of Chemical Physics, 2020, 153, 010903.	1.2	37
143	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
144	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

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145	Simulations of phase transitions and free energies for ionic systems. Molecular Physics, 2008, 106, 2039-2051.	0.8	36
146	Aggregation phenomena in telechelic star polymer solutions. Physical Review E, 2009, 79, 010401.	0.8	36
147	Effect of Chain Stiffness on Polymer Phase Behavior. Macromolecules, 1996, 29, 4444-4446.	2.2	35
148	Dipolar origin of the gas-liquid coexistence of the hard-core 1:1 electrolyte model. Physical Review E, 2002, 66, 041204.	0.8	35
149	Shear Ordering in Thin Films of Spherical Block Copolymer. Langmuir, 2005, 21, 11518-11527.	1.6	35
150	Optimization of Intermolecular Potential Parameters for the CO₂/H₂O Mixture. Journal of Physical Chemistry B, 2014, 118, 11504-11511.	1.2	35
151	The heat capacity of the restricted primitive model electrolyte. Journal of Chemical Physics, 2001, 114, 5468-5471.	1.2	34
152	Flat-Histogram Dynamics and Optimization in Density of States Simulations of Fluidsâ€. Journal of Physical Chemistry B, 2004, 108, 19748-19755.	1.2	34
153	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
154	Gaussian-Charge Polarizable and Nonpolarizable Models for CO₂. Journal of Physical Chemistry B, 2016, 120, 984-994.	1.2	34
155	Thin Films of Homopolymers and Cylinder-Forming Diblock Copolymers under Shear. ACS Nano, 2014, 8, 8015-8026.	7.3	33
156	Structured Nanoparticles from the Self-Assembly of Polymer Blends through Rapid Solvent Exchange. Langmuir, 2017, 33, 6021-6028.	1.6	33
157	Gibbs Ensemble Techniques. , 1995, , 463-501.		33
158	Phase equilibria in ternary Lennard-Jones systems. Fluid Phase Equilibria, 1995, 107, 31-43.	1.4	32
159	Simulations of shear-induced morphological transitions in block copolymers. Soft Matter, 2013, 9, 9960.	1.2	32
160	Bottom-Up Colloidal Crystal Assembly with a Twist. ACS Nano, 2016, 10, 5459-5467.	7.3	32
161	Vaporâ€"liquid equilibrium of water with the MB-pol many-body potential. Journal of Chemical Physics, 2021, 154, 211103.	1.2	32
162	Current advances in Monte Carlo methods. Fluid Phase Equilibria, 1996, 116, 257-266.	1.4	31

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163	Thermodynamic properties of lattice hard-sphere models. Journal of Chemical Physics, 2005, 123, 104504.	1.2	31
164	Surfactant and Hydrocarbon Aggregates on Defective Graphite Surface: Structure and Dynamics. Journal of Physical Chemistry B, 2008, 112, 12954-12961.	1.2	31
165	Phase behavior and structure formation in linear multiblock copolymer solutions by Monte Carlo simulation. Journal of Chemical Physics, 2008, 128, 164906.	1.2	31
166	Implicit-Solvent Models for Micellization: Nonionic Surfactants and Temperature-Dependent Properties. Journal of Physical Chemistry B, 2011, 115, 990-1001.	1.2	31
167	Equilibrium crystal phases of triblock Janus colloids. Journal of Chemical Physics, 2016, 145, 094505.	1.2	31
168	Automated crystal characterization with a fast neighborhood graph analysis method. Soft Matter, 2018, 14, 6083-6089.	1.2	30
169	Dynamic properties of aqueous electrolyte solutions from non-polarisable, polarisable, and scaled-charge models. Molecular Physics, 2019, 117, 3538-3549.	0.8	30
170	Ternary oilâ€"waterâ€"amphiphile systems: self-assembly and phase equilibria. Molecular Physics, 2002, 100, 2213-2220.	0.8	29
171	Molecular simulation of the solubility of carbon dioxide in aqueous solutions of sodium chloride. Fluid Phase Equilibria, 2004, 226, 237-250.	1.4	29
172	Coarse-grained computations for a micellar system. Journal of Chemical Physics, 2005, 122, 044907.	1.2	29
173	Charge correlation effects on ionization of weak polyelectrolytes. Journal of Physics Condensed Matter, 2009, 21, 424113.	0.7	29
174	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
175	Thermodynamic signatures and cluster properties of self-assembly in systems with competing interactions. Soft Matter, 2017, 13, 8055-8063.	1.2	29
176	High-Pressure Phase Equilibria in Ternary Fluid Mixtures with a Supercritical Component. ACS Symposium Series, 1987, , 115-129.	0.5	28
177	Critical point of electrolyte mixtures. Journal of Chemical Physics, 2005, 123, 084903.	1.2	28
178	Universality of Ionic Criticality: Size- and Charge-Asymmetric Electrolytes. Physical Review Letters, 2005, 95, 195703.	2.9	28
179	Competing Ranges of Attractive and Repulsive Interactions in the Micellization of Model Surfactants. Langmuir, 2003, 19, 5164-5168.	1.6	27
180	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

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181	Explicit- and Implicit-Solvent Simulations of Micellization in Surfactant Solutions. Langmuir, 2015, 31, 3283-3292.	1.6	27
182	Influence of hydrodynamic interactions on stratification in drying mixtures. Journal of Chemical Physics, 2018, 149, 024902.	1.2	27
183	Phase equilibria of binary Lennard-Jones mixtures with cubic equations of state. Fluid Phase Equilibria, 1994, 94, 1-18.	1.4	26
184	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
185	Coarse-Graining of Chain Models in Dissipative Particle Dynamics Simulations. Industrial & Engineering Chemistry Research, 2011, 50, 69-77.	1.8	26
186	Molecular Dynamics Simulations of Water Permeation across Nafion Membrane Interfaces. Journal of Physical Chemistry B, 2014, 118, 8798-8807.	1.2	26
187	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
188	Molecular Modeling of Thermodynamic and Transport Properties for CO₂ and Aqueous Brines. Accounts of Chemical Research, 2017, 50, 751-758.	7.6	26
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