Pablo Debenedetti

List of Publications by Year
in descending order

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326 papers	28,978 citations	4658 85 h-index	5988 160 g-index
344 all docs	344 docs citations	344 times ranked	15270 citing authors

#	Article	IF	Citations
1	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.	4.6	25
2	Liquidâ€“liquid criticality in the WAIL water model. Journal of Chemical Physics, 2022, 157, .	3.0	20
3	Thermodynamics of DNA Hybridization from Atomistic Simulations. Journal of Physical Chemistry B, 2021, 125, 771-779.	2.6	15
4	Phase Equilibrium of Water with Hexagonal and Cubic Ice Using the SCAN Functional. Journal of Chemical Theory and Computation, 2021, 17, 3065-3077.	5.3	37
5	Effects of Trehalose on Lipid Membranes under Rapid Cooling using All-Atom and Coarse-Grained Molecular Simulations. Journal of Physical Chemistry B, 2021, 125, 5346-5357.	2.6	3
6	Manifestations of metastable criticality in the long-range structure of model water glasses. Nature Communications, 2021, 12, 3398.	12.8	14
7	Effect of configuration-dependent multi-body forces on interconversion kinetics of a chiral tetramer model. Journal of Chemical Physics, 2021, 155, 084105.	3.0	8
8	Thermodynamics and kinetics of crystallization in deeply supercooled Stillingerâ€“Weber silicon. Journal of Chemical Physics, 2021, 155, 194502.	3.0	7
9	Interconversion-controlled liquidâ€“liquid phase separation in a molecular chiral model. Journal of Chemical Physics, 2021, 155, 204502.	3.0	9
10	A Computational Study of RNA Tetraloop Thermodynamics, Including Misfolded States. Journal of Physical Chemistry B, 2021, 125, 13685-13695.	2.6	5
11	Computational investigation of retroâ€isomer equilibrium structures: Intrinsically disordered, foldable, and cyclic peptides. FEBS Letters, 2020, 594, 104-113.	2.8	4
12	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.	7.1	112
13	Second critical point in two realistic models of water. Science, 2020, 369, 289-292.	12.6	176
14	Genetic Algorithm Approach for the Optimization of Protein Antifreeze Activity Using Molecular Simulations. Journal of Chemical Theory and Computation, 2020, 16, 7866-7873.	5.3	4
15	Stability of Protein Structure during Nanocarrier Encapsulation: Insights on Solvent Effects from Simulations and Spectroscopic Analysis. ACS Nano, 2020, 14, 16962-16972.	14.6	1
16	The Handedness of DNA Assembly around Carbon Nanotubes Is Determined by the Chirality of DNA. Journal of Physical Chemistry B, 2020, 124, 5362-5369.	2.6	6
17	Insights into Hydrophobic Ion Pairing from Molecular Simulation and Experiment. ACS Nano, 2020, 14, 6097-6106.	14.6	18
18	Preparation of Microparticulates Using Supercritical Fluids. , 2020, , 89-125.		2

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19	Waterâ€™s two-critical-point scenario in the Ising paradigm. Journal of Chemical Physics, 2019, 150, 244509.	3.0	19
20	A computational investigation of the thermodynamics of the Stillinger-Weber family of models at supercooled conditions. Molecular Physics, 2019, 117, 3254-3268.	1.7	9
21	Computational Investigation of the Effect of Backbone Chiral Inversions on Polypeptide Structure. Biophysical Journal, 2019, 116, 46a.	0.5	1
22	Thermodynamic analysis of the stability of planar interfaces between coexisting phases and its application to supercooled water. Journal of Chemical Physics, 2019, 150, 224503.	3.0	7
23	Nucleation in aqueous NaCl solutions shifts from 1-step to 2-step mechanism on crossing the spinodal. Journal of Chemical Physics, 2019, 150, 124502.	3.0	70
24	Computational Investigation of the Effect of Pressure on Protein Stability. Journal of Physical Chemistry Letters, 2019, 10, 1894-1899.	4.6	11
25	Effect of heterochiral inversions on the structure of a Î²â€hairpin peptide. Proteins: Structure, Function and Bioinformatics, 2019, 87, 569-578.	2.6	9
26	Pattern of property extrema in supercooled and stretched water models and a new correlation for predicting the stability limit of the liquid state. Journal of Chemical Physics, 2019, 150, 064503.	3.0	9
27	Low temperature protein refolding suggested by molecular simulation. Journal of Chemical Physics, 2019, 151, 185101.	3.0	13
28	Forward flux sampling calculation of homogeneous nucleation rates from aqueous NaCl solutions. Journal of Chemical Physics, 2018, 148, 044505.	3.0	47
29	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.	3.0	58
30	A Computational Study of the Ionic Liquid-Induced Destabilization of the Miniprotein Trp-Cage. Journal of Physical Chemistry B, 2018, 122, 5707-5715.	2.6	8
31	Cavitation transition in the energy landscape: Distinct tensile yielding behavior in strongly and weakly attractive systems. Journal of Chemical Physics, 2018, 148, 114501.	3.0	6
32	Waterâ€™s Thermal Pressure Drives the Temperature Dependence of Hydrophobic Hydration. Journal of Physical Chemistry B, 2018, 122, 3620-3625.	2.6	8
33	Combined molecular dynamics and neural network method for predicting protein antifreeze activity. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, 13252-13257.	7.1	40
34	Communication: Nucleation rates of supersaturated aqueous NaCl using a polarizable force field. Journal of Chemical Physics, 2018, 149, 141102.	3.0	16
35	Computational Investigation of the Effect of Backbone Chiral Inversions on Polypeptide Structure. Journal of Physical Chemistry B, 2018, 122, 6357-6363.	2.6	10
36	Advances in Computational Studies of the Liquidâ€“Liquid Transition in Water and Water-Like Models. Chemical Reviews, 2018, 118, 9129-9151.	47.7	152

