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	Supercooled liquids and the glass transition. Nature, 2001, 410, 259-267.	27.8	3,877
2	Relationship between structural order and the anomalies of liquid water. Nature, 2001, 409, 318-321.	27.8	1,320
3	Is Random Close Packing of Spheres Well Defined?. Physical Review Letters, 2000, 84, 2064-2067.	7.8	1,173
4	Supercooled and glassy water. Journal of Physics Condensed Matter, 2003, 15, R1669-R1726.	1.8	956
5	Supercritical fluids as solvents for chemical and materials processing. Nature, 1996, 383, 313-318.	27.8	849
6	Signatures of distinct dynamical regimes in the energy landscape of a glass-forming liquid. Nature, 1998, 393, 554-557.	27.8	676
7	Singularity-free interpretation of the thermodynamics of supercooled water. Physical Review E, 1996, 53, 6144-6154.	2.1	499
8	Supercooled and Glassy Water. Physics Today, 2003, 56, 40-46.	0.3	470
9	Metastable liquidâ€“liquid transition in a molecular model of water. Nature, 2014, 510, 385-388.	27.8	431
10	Effect of Surface Polarity on Water Contact Angle and Interfacial Hydration Structure. Journal of Physical Chemistry B, 2007, 111, 9581-9587.	2.6	416
11	Particle formation with supercritical fluidsâ€”a review. Journal of Aerosol Science, 1991, 22, 555-584.	3.8	330
12	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
13	Formation of microparticulate protein powder using a supercritical fluid antisolvent. Biotechnology and Bioengineering, 1993, 41, 341-346.	3.3	286
14	Towards a quantification of disorder in materials: Distinguishing equilibrium and glassy sphere packings. Physical Review E, 2000, 62, 993-1001.	2.1	258
15	The evaporation rate, free energy, and entropy of amorphous water at 150 K. Journal of Chemical Physics, 1996, 105, 240-244.	3.0	251
16	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
17	Hydration Behavior under Confinement by Nanoscale Surfaces with Patterned Hydrophobicity and Hydrophilicity. Journal of Physical Chemistry C, 2007, 111, 1323-1332.	3.1	224
18	Glass Transition Thermodynamics and Kinetics. Annual Review of Condensed Matter Physics, 2013, 4, 263-285.	14.5	217

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19	Molecular structural order and anomalies in liquid silica. Physical Review E, 2002, 66, 011202.	2.1	215
20	Generalization of the Wang-Landau method for off-lattice simulations. Physical Review E, 2002, 66, 056703.	2.1	209
21	Phase Transitions Induced by Nanoconfinement in Liquid Water. Physical Review Letters, 2009, 102, 050603.	7.8	208
22	Soluteâ€“solvent interactions in infinitely dilute supercritical mixtures: A molecular dynamics investigation. Journal of Chemical Physics, 1989, 91, 7075-7084.	3.0	201
23	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
24	Precipitation of Proteins in Supercritical Carbon Dioxide. Journal of Pharmaceutical Sciences, 1996, 85, 586-594.	3.3	185
25	Formation of bioerodible polymeric microspheres and microparticles by rapid expansion of supercritical solutions. Biotechnology Progress, 1991, 7, 403-411.	2.6	182
26	Second critical point in two realistic models of water. Science, 2020, 369, 289-292.	12.6	176
27	Atomistic Simulation of Aging and Rejuvenation in Glasses. Physical Review Letters, 2000, 84, 1471-1474.	7.8	175
28	Clustering in dilute, binary supercritical mixtures: A fluctuation analysis. Chemical Engineering Science, 1987, 42, 2203-2212.	3.8	166
29	A computational study of hydration, solution structure, and dynamics in dilute carbohydrate solutions. Journal of Chemical Physics, 2005, 122, 204511.	3.0	166
30	Rapid expansion of supercritical solutions (ress): fundamentals and applications. Fluid Phase Equilibria, 1993, 82, 311-321.	2.5	162
31	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
32	Homogeneous Nucleation of Methane Hydrate in Microsecond Molecular Dynamics Simulations. Journal of Physical Chemistry Letters, 2012, 3, 2942-2947.	4.6	156
33	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
34	Advances in Computational Studies of the Liquidâ€“Liquid Transition in Water and Water-Like Models. Chemical Reviews, 2018, 118, 9129-9151.	47.7	152
35	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
36	Attractive, weakly attractive, and repulsive nearâ€critical systems. Journal of Chemical Physics, 1989, 90, 4528-4536.	3.0	148

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37	Structural precursor to freezing in the hard-disk and hard-sphere systems. Physical Review E, 1998, 58, 3083-3088.	2.1	147
38	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
39	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
40	Liquid-liquid transition in ST2 water. Journal of Chemical Physics, 2012, 137, 214505.	3.0	144
41	Diffusion and mass transfer in supercritical fluids. AICHE Journal, 1986, 32, 2034-2046.	3.6	143
42	Homogeneous nucleation in supercritical fluids. AICHE Journal, 1990, 36, 1289-1298.	3.6	143
43	Thermodynamic implications of confinement for a waterlike fluid. Journal of Chemical Physics, 2001, 114, 2401-2418.	3.0	143
44	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
45	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
46	Nonlinear dimensionality reduction in molecular simulation: The diffusion map approach. Chemical Physics Letters, 2011, 509, 1-11.	2.6	141
47	Low-temperature fluid-phase behavior of ST2 water. Journal of Chemical Physics, 2009, 131, 104508.	3.0	139
48	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
49	A computational investigation of thermodynamics, structure, dynamics and solvation behavior in modified water models. Journal of Chemical Physics, 2008, 128, 124511.	3.0	134
50	The Kauzmann Paradox Revisitedâ€. Journal of Physical Chemistry B, 2001, 105, 11809-11816.	2.6	131
51	Solubility and Molecular Conformations of n-Alkane Chains in Water. Journal of Physical Chemistry B, 2009, 113, 6405-6414.	2.6	131
52	Application of supercritical fluids for the production of sustained delivery devices. Journal of Controlled Release, 1993, 24, 27-44.	9.9	128
53	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
54	An improved Monte Carlo method for direct calculation of the density of states. Journal of Chemical Physics, 2003, 119, 9406-9411.	3.0	128

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55	Quantification of order in the Lennard-Jones system. Journal of Chemical Physics, 2003, 118, 2256-2263.	3.0	124
56	Polyamorphism and density anomalies in networkâ€forming fluids: Zerothâ€and firstâ€order approximations. Journal of Chemical Physics, 1996, 105, 658-672.	3.0	122
57	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
58	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
59	A simple molecular thermodynamic theory of hydrophobic hydration. Journal of Chemical Physics, 2002, 116, 2907-2921.	3.0	118
60	Liquid-Liquid Immiscibility in Pure Fluids: Polyamorphism in Simulations of a Network-Forming Fluid. Physical Review Letters, 1996, 77, 4386-4389.	7.8	117
61	Numerical modeling of mass transfer in the supercritical antisolvent process: miscible conditions. Journal of Supercritical Fluids, 2000, 18, 11-24.	3.2	114
62	Free volume in the hard sphere liquid. Molecular Physics, 1998, 95, 289-297.	1.7	112
63	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
64	Numerical modeling of mass transfer in the supercritical antisolvent process. Journal of Supercritical Fluids, 1999, 16, 167-181.	3.2	111
65	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
66	Molecular Dynamics Study of Carbon Dioxide Hydrate Dissociation. Journal of Physical Chemistry A, 2011, 115, 6102-6111.	2.5	107
67	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
68	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
69	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
70	Effects of process conditions on crystals obtained from supercritical mixtures. AICHE Journal, 1989, 35, 325-328.	3.6	104
71	The Equation of State of an Energy Landscape. Journal of Physical Chemistry B, 1999, 103, 7390-7397.	2.6	103
72	Cooperative Origin of Low-Density Domains in Liquid Water. Physical Review Letters, 2002, 89, 215503.	7.8	103