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37	Microscopic Origin of Hysteresis in Water Sorption on Protein Matrices. Journal of Physical Chemistry Letters, 2017, 8, 1185-1190.	4.6	3
38	Structural and dynamic properties of liquid tin from a new modified embedded-atom method force field. Physical Review B, 2017, 95, .	3.2	22
39	Molecular modeling and structural characterization of a high glycineâ€“tyrosine hair keratin associated protein. Physical Chemistry Chemical Physics, 2017, 19, 8575-8583.	2.8	16
40	Effect of material flexibility on the thermodynamics and kinetics of hydrophobically induced evaporation of water. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, E2548-E2555.	7.1	56
41	Computational investigation of surface freezing in a molecular model of water. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, 3316-3321.	7.1	58
42	Two-structure thermodynamics for the TIP4P/2005 model of water covering supercooled and deeply stretched regions. Journal of Chemical Physics, 2017, 146, 034502.	3.0	107
43	Thermodynamic Anomalies in Stretched Water. Langmuir, 2017, 33, 11771-11778.	3.5	27
44	Effects of disulfide bridges and backbone connectivity on water sorption by protein matrices. Scientific Reports, 2017, 7, 7957.	3.3	4
45	Characterization of the liquid Li-solid Mo (1â€‰1â€‰0) interface from classical molecular dynamics for plasma-facing applications. Nuclear Fusion, 2017, 57, 116036.	3.5	7
46	Perspective: Surface freezing in water: A nexus of experiments and simulations. Journal of Chemical Physics, 2017, 147, 060901.	3.0	24
47	A free energy study of the liquid-liquid phase transition of the Jagla two-scale potential. Journal of Chemical Sciences, 2017, 129, 801-823.	1.5	14
48	Chemical physics of water. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, 13325-13326.	7.1	13
49	Communication: Relationship between local structure and the stability of water in hydrophobic confinement. Journal of Chemical Physics, 2017, 147, 241102.	3.0	13
50	Water anomalous thermodynamics, attraction, repulsion, and hydrophobic hydration. Journal of Chemical Physics, 2016, 144, 164501.	3.0	14
51	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.	3.0	80
52	Molecular model for chirality phenomena. Journal of Chemical Physics, 2016, 145, 154503.	3.0	20
53	Two-state thermodynamics and the possibility of a liquid-liquid phase transition in supercooled TIP4P/2005 water. Journal of Chemical Physics, 2016, 144, 144504.	3.0	145
54	A cavitation transition in the energy landscape of simple cohesive liquids and glasses. Journal of Chemical Physics, 2016, 145, 211905.	3.0	7

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55	Computational investigation of cold denaturation in the Trp-cage miniprotein. Proceedings of the National Academy of Sciences of the United States of America, 2016, 113, 8991-8996.	7.1	48
56	Computational investigation of dynamical transitions in Trp-cage miniprotein powders. Scientific Reports, 2016, 6, 25612.	3.3	15
57	Density and bond-orientational relaxations in supercooled water. Molecular Physics, 2016, 114, 2580-2585.	1.7	14
58	Concentration Fluctuations and Capacitive Response in Dense Ionic Solutions. Journal of Physical Chemistry Letters, 2016, 7, 2333-2338.	4.6	60
59	Formation of cyclopentane methane binary clathrate hydrate in brine solutions. Chemical Engineering Science, 2016, 141, 125-132.	3.8	61
60	Palmer et al. reply. Nature, 2016, 531, E2-E3.	27.8	17
61	Computational investigation of structure, dynamics and nucleation kinetics of a family of modified Stillingerâ€“Weber model fluids in bulk and free-standing thin films. Physical Chemistry Chemical Physics, 2016, 18, 4102-4111.	2.8	28
62	Thermodynamic and kinetic anisotropies in octane thin films. Journal of Chemical Physics, 2015, 143, 214501.	3.0	18
63	Liquid li structure and dynamics: A comparison between OFDFT and second nearestâ€neighbor embeddedâ€atom method. AICHE Journal, 2015, 61, 2841-2853.	3.6	24
64	A Computational Study of the Effect of Matrix Structural Order on Water Sorption by Trp-Cage Miniproteins. Journal of Physical Chemistry B, 2015, 119, 1847-1856.	2.6	9
65	Recent advances in molecular simulation: A chemical engineering perspective. AICHE Journal, 2015, 61, 370-383.	3.6	53
66	Anomalous Capacitance Maximum of the Glassy Carbonâ€“Ionic Liquid Interface through Dilution with Organic Solvents. Journal of Physical Chemistry Letters, 2015, 6, 2644-2648.	4.6	69
67	Direct calculation of ice homogeneous nucleation rate for a molecular model of water. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, 10582-10588.	7.1	199
68	Pathways to dewetting in hydrophobic confinement. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, 8181-8186.	7.1	95
69	Systematic characterization of protein folding pathways using diffusion maps: Application to Trp-cage miniprotein. Journal of Chemical Physics, 2015, 142, 085101.	3.0	53
70	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.	2.6	27
71	The effect of substrate on thermodynamic and kinetic anisotropies in atomic thin films. Journal of Chemical Physics, 2014, 141, 024506.	3.0	34
72	The role of material flexibility on the drying transition of water between hydrophobic objects: A thermodynamic analysis. Journal of Chemical Physics, 2014, 141, 18C531.	3.0	25

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73	Two-state thermodynamics of the ST2 model for supercooled water. Journal of Chemical Physics, 2014, 140, 104502.	3.0	96
74	Suppression of sub-surface freezing in free-standing thin films of a coarse-grained model of water. Physical Chemistry Chemical Physics, 2014, 16, 25916-25927.	2.8	65
75	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.	2.6	11
76	Formation kinetics of cyclopentaneâ€“methane binary clathrate hydrate. Chemical Engineering Science, 2014, 119, 147-157.	3.8	37
77	Molecular Dynamics Simulations of Water Permeation across Nafion Membrane Interfaces. Journal of Physical Chemistry B, 2014, 118, 8798-8807.	2.6	26
78	Computational Study of the Stability of the Miniprotein Trp-Cage, the GB1 Î²-Hairpin, and the AK16 Peptide, under Negative Pressure. Journal of Physical Chemistry B, 2014, 118, 7761-7769.	2.6	37
79	Metastable liquidâ€“liquid transition in a molecular model of water. Nature, 2014, 510, 385-388.	27.8	431
80	Simulations of vaporâ€“liquid phase equilibrium and interfacial tension in the CO₂â€“H₂Oâ€“NaCl system. AICHE Journal, 2013, 59, 3514-3522.	3.6	43
81	Molecular Dynamics Simulations of Water Sorption in a Perfluorosulfonic Acid Membrane. Journal of Physical Chemistry B, 2013, 117, 12649-12660.	2.6	40
82	A computational investigation of attrition-enhanced chiral symmetry breaking in conglomerate crystals. Journal of Chemical Physics, 2013, 139, 174503.	3.0	27
83	The liquidâ€“liquid transition in supercooled ST2 water: a comparison between umbrella sampling and well-tempered metadynamics. Faraday Discussions, 2013, 167, 77.	3.2	85
84	Glass Transition Thermodynamics and Kinetics. Annual Review of Condensed Matter Physics, 2013, 4, 263-285.	14.5	217
85	Creation and Persistence of Chiral Asymmetry in a Microscopically Reversible Molecular Model. Journal of Physical Chemistry B, 2013, 117, 602-614.	2.6	10
86	Stretched to the limit. Nature Physics, 2013, 9, 7-8.	16.7	12
87	Temperature and length scale dependence of solvophobic solvation in a single-site water-like liquid. Journal of Chemical Physics, 2013, 138, 064506.	3.0	15
88	Relaxation processes in liquids: Variations on a theme by Stokes and Einstein. Journal of Chemical Physics, 2013, 138, 12A526.	3.0	83
89	A Coarse-Grained Protein Model in a Water-like Solvent. Scientific Reports, 2013, 3, 1841.	3.3	12
90	Modeling simple amphiphilic solutes in a Jagla solvent. Journal of Chemical Physics, 2012, 136, 044511.	3.0	18

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91	Molecular modeling of mechanical stresses on proteins in glassy matrices: Formalism. Journal of Chemical Physics, 2012, 137, 035103.	3.0	16
92	A computational investigation of the phase behavior and capillary sublimation of water confined between nanoscale hydrophobic plates. Journal of Chemical Physics, 2012, 137, 144501.	3.0	40
93	Thermal Stability of Hydrophobic Helical Oligomers: A Lattice Simulation Study in Explicit Water. Journal of Physical Chemistry B, 2012, 116, 9963-9970.	2.6	0
94	Free Energy Barriers to Evaporation of Water in Hydrophobic Confinement. Journal of Physical Chemistry B, 2012, 116, 13282-13289.	2.6	62
95	Evaporation rate of water in hydrophobic confinement. Proceedings of the National Academy of Sciences of the United States of America, 2012, 109, 4365-4370.	7.1	150
96	Massively parallel chemical potential calculation on graphics processing units. Computer Physics Communications, 2012, 183, 2054-2062.	7.5	25
97	Phase Behavior of a Lattice Hydrophobic Oligomer in Explicit Water. Journal of Physical Chemistry B, 2012, 116, 9540-9548.	2.6	3
98	Role of Hydrophobic Hydration in Protein Stability: A 3D Water-Explicit Protein Model Exhibiting Cold and Heat Denaturation. Journal of Physical Chemistry B, 2012, 116, 8095-8104.	2.6	52
99	Computational Studies of Pressure, Temperature, and Surface Effects on the Structure and Thermodynamics of Confined Water. Annual Review of Physical Chemistry, 2012, 63, 179-200.	10.8	120
100	Liquid-liquid transition in ST2 water. Journal of Chemical Physics, 2012, 137, 214505.	3.0	144
101	Computer Simulation of Water Sorption on Flexible Protein Crystals. Journal of Physical Chemistry Letters, 2012, 3, 2713-2718.	4.6	16
102	Homogeneous Nucleation of Methane Hydrate in Microsecond Molecular Dynamics Simulations. Journal of Physical Chemistry Letters, 2012, 3, 2942-2947.	4.6	156
103	Hydrogen bond strength and network structure effects on hydration of non-polar molecules. Physical Chemistry Chemical Physics, 2011, 13, 2748-2757.	2.8	28
104	Non-monotonic dependence of water reorientation dynamics on surface hydrophilicity: competing effects of the hydration structure and hydrogen-bond strength. Physical Chemistry Chemical Physics, 2011, 13, 19911.	2.8	60
105	Dissecting the Energetics of Hydrophobic Hydration of Polypeptides. Journal of Physical Chemistry B, 2011, 115, 14859-14865.	2.6	34
106	Tribute to H. Eugene Stanley. Journal of Physical Chemistry B, 2011, 115, 13963-13964.	2.6	0
107	Evaporation Length Scales of Confined Water and Some Common Organic Liquids. Journal of Physical Chemistry Letters, 2011, 2, 1000-1003.	4.6	48
108	Properties of model atomic free-standing thin films. Journal of Chemical Physics, 2011, 134, 114524.	3.0	38

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109	Structure, dynamics, and thermodynamics of a family of potentials with tunable softness. Journal of Chemical Physics, 2011, 135, 084513.	3.0	34
110	Molecular Dynamics Study of Carbon Dioxide Hydrate Dissociation. Journal of Physical Chemistry A, 2011, 115, 6102-6111.	2.5	107
111	Monte Carlo Simulations of High-Pressure Phase Equilibria of CO₂â€“H₂O Mixtures. Journal of Physical Chemistry B, 2011, 115, 6629-6635.	2.6	45
112	Waterlike glass polyamorphism in a monoatomic isotropic Jagla model. Journal of Chemical Physics, 2011, 134, 064507.	3.0	46
113	Physics and chemistry of water and ice. Physical Chemistry Chemical Physics, 2011, 13, 19660.	2.8	12
114	Structure and Energetics of Thin Film Water. Journal of Physical Chemistry C, 2011, 115, 4624-4635.	3.1	33
115	Nonlinear dimensionality reduction in molecular simulation: The diffusion map approach. Chemical Physics Letters, 2011, 509, 1-11.	2.6	141
116	Integrating diffusion maps with umbrella sampling: Application to alanine dipeptide. Journal of Chemical Physics, 2011, 134, 135103.	3.0	64
117	Properties of Liquids Made from Modified Water Models. , 2010, , 89-99.		0
118	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.	7.1	142
119	An Experimental and Computational Investigation of Spontaneous Lasso Formation in Microcin J25. Biophysical Journal, 2010, 99, 3056-3065.	0.5	58
120	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.	3.0	29
121	Chiral symmetry breaking in a microscopic model with asymmetric autocatalysis and inhibition. Journal of Chemical Physics, 2010, 133, 224502.	3.0	19
122	Enhanced surface hydrophobicity by coupling of surface polarity and topography. Proceedings of the National Academy of Sciences of the United States of America, 2009, 106, 15181-15185.	7.1	106
123	Low-temperature fluid-phase behavior of ST2 water. Journal of Chemical Physics, 2009, 131, 104508.	3.0	139
124	Hydrate Molecular Ballet. Science, 2009, 326, 1070-1071.	12.6	24
125	Thermodynamic mechanism for solution phase chiral amplification via a lattice model. Proceedings of the National Academy of Sciences of the United States of America, 2009, 106, 15131-15135.	7.1	28
126	Phase Transitions Induced by Nanoconfinement in Liquid Water. Physical Review Letters, 2009, 102, 050603.	7.8	208