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73	Differential Scanning Calorimetry Studies of Clathrate Hydrate Formation. Journal of Physical Chemistry B, 2004, 108, 16717-16722.	2.6	102
74	Spinodal curve of some supercooled liquids. The Journal of Physical Chemistry, 1991, 95, 4540-4551.	2.9	101
75	Influence of solute-solvent asymmetry upon the behavior of dilute supercritical mixtures. The Journal of Physical Chemistry, 1991, 95, 386-399.	2.9	98
76	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
77	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
78	Evolution from Surface-Influenced to Bulk-Like Dynamics in Nanoscopically Confined Water. Journal of Physical Chemistry B, 2009, 113, 7973-7976.	2.6	97
79	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
80	Two-state thermodynamics of the ST2 model for supercooled water. Journal of Chemical Physics, 2014, 140, 104502.	3.0	96
81	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
82	Constraints, metastability, and inherent structures in liquids. Physical Review E, 1997, 55, 5522-5534.	2.1	94
83	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
84	Computational Investigation of Order, Structure, and Dynamics in Modified Water Modelsâ€. Journal of Physical Chemistry B, 2005, 109, 6527-6534.	2.6	88
85	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
86	Statistical geometry of particle packings.â€ƒII. â€œWeak spotsâ€•in liquids. Physical Review E, 1997, 56, 5533-5543.	2.1	83
87	Lindemann measures for the solid-liquid phase transition. Journal of Chemical Physics, 2007, 126, 204508.	3.0	83
88	Relaxation processes in liquids: Variations on a theme by Stokes and Einstein. Journal of Chemical Physics, 2013, 138, 12A526.	3.0	83
89	Engineering pharmaceutical stability with amorphous solids. AICHE Journal, 2002, 48, 1140-1144.	3.6	82
90	Supercritical antisolvent process for substituted para-linked aromatic polyamides: phase equilibrium and morphology study. Macromolecules, 1993, 26, 6207-6210.	4.8	81

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91	A computational study of homogeneous liquidâ€“vapor nucleation in the Lennard-Jones fluid. Journal of Chemical Physics, 1999, 111, 3581-3589.	3.0	81
92	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
93	The molecular basis of temperature effects in supercritical extraction. AICHE Journal, 1988, 34, 645-657.	3.6	77
94	Density-functional study of homogeneous bubble nucleation in the stretched Lennard-Jones fluid. Journal of Chemical Physics, 2001, 114, 4149-4159.	3.0	75
95	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
96	Energy landscape diversity and supercooled liquid properties. Journal of Chemical Physics, 2002, 116, 3353-3361.	3.0	70
97	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
98	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
99	Secondary Structure Characterization of Microparticulate Insulin Powdersâ€. Journal of Pharmaceutical Sciences, 1994, 83, 1651-1656.	3.3	67
100	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
101	Integrating diffusion maps with umbrella sampling: Application to alanine dipeptide. Journal of Chemical Physics, 2011, 134, 135103.	3.0	64
102	Free Energy Barriers to Evaporation of Water in Hydrophobic Confinement. Journal of Physical Chemistry B, 2012, 116, 13282-13289.	2.6	62
103	Formation of cyclopentane methane binary clathrate hydrate in brine solutions. Chemical Engineering Science, 2016, 141, 125-132.	3.8	61
104	Estimation of the Characteristic Time Scales in the Supercritical Antisolvent Process. Industrial & Engineering Chemistry Research, 2003, 42, 3156-3162.	3.7	60
105	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
106	Concentration Fluctuations and Capacitive Response in Dense Ionic Solutions. Journal of Physical Chemistry Letters, 2016, 7, 2333-2338.	4.6	60
107	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
108	Theory of supercooled liquids and glasses: Energy landscape and statistical geometry perspectives. Advances in Chemical Engineering, 2001, 28, 21-79.	0.9	58

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109	An Experimental and Computational Investigation of Spontaneous Lasso Formation in Microcin J25. Biophysical Journal, 2010, 99, 3056-3065.	0.5	58
110	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
111	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
112	Applications of Supercritical Fluids in the Controlled Release of Drugs. ACS Symposium Series, 1992, , 238-257.	0.5	57
113	A kinetic theory of homogeneous bubble nucleation. Journal of Chemical Physics, 2003, 118, 768-783.	3.0	57
114	The distribution of tetravalent network glasses. Molecular Physics, 1996, 88, 1293-1316.	1.7	56
115	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
116	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
117	Computational probes of molecular motion in the Lewis-WahnstrÃ¶m model for ortho-terphenyl. Journal of Chemical Physics, 2006, 125, 174507.	3.0	55
118	Molecular dynamics study of solute-solute microstructure in attractive and repulsive supercritical mixtures. Industrial & Engineering Chemistry Research, 1992, 31, 1391-1397.	3.7	54
119	One substance, two liquids?. Nature, 1998, 392, 127-128.	27.8	54
120	Dynamic heterogeneity and non-Gaussian behaviour in a model supercooled liquid. Journal of Physics Condensed Matter, 2005, 17, S4035-S4046.	1.8	54
121	Energy landscapes, ideal glasses, and their equation of state. Journal of Chemical Physics, 2003, 118, 8821-8830.	3.0	53
122	Recent advances in molecular simulation: A chemical engineering perspective. AICHE Journal, 2015, 61, 370-383.	3.6	53
123	Systematic characterization of protein folding pathways using diffusion maps: Application to Trp-cage miniprotein. Journal of Chemical Physics, 2015, 142, 085101.	3.0	53
124	Cross-flow, solid-state electrochemical reactors: a steady state analysis. Industrial & Engineering Chemistry Fundamentals, 1985, 24, 316-324.	0.7	52
125	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
126	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

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127	A Calorimetric and Spectroscopic Study of DNA at Low Hydration. Journal of Physical Chemistry B, 2004, 108, 3098-3106.	2.6	50
128	Structural and mechanical properties of glassy water in nanoscale confinement. Faraday Discussions, 2009, 141, 359-376.	3.2	49
129	A computational study of metastability in vaporâ€"liquid equilibrium. Chemical Engineering Science, 1994, 49, 2717-2734.	3.8	48
130	Structural order in glassy water. Physical Review E, 2005, 71, 061505.	2.1	48
131	Evaporation Length Scales of Confined Water and Some Common Organic Liquids. Journal of Physical Chemistry Letters, 2011, 2, 1000-1003.	4.6	48
132	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
133	Infinite dilution fugacity coefficients and the general behavior of dilute binary systems. AICHE Journal, 1986, 32, 1253-1262.	3.6	47
134	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
135	Disproportionation of toluene over ZSMâ€“5 under near-critical conditions. AICHE Journal, 1988, 34, 1211-1214.	3.6	47
136	Phase transitions, Kauzmann curves, and inverse melting. Biophysical Chemistry, 2003, 105, 211-220.	2.8	47
137	Forward flux sampling calculation of homogeneous nucleation rates from aqueous NaCl solutions. Journal of Chemical Physics, 2018, 148, 044505.	3.0	47
138	On the use of the Verlet neighbor list in molecular dynamics. Computer Physics Communications, 1990, 60, 215-224.	7.5	46
139	Waterlike glass polyamorphism in a monoatomic isotropic Jagla model. Journal of Chemical Physics, 2011, 134, 064507.	3.0	46
140	Monte Carlo Simulations of High-Pressure Phase Equilibria of CO₂â€“H₂O Mixtures. Journal of Physical Chemistry B, 2011, 115, 6629-6635.	2.6	45
141	Supercritical Fluids: Fundamentals and Applications. , 1994, , 30-35.		45
142	Protein purification with vapor-phase carbon dioxide. , 1999, 62, 247-258.		44
143	Local Density Augmentation in Supercritical Solutions. ACS Symposium Series, 1992, , 60-72.	0.5	43
144	Simulations of vaporâ€“liquid phase equilibrium and interfacial tension in the CO₂â€“H₂Oâ€“NaCl system. AICHE Journal, 2013, 59, 3514-3522.	3.6	43