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127	Effect of Surface Polarity on the Structure and Dynamics of Water in Nanoscale Confinement. Journal of Physical Chemistry B, 2009, 113, 1438-1446.	2.6	143
128	Evolution from Surface-Influenced to Bulk-Like Dynamics in Nanoscopically Confined Water. Journal of Physical Chemistry B, 2009, 113, 7973-7976.	2.6	97
129	Structural and mechanical properties of glassy water in nanoscale confinement. Faraday Discussions, 2009, 141, 359-376.	3.2	49
130	Structureâ€“energy relations in hen egg white lysozyme observed during refolding from a quenched unfolded state. Chemical Communications, 2009, , 4441.	4.1	10
131	Solubility and Molecular Conformations of n-Alkane Chains in Water. Journal of Physical Chemistry B, 2009, 113, 6405-6414.	2.6	131
132	Effect of Temperature on the Structure and Phase Behavior of Water Confined by Hydrophobic, Hydrophilic, and Heterogeneous Surfaces. Journal of Physical Chemistry B, 2009, 113, 13723-13734.	2.6	155
133	Hydrophobicity of protein surfaces: Separating geometry from chemistry. Proceedings of the National Academy of Sciences of the United States of America, 2008, 105, 2274-2279.	7.1	242
134	The effect of sequence on the conformational stability of a model heteropolymer in explicit water. Journal of Chemical Physics, 2008, 128, 175102.	3.0	15
135	A computational investigation of thermodynamics, structure, dynamics and solvation behavior in modified water models. Journal of Chemical Physics, 2008, 128, 124511.	3.0	134
136	Lindemann measures for the solid-liquid phase transition. Journal of Chemical Physics, 2007, 126, 204508.	3.0	83
137	Water-like solvation thermodynamics in a spherically symmetric solvent model with two characteristic lengths. Proceedings of the National Academy of Sciences of the United States of America, 2007, 104, 20177-20182.	7.1	93
138	Structure of the first- and second-neighbor shells of simulated water: Quantitative relation to translational and orientational order. Physical Review E, 2007, 76, 051201.	2.1	109
139	Hydration Behavior under Confinement by Nanoscale Surfaces with Patterned Hydrophobicity and Hydrophilicity. Journal of Physical Chemistry C, 2007, 111, 1323-1332.	3.1	224
140	Effect of Surface Polarity on Water Contact Angle and Interfacial Hydration Structure. Journal of Physical Chemistry B, 2007, 111, 9581-9587.	2.6	416
141	Method for Efficient Computation of the Density of States in Water-Explicit Biopolymer Simulations on a Lattice. Journal of Physical Chemistry A, 2007, 111, 12651-12658.	2.5	6
142	A Water-Explicit Lattice Model of Heat-, Cold-, and Pressure-Induced Protein Unfolding. Biophysical Journal, 2007, 93, 4116-4127.	0.5	42
143	Stability of proteins in the presence of carbohydrates; experiments and modeling using scaled particle theory. Biophysical Chemistry, 2007, 127, 51-63.	2.8	32
144	Recent developments in the theory of amorphous aqueous systems. Special Publication - Royal Society of Chemistry, 2007, , 115-120.	0.0	0

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145	Fluid-phase behavior of binary mixtures in which one component can have two critical points. Journal of Chemical Physics, 2006, 124, 154503.	3.0	55
146	Scaled particle theory for hard sphere pairs. I. Mathematical structure. Journal of Chemical Physics, 2006, 125, 204504.	3.0	17
147	In Honor of Eduardo Glandt. Industrial & Engineering Chemistry Research, 2006, 45, 5419-5420.	3.7	0
148	Bill Russel:Â A Tribute. Industrial & Engineering Chemistry Research, 2006, 45, 6877-6879.	3.7	0
149	When a phase is born. Nature, 2006, 441, 168-169.	27.8	36
150	A conformal solution theory for the energy landscape and glass transition of mixtures. Fluid Phase Equilibria, 2006, 241, 147-154.	2.5	17
151	Accurate prediction of clathrate hydrate phase equilibria below 300 K from a simple model. Journal of Petroleum Science and Engineering, 2006, 51, 45-53.	4.2	25
152	Solid-State Stabilization of Î±-Chymotrypsin and Catalase with Carbohydrates. Industrial & Engineering Chemistry Research, 2006, 45, 5134-5147.	3.7	32
153	Family of tunable spherically symmetric potentials that span the range from hard spheres to waterlike behavior. Physical Review E, 2006, 73, 051204.	2.1	106
154	Computational probes of molecular motion in the Lewis-WahnstrÃ¶m model for ortho-terphenyl. Journal of Chemical Physics, 2006, 125, 174507.	3.0	55
155	Scaled particle theory for hard sphere pairs. II. Numerical analysis. Journal of Chemical Physics, 2006, 125, 204505.	3.0	13
156	Effect of pressure on the phase behavior and structure of water confined between nanoscale hydrophobic and hydrophilic plates. Physical Review E, 2006, 73, 041604.	2.1	319
157	Culmination of the 50th year and some changes for the 51st year. AICHE Journal, 2005, 51, 1836-1838.	3.6	0
158	Preface to perspectives. AICHE Journal, 2005, 51, 2370-2370.	3.6	0
159	Structure, dynamics and thermodynamics in complex systems: Theoretical challenges and opportunities. AICHE Journal, 2005, 51, 2391-2395.	3.6	12
160	Preface to perspectives. AICHE Journal, 2005, 51, 3082-3082.	3.6	0
161	Computational characterization of the sequence landscape in simple protein alphabets. Proteins: Structure, Function and Bioinformatics, 2005, 62, 232-243.	2.6	11
162	Dynamic heterogeneity and non-Gaussian behaviour in a model supercooled liquid. Journal of Physics Condensed Matter, 2005, 17, S4035-S4046.	1.8	54

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163	Generating inherent structures of liquids: Comparison of local minimization algorithms. Journal of Chemical Physics, 2005, 123, 206101.	3.0	13
164	Structural order in glassy water. Physical Review E, 2005, 71, 061505.	2.1	48
165	Reply to â€œComment on Test of nonequilibrium thermodynamics in glassy systems: The soft-sphere caseâ€• Physical Review E, 2005, 71, .	2.1	2
166	Effects of nonpolar solutes on the thermodynamic response functions of aqueous mixtures. Journal of Chemical Physics, 2005, 123, 164503.	3.0	28
167	A computational study of hydration, solution structure, and dynamics in dilute carbohydrate solutions. Journal of Chemical Physics, 2005, 122, 204511.	3.0	166
168	Computational Investigation of Order, Structure, and Dynamics in Modified Water Modelsâ€. Journal of Physical Chemistry B, 2005, 109, 6527-6534.	2.6	88
169	Novel Computational Probes of Diffusive Motion. Journal of Physical Chemistry B, 2005, 109, 21329-21333.	2.6	1
170	Alternative View of Self-Diffusion and Shear Viscosityâ€. Journal of Physical Chemistry B, 2005, 109, 6604-6609.	2.6	20
171	Reply to Comment on ÂSupercooled and glassy waterÂ. Journal of Physics Condensed Matter, 2004, 16, 6815-6817.	1.8	13
172	Saddles in the Energy Landscape: Extensivity and Thermodynamic Formalism. Physical Review Letters, 2004, 92, 035506.	7.8	25
173	Flat-Histogram Dynamics and Optimization in Density of States Simulations of Fluidsâ€. Journal of Physical Chemistry B, 2004, 108, 19748-19755.	2.6	34
174	From molecular dynamics to coarse self-similar solutions: a simple example using equation-free computation. Journal of Non-Newtonian Fluid Mechanics, 2004, 120, 215-223.	2.4	28
175	A Calorimetric and Spectroscopic Study of DNA at Low Hydration. Journal of Physical Chemistry B, 2004, 108, 3098-3106.	2.6	50
176	Simultaneous Determination of Structural and Thermodynamic Effects of Carbohydrate Solutes on the Thermal Stability of Ribonuclease A. Journal of the American Chemical Society, 2004, 126, 11794-11795.	13.7	31
177	Frank H. Stillinger, Theoretical Chemist:Â A Tribute. Journal of Physical Chemistry B, 2004, 108, 19569-19570.	2.6	2
178	Differential Scanning Calorimetry Studies of Clathrate Hydrate Formation. Journal of Physical Chemistry B, 2004, 108, 16717-16722.	2.6	102
179	Thermodynamics and the glass transition in model energy landscapes. Physical Review E, 2004, 69, 051102.	2.1	20
180	Inherent-Structure View of Self-Diffusion in Liquids. Journal of Physical Chemistry B, 2004, 108, 6772-6777.	2.6	21

#	Article	IF	Citations
181	Recent Developments in the Theory of Amorphous Aqueous Systems. ChemInform, 2003, 34, no.	0.0	0
182	Phase transitions, Kauzmann curves, and inverse melting. Biophysical Chemistry, 2003, 105, 211-220.	2.8	47
183	Quantification of order in the Lennard-Jones system. Journal of Chemical Physics, 2003, 118, 2256-2263.	3.0	124
184	Estimation of the Characteristic Time Scales in the Supercritical Antisolvent Process. Industrial & Engineering Chemistry Research, 2003, 42, 3156-3162.	3.7	60
185	In Honor of Charles A. Eckert. Industrial & Engineering Chemistry Research, 2003, 42, 6263-6266.	3.7	1
186	Supercooled and glassy water. Journal of Physics Condensed Matter, 2003, 15, R1669-R1726.	1.8	956
187	Model Energy Landscapes. Journal of Physical Chemistry B, 2003, 107, 14434-14442.	2.6	40
188	A Theoretical Study of the Interfacial Properties of Supercooled Water. Industrial & Engineering Chemistry Research, 2003, 42, 6396-6405.	3.7	13
189	A kinetic theory of homogeneous bubble nucleation. Journal of Chemical Physics, 2003, 118, 768-783.	3.0	57
190	Energy landscapes, ideal glasses, and their equation of state. Journal of Chemical Physics, 2003, 118, 8821-8830.	3.0	53
191	A statistical mechanical model for inverse melting. Journal of Chemical Physics, 2003, 119, 4582-4591.	3.0	36
192	Test of nonequilibrium thermodynamics in glassy systems: The soft-sphere case. Physical Review E, 2003, 68, 032103.	2.1	23
193	An improved Monte Carlo method for direct calculation of the density of states. Journal of Chemical Physics, 2003, 119, 9406-9411.	3.0	128
194	Response to â€œComment on â€˜A simple molecular thermodynamic theory of hydrophobic hydrationâ€™â€Šâ€•[J. Chem. Phys. 119, 10448 (2003)]. Journal of Chemical Physics, 2003, 119, 10450-10451.	3.0	5
195	Supercooled and Glassy Water. Physics Today, 2003, 56, 40-46.	0.3	470
196	Generalization of the Wang-Landau method for off-lattice simulations. Physical Review E, 2002, 66, 056703.	2.1	209
197	Cooperative Origin of Low-Density Domains in Liquid Water. Physical Review Letters, 2002, 89, 215503.	7.8	103
198	Energy landscape diversity and supercooled liquid properties. Journal of Chemical Physics, 2002, 116, 3353-3361.	3.0	70