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145	A Water-Explicit Lattice Model of Heat-, Cold-, and Pressure-Induced Protein Unfolding. Biophysical Journal, 2007, 93, 4116-4127.	0.5	42
146	Loss of tensile strength in liquids without property discontinuities: A thermodynamic analysis. Journal of Chemical Physics, 1987, 86, 2229-2235.	3.0	41
147	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
148	Model Energy Landscapes. Journal of Physical Chemistry B, 2003, 107, 14434-14442.	2.6	40
149	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
150	Molecular Dynamics Simulations of Water Sorption in a Perfluorosulfonic Acid Membrane. Journal of Physical Chemistry B, 2013, 117, 12649-12660.	2.6	40
151	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
152	Steady-state analysis of high temperature fuel cells. Chemical Engineering Science, 1983, 38, 1817-1829.	3.8	39
153	Stability and tensile strength of liquids exhibiting density maxima. AICHE Journal, 1988, 34, 447-455.	3.6	38
154	Clustering in supercritical mixtures: Theory, applications and simulations. Fluid Phase Equilibria, 1989, 52, 347-356.	2.5	38
155	Solids Formation After the Expansion of Supercritical Mixtures. ACS Symposium Series, 1989, , 355-378.	0.5	38
156	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
157	Properties of model atomic free-standing thin films. Journal of Chemical Physics, 2011, 134, 114524.	3.0	38
158	Formation kinetics of cyclopentaneâ€“methane binary clathrate hydrate. Chemical Engineering Science, 2014, 119, 147-157.	3.8	37
159	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
160	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
161	Statistical geometry of cavities in a metastable confined fluid. Physical Review E, 2000, 62, 538-544.	2.1	36
162	A statistical mechanical model for inverse melting. Journal of Chemical Physics, 2003, 119, 4582-4591.	3.0	36

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163	When a phase is born. Nature, 2006, 441, 168-169.	27.8	36
164	Distinguishing Vibrational and Structural Equilibration Contributions to Thermal Expansion. Journal of Physical Chemistry B, 1999, 103, 4052-4059.	2.6	35
165	Resolving vibrational and structural contributions to isothermal compressibility. Journal of Chemical Physics, 1998, 109, 3983-3988.	3.0	34
166	Flat-Histogram Dynamics and Optimization in Density of States Simulations of Fluidsâ€. Journal of Physical Chemistry B, 2004, 108, 19748-19755.	2.6	34
167	Dissecting the Energetics of Hydrophobic Hydration of Polypeptides. Journal of Physical Chemistry B, 2011, 115, 14859-14865.	2.6	34
168	Structure, dynamics, and thermodynamics of a family of potentials with tunable softness. Journal of Chemical Physics, 2011, 135, 084513.	3.0	34
169	The effect of substrate on thermodynamic and kinetic anisotropies in atomic thin films. Journal of Chemical Physics, 2014, 141, 024506.	3.0	34
170	Long-term and high-temperature storage of supercritically-processed microparticulate protein powders. Pharmaceutical Research, 1997, 14, 1370-1378.	3.5	33
171	Structure and Energetics of Thin Film Water. Journal of Physical Chemistry C, 2011, 115, 4624-4635.	3.1	33
172	Supercritical antisolvent process for a series of substituted para-linked aromatic polyamides. Macromolecules, 1995, 28, 1316-1317.	4.8	32
173	Molecular dynamics simulation of infinitely dilute solutions of benzene in supercritical CO2. Fluid Phase Equilibria, 1996, 116, 282-288.	2.5	32
174	Solid-State Stabilization of Î±-Chymotrypsin and Catalase with Carbohydrates. Industrial & Engineering Chemistry Research, 2006, 45, 5134-5147.	3.7	32
175	Stability of proteins in the presence of carbohydrates; experiments and modeling using scaled particle theory. Biophysical Chemistry, 2007, 127, 51-63.	2.8	32
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	Density fluctuations in many-body systems. Physical Review E, 1998, 58, 7369-7380.	2.1	30
178	Soluteâ€“solute correlations in infinitely dilute supercritical mixtures. Journal of Chemical Physics, 1992, 97, 504-507.	3.0	29
179	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
180	On the relationship between principal fluctuations and stability coefficients in multicomponent systems. Journal of Chemical Physics, 1986, 84, 1778-1787.	3.0	28

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181	On the entropy changes and fluctuations occurring near a tensile instability. Journal of Chemical Physics, 1986, 85, 4005-4010.	3.0	28
182	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
183	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
184	Effects of nonpolar solutes on the thermodynamic response functions of aqueous mixtures. Journal of Chemical Physics, 2005, 123, 164503.	3.0	28
185	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
186	Hydrogen bond strength and network structure effects on hydration of non-polar molecules. Physical Chemistry Chemical Physics, 2011, 13, 2748-2757.	2.8	28
187	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
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