#	Article	IF	Citations
199	A simple molecular thermodynamic theory of hydrophobic hydration. Journal of Chemical Physics, 2002, 116, 2907-2921.	3.0	118
200	Comment on â€œObservations on an equation of state for water confined in narrow slit-poresâ€•[J. Chem. Phys. 116, 2565 (2002)]. Journal of Chemical Physics, 2002, 117, 8162-8163.	3.0	3
201	Molecular structural order and anomalies in liquid silica. Physical Review E, 2002, 66, 011202.	2.1	215
202	Energy Landscape and Isotropic Tensile Strength ofn-Alkane Glasses. Journal of Physical Chemistry B, 2002, 106, 10447-10459.	2.6	14
203	Engineering pharmaceutical stability with amorphous solids. AICHE Journal, 2002, 48, 1140-1144.	3.6	82
204	Mathematical modeling of nucleation and growth of particles formed by the rapid expansion of a supercritical solution under subsonic conditions. Journal of Supercritical Fluids, 2002, 23, 65-80.	3.2	96
205	Density-functional study of homogeneous bubble nucleation in the stretched Lennard-Jones fluid. Journal of Chemical Physics, 2001, 114, 4149-4159.	3.0	75
206	The Kauzmann Paradox Revisitedâ€. Journal of Physical Chemistry B, 2001, 105, 11809-11816.	2.6	131
207	Isotropic tensile strength of molecular glasses. Journal of Chemical Physics, 2001, 114, 10049-10057.	3.0	22
208	Incoherent Quasi-elastic Neutron Scattering from Fructoseâ^'Water Solutions. Journal of Physical Chemistry B, 2001, 105, 7799-7804.	2.6	19
209	Relationship between structural order and the anomalies of liquid water. Nature, 2001, 409, 318-321.	27.8	1,320
210	Supercooled liquids and the glass transition. Nature, 2001, 410, 259-267.	27.8	3,877
211	Theory of supercooled liquids and glasses: Energy landscape and statistical geometry perspectives. Advances in Chemical Engineering, 2001, 28, 21-79.	0.9	58
212	Thermodynamic implications of confinement for a waterlike fluid. Journal of Chemical Physics, 2001, 114, 2401-2418.	3.0	143
213	Numerical modeling of mass transfer in the supercritical antisolvent process: miscible conditions. Journal of Supercritical Fluids, 2000, 18, 11-24.	3.2	114
214	Triangle Distribution and Equation of State for Classical Rigid Disks. Journal of Statistical Physics, 2000, 100, 49-72.	1.2	16
215	Towards a quantification of disorder in materials: Distinguishing equilibrium and glassy sphere packings. Physical Review E, 2000, 62, 993-1001.	2.1	258
216	Statistical geometry of cavities in a metastable confined fluid. Physical Review E, 2000, 62, 538-544.	2.1	36

#	Article	IF	Citations
217	Atomistic Simulation of Aging and Rejuvenation in Glasses. Physical Review Letters, 2000, 84, 1471-1474.	7.8	175
218	Equation of state of the rigid disk fluid from its triangle distribution. Journal of Chemical Physics, 2000, 113, 10186-10190.	3.0	6
219	Is Random Close Packing of Spheres Well Defined?. Physical Review Letters, 2000, 84, 2064-2067.	7.8	1,173
220	Phase Separation By Nucleation and Ly Spinodal Decomposition: Fundamentals. , 2000, , 123-166.		11
221	A computational study of homogeneous liquidâ€“vapor nucleation in the Lennard-Jones fluid. Journal of Chemical Physics, 1999, 111, 3581-3589.	3.0	81
222	A single-bond approach to orientation-dependent interactions and its implications for liquid water. Journal of Chemical Physics, 1999, 111, 2647-2656.	3.0	157
223	Potential energy landscape signatures of slow dynamics in glass forming liquids. Physica A: Statistical Mechanics and Its Applications, 1999, 270, 301-308.	2.6	50
224	Numerical modeling of mass transfer in the supercritical antisolvent process. Journal of Supercritical Fluids, 1999, 16, 167-181.	3.2	111
225	The statistical geometry of voids in liquids. Fluid Phase Equilibria, 1999, 158-160, 549-556.	2.5	19
226	Direct coal gasification with simultaneous production of electricity in a novel fused metal anode SOFC: a theoretical approach. Ionics, 1999, 5, 460-471.	2.4	2
227	Protein purification with vapor-phase carbon dioxide. , 1999, 62, 247-258.		44
228	The Equation of State of an Energy Landscape. Journal of Physical Chemistry B, 1999, 103, 7390-7397.	2.6	103
229	Equation of State of the Energy Landscape of SPC/E Water. Journal of Physical Chemistry B, 1999, 103, 10258-10265.	2.6	26
230	Structure and Dynamics in Concentrated, Amorphous Carbohydrateâ^'Water Systems by Molecular Dynamics Simulation. Journal of Physical Chemistry B, 1999, 103, 7308-7318.	2.6	128
231	Distinguishing Vibrational and Structural Equilibration Contributions to Thermal Expansion. Journal of Physical Chemistry B, 1999, 103, 4052-4059.	2.6	35
232	Response to â€œComment on â€˜Reversible work of formation of an embryo of a new phase within a uniform macroscopic mother phaseâ€™â€‰â€•[J. Chem. Phys. 111, 3769 (1999)]. Journal of Chemical Physics, 1999, 111, 3771-3772.	3.0	12
233	Free volume in the hard sphere liquid. Molecular Physics, 1998, 95, 289-297.	1.7	112
234	Signatures of distinct dynamical regimes in the energy landscape of a glass-forming liquid. Nature, 1998, 393, 554-557.	27.8	676

#	Article	IF	Citations
235	One substance, two liquids?. Nature, 1998, 392, 127-128.	27.8	54
236	Chain-packing effects in the thermodynamics of polymers. Journal of Polymer Science, Part B: Polymer Physics, 1998, 36, 3001-3005.	2.1	11
237	A molecular dynamics study of intermolecular structure, thermodynamics and miscibility in hydrocarbon polymers. Computers and Chemical Engineering, 1998, 22, S19-S26.	3.8	2
238	Liquidâ^'Liquid Immiscibility in Single-Component Network-Forming Fluids:Â Model Calculations and Implications for Polyamorphism in Water. Industrial & Engineering Chemistry Research, 1998, 37, 3012-3020.	3.7	13
239	Density fluctuations in many-body systems. Physical Review E, 1998, 58, 7369-7380.	2.1	30
240	Liquid Structure, Thermodynamics, and Mixing Behavior of Saturated Hydrocarbon Polymers. 2. Pair Distribution Functions and the Regularity of Mixing. Macromolecules, 1998, 31, 6998-7002.	4.8	38
241	Liquid Structure, Thermodynamics, and Mixing Behavior of Saturated Hydrocarbon Polymers. 1. Cohesive Energy Density and Internal Pressure. Macromolecules, 1998, 31, 6991-6997.	4.8	59
242	Structural precursor to freezing in the hard-disk and hard-sphere systems. Physical Review E, 1998, 58, 3083-3088.	2.1	147
243	Singularity-free interpretation of the thermodynamics of supercooled water. II. Thermal and volumetric behavior. Journal of Chemical Physics, 1998, 109, 626-633.	3.0	119
244	A theoretical study of Gemini surfactant phase behavior. Journal of Chemical Physics, 1998, 109, 5651-5658.	3.0	22
245	Resolving vibrational and structural contributions to isothermal compressibility. Journal of Chemical Physics, 1998, 109, 3983-3988.	3.0	34
246	Reversible work of formation of an embryo of a new phase within a uniform macroscopic mother phase. Journal of Chemical Physics, 1998, 108, 5498-5505.	3.0	70
247	Statistical mechanics of fluids under internal constraints: Rigorous results for the one-dimensional hard rod fluid. Physical Review E, 1998, 57, 4211-4226.	2.1	26
248	Free volume in the hard sphere liquid. Molecular Physics, 1998, 95, 289-297.	1.7	25
249	Statistical geometry of particle packings.â€ƒII. â€œWeak spotsâ€•in liquids. Physical Review E, 1997, 56, 5533-5543.	2.1	83
250	Constraints, metastability, and inherent structures in liquids. Physical Review E, 1997, 55, 5522-5534.	2.1	94
251	Statistical geometry of particle packings.â€ƒI.â€ƒAlgorithm for exact determination of connectivity, volume, and surface areas of void space in monodisperse and polydisperse sphere packings. Physical Review E, 1997, 56, 5524-5532.	2.1	145
252	Compressibility Effects in Neutron Scattering by Polymer Blends. Macromolecules, 1997, 30, 6943-6946.	4.8	9

#	Article	IF	Citations
253	Long-term and high-temperature storage of supercritically-processed microparticulate protein powders. Pharmaceutical Research, 1997, 14, 1370-1378.	3.5	33
254	Effects of Compressed Carbon Dioxide on the Phase Equilibrium and Molecular Order of a Lyotropic Polyamide Solution. Macromolecules, 1996, 29, 4904-4909.	4.8	3
255	Liquid-Liquid Immiscibility in Pure Fluids: Polyamorphism in Simulations of a Network-Forming Fluid. Physical Review Letters, 1996, 77, 4386-4389.	7.8	117
256	Compressibility Effects in the Analysis and Interpretation of Neutron Scattering Data from Polymer Blends. Macromolecules, 1996, 29, 764-773.	4.8	21
257	Singularity-free interpretation of the thermodynamics of supercooled water. Physical Review E, 1996, 53, 6144-6154.	2.1	499
258	Comment on â€˜â€˜Entropy catastrophe and configurational entropies in supercooled and superheated regimesâ€™â€™ [J. Chem. Phys. 101, 7037 (1994)]. Journal of Chemical Physics, 1996, 104, 5349-5350.	3.0	1
259	Molecular dynamics simulation of infinitely dilute solutions of benzene in supercritical CO2. Fluid Phase Equilibria, 1996, 116, 282-288.	2.5	32
260	Supercritical fluids as solvents for chemical and materials processing. Nature, 1996, 383, 313-318.	27.8	849
261	Freeze Crystallization of Imipenem. Journal of Pharmaceutical Sciences, 1996, 85, 174-177.	3.3	9
262	Precipitation of Proteins in Supercritical Carbon Dioxide. Journal of Pharmaceutical Sciences, 1996, 85, 586-594.	3.3	185
263	The distribution of tetravalent network glasses. Molecular Physics, 1996, 88, 1293-1316.	1.7	56
264	The evaporation rate, free energy, and entropy of amorphous water at 150 K. Journal of Chemical Physics, 1996, 105, 240-244.	3.0	251
265	Polyamorphism and density anomalies in networkâ€forming fluids: Zerothâ€and firstâ€order approximations. Journal of Chemical Physics, 1996, 105, 658-672.	3.0	122
266	The distribution of tetravalent network glasses. Molecular Physics, 1996, 88, 1293-1316.	1.7	17
267	Persistence time for bonds in a tetravalent network fluid. Molecular Physics, 1995, 86, 1375-1386.	1.7	24
268	Supercritical antisolvent process for a series of substituted para-linked aromatic polyamides. Macromolecules, 1995, 28, 1316-1317.	4.8	32
269	A Lattice Model of Network-Forming Fluids with Orientation-Dependent Bonding: Equilibrium, Stability, and Implications for the Phase Behavior of Supercooled Water. The Journal of Physical Chemistry, 1995, 99, 3781-3792.	2.9	98
270	Metastability and Constraints: A Study of the Superheated Leonard-Jones Liquid in the Void-Constrained Ensemble. Industrial & Engineering Chemistry Research, 1995, 34, 3573-3580.	3.7	13

#	Article	IF	Citations
271	The entropy of a network crystal, fluid and glass. Molecular Physics, 1994, 81, 237-249.	1.7	27
272	Thermal Expansion and Stability Limits of Generalized van der Waals Fluids. The Journal of Physical Chemistry, 1994, 98, 6876-6884.	2.9	2
273	Secondary Structure Characterization of Microparticulate Insulin Powdersâ€. Journal of Pharmaceutical Sciences, 1994, 83, 1651-1656.	3.3	67
274	A computational study of metastability in vaporâ€"liquid equilibrium. Chemical Engineering Science, 1994, 49, 2717-2734.	3.8	48
275	Precipitation of poly(l-lactic acid) and composite poly(l-lactic acid)-pyrene particles by rapid expansion of supercritical solutions. Journal of Supercritical Fluids, 1994, 7, 9-29.	3.2	136
276	Supercritical Fluids: Fundamentals and Applications. , 1994, , 30-35.		45
277	Supercritical Fluids as Particle Formation Media. , 1994, , 719-729.		16
278	Solute-Solute Interactions: Theory and Simulations. , 1994, , 439-445.		0
279	Formation of microparticulate protein powder using a supercritical fluid antisolvent. Biotechnology and Bioengineering, 1993, 41, 341-346.	3.3	286
280	Application of supercritical fluids for the production of sustained delivery devices. Journal of Controlled Release, 1993, 24, 27-44.	9.9	128
281	Rapid expansion of supercritical solutions (ress): fundamentals and applications. Fluid Phase Equilibria, 1993, 82, 311-321.	2.5	162
282	Mathematical modeling of aerosol formation by rapid expansion of supercritical solutions in a converging nozzle. Journal of Aerosol Science, 1993, 24, 445-469.	3.8	97
283	Supercritical antisolvent process for substituted para-linked aromatic polyamides: phase equilibrium and morphology study. Macromolecules, 1993, 26, 6207-6210.	4.8	81
284	Integral equation study of microstructure and solvation in model attractive and repulsive supercritical mixtures. Industrial & Engineering Chemistry Research, 1993, 32, 2118-2128.	3.7	41
285	Equilibrium, stability, and density anomalies in a lattice model with core-softening and directional bonding. The Journal of Physical Chemistry, 1993, 97, 6292-6303.	2.9	25
286	Soluteâ€"solute correlations in infinitely dilute supercritical mixtures. Journal of Chemical Physics, 1992, 97, 504-507.	3.0	29
287	Local Density Augmentation in Supercritical Solutions. ACS Symposium Series, 1992, , 60-72.	0.5	43
288	Applications of Supercritical Fluids in the Controlled Release of Drugs. ACS Symposium Series, 1992, , 238-257.	0.5	57

#	Article	IF	Citations
289	Molecular dynamics study of solute-solute microstructure in attractive and repulsive supercritical mixtures. Industrial & Engineering Chemistry Research, 1992, 31, 1391-1397.	3.7	54
290	An automated Verlet neighbor list algorithm with a multiple time-step approach for the simulation of large systems. Computer Physics Communications, 1992, 70, 467-477.	7.5	9
291	Spinodal curve of some supercooled liquids. The Journal of Physical Chemistry, 1991, 95, 4540-4551.	2.9	101
292	Particle formation with supercritical fluidsâ€"a review. Journal of Aerosol Science, 1991, 22, 555-584.	3.8	330
293	Influence of solute-solvent asymmetry upon the behavior of dilute supercritical mixtures. The Journal of Physical Chemistry, 1991, 95, 386-399.	2.9	98
294	A Study of Solute-Solvent Interactions at Infinite Dilution via the Coupling Parameter Approach. Molecular Simulation, 1991, 7, 265-283.	2.0	8
295	Formation of bioerodible polymeric microspheres and microparticles by rapid expansion of supercritical solutions. Biotechnology Progress, 1991, 7, 403-411.	2.6	182
296	On the performance of an automated Verlet neighbor list algorithm for large systems on a vector processor. Computer Physics Communications, 1991, 64, 15-18.	7.5	18
297	Use of the McQuarrie equation for the computation of shear viscosity via equilibrium molecular dynamics. Physical Review A, 1991, 43, 4289-4295.	2.5	23
298	Homogeneous nucleation in supercritical fluids. AICHE Journal, 1990, 36, 1289-1298.	3.6	143
299	On the use of the Verlet neighbor list in molecular dynamics. Computer Physics Communications, 1990, 60, 215-224.	7.5	46
300	Attractive, weakly attractive, and repulsive nearâ€critical systems. Journal of Chemical Physics, 1989, 90, 4528-4536.	3.0	148
301	A molecular dynamics study of the influence of elongation and quadrupole moment upon some thermodynamic and transport properties of linear heteronuclear triatomic fluids. Journal of Chemical Physics, 1989, 91, 7818-7830.	3.0	6
302	Fluctuation Simulations and the Calculation of Mechanical Partial Molar Properties. Molecular Simulation, 1989, 2, 33-53.	2.0	6
303	Effects of process conditions on crystals obtained from supercritical mixtures. AICHE Journal, 1989, 35, 325-328.	3.6	104
304	Clustering in supercritical mixtures: Theory, applications and simulations. Fluid Phase Equilibria, 1989, 52, 347-356.	2.5	38
305	Soluteâ€"solvent interactions in infinitely dilute supercritical mixtures: A molecular dynamics investigation. Journal of Chemical Physics, 1989, 91, 7075-7084.	3.0	201
306	A novel fused metal anode solid electrolyte fuel cell for direct coal gasification: a steady-state model. Industrial & Engineering Chemistry Research, 1989, 28, 1414-1424.	3.7	23

#	Article	IF	Citations
307	Solids Formation After the Expansion of Supercritical Mixtures. ACS Symposium Series, 1989, , 355-378.	0.5	38
308	The molecular basis of temperature effects in supercritical extraction. AICHE Journal, 1988, 34, 645-657.	3.6	77
309	Disproportionation of toluene over ZSMâ€“5 under near-critical conditions. AICHE Journal, 1988, 34, 1211-1214.	3.6	47
310	Stability and tensile strength of liquids exhibiting density maxima. AICHE Journal, 1988, 34, 447-455.	3.6	38
311	Fluctuationâ€based computer calculation of partial molar properties. II. A numerically accurate method for the determination of partial molar energies and enthalpies. Journal of Chemical Physics, 1988, 88, 2681-2684.	3.0	16
312	Thermodynamic stability of singleâ€phase fluids and fluid mixtures under the influence of gravity. Journal of Chemical Physics, 1988, 89, 6881-6888.	3.0	8
313	Loss of tensile strength in liquids without property discontinuities: A thermodynamic analysis. Journal of Chemical Physics, 1987, 86, 2229-2235.	3.0	41
314	Fluctuationâ€based computer calculation of partial molar properties. I. Molecular dynamics simulation of constant volume fluctuations. Journal of Chemical Physics, 1987, 86, 7126-7137.	3.0	28
315	The statistical mechanical theory of concentration fluctuations in mixtures. Journal of Chemical Physics, 1987, 87, 1256-1260.	3.0	8
316	Clustering in dilute, binary supercritical mixtures: A fluctuation analysis. Chemical Engineering Science, 1987, 42, 2203-2212.	3.8	166
317	Derivation of operational definitions for the computer calculation of partial molar properties in multicomponent mixtures. Chemical Physics Letters, 1986, 132, 325-329.	2.6	6
318	Infinite dilution fugacity coefficients and the general behavior of dilute binary systems. AICHE Journal, 1986, 32, 1253-1262.	3.6	47
319	Diffusion and mass transfer in supercritical fluids. AICHE Journal, 1986, 32, 2034-2046.	3.6	143
320	On the relationship between principal fluctuations and stability coefficients in multicomponent systems. Journal of Chemical Physics, 1986, 84, 1778-1787.	3.0	28
321	On the entropy changes and fluctuations occurring near a tensile instability. Journal of Chemical Physics, 1986, 85, 4005-4010.	3.0	28
322	Generalized Massieuâ€“Planck functions: Geometric representation, extrema and uniqueness properties. Journal of Chemical Physics, 1986, 85, 2132-2139.	3.0	5
323	On the nature of the tensile instability in metastable liquids and its relationship to density anomalies. Journal of Chemical Physics, 1986, 84, 3339-3345.	3.0	47
324	Cross-flow, solid-state electrochemical reactors: a steady state analysis. Industrial & Engineering Chemistry Fundamentals, 1985, 24, 316-324.	0.7	52

#	Article	IF	Citations
325	Steady-state analysis of high temperature fuel cells. Chemical Engineering Science, 1983, 38, 1817-1829.	3.8	39
326	Plea for Argentinians. Nature, 1976, 262, 253-253.	27.8	1