

Pablo Debenedetti

List of Publications by Year in descending order

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324
papers

28,978
citations

5430

85
h-index

6872

160
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344
all docs

344
docs citations

344
times ranked

17376
citing authors

#	ARTICLE	IF	CITATIONS
1	Supercooled liquids and the glass transition. <i>Nature</i> , 2001, 410, 259-267.	13.7	3,877
2	Relationship between structural order and the anomalies of liquid water. <i>Nature</i> , 2001, 409, 318-321.	13.7	1,320
3	Is Random Close Packing of Spheres Well Defined?. <i>Physical Review Letters</i> , 2000, 84, 2064-2067.	2.9	1,173
4	Supercooled and glassy water. <i>Journal of Physics Condensed Matter</i> , 2003, 15, R1669-R1726.	0.7	956
5	Supercritical fluids as solvents for chemical and materials processing. <i>Nature</i> , 1996, 383, 313-318.	13.7	849
6	Signatures of distinct dynamical regimes in the energy landscape of a glass-forming liquid. <i>Nature</i> , 1998, 393, 554-557.	13.7	676
7	Singularity-free interpretation of the thermodynamics of supercooled water. <i>Physical Review E</i> , 1996, 53, 6144-6154.	0.8	499
8	Supercooled and Glassy Water. <i>Physics Today</i> , 2003, 56, 40-46.	0.3	470
9	Metastable liquidâ€“liquid transition in a molecular model of water. <i>Nature</i> , 2014, 510, 385-388.	13.7	431
10	Effect of Surface Polarity on Water Contact Angle and Interfacial Hydration Structure. <i>Journal of Physical Chemistry B</i> , 2007, 111, 9581-9587.	1.2	416
11	Particle formation with supercritical fluidsâ€”a review. <i>Journal of Aerosol Science</i> , 1991, 22, 555-584.	1.8	330
12	Effect of pressure on the phase behavior and structure of water confined between nanoscale hydrophobic and hydrophilic plates. <i>Physical Review E</i> , 2006, 73, 041604.	0.8	319
13	Formation of microparticulate protein powder using a supercritical fluid antisolvent. <i>Biotechnology and Bioengineering</i> , 1993, 41, 341-346.	1.7	286
14	Towards a quantification of disorder in materials: Distinguishing equilibrium and glassy sphere packings. <i>Physical Review E</i> , 2000, 62, 993-1001.	0.8	258
15	The evaporation rate, free energy, and entropy of amorphous water at 150 K. <i>Journal of Chemical Physics</i> , 1996, 105, 240-244.	1.2	251
16	Hydrophobicity of protein surfaces: Separating geometry from chemistry. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2008, 105, 2274-2279.	3.3	242
17	Hydration Behavior under Confinement by Nanoscale Surfaces with Patterned Hydrophobicity and Hydrophilicity. <i>Journal of Physical Chemistry C</i> , 2007, 111, 1323-1332.	1.5	224
18	Glass Transition Thermodynamics and Kinetics. <i>Annual Review of Condensed Matter Physics</i> , 2013, 4, 263-285.	5.2	217

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19	Molecular structural order and anomalies in liquid silica. <i>Physical Review E</i> , 2002, 66, 011202.	0.8	215
20	Generalization of the Wang-Landau method for off-lattice simulations. <i>Physical Review E</i> , 2002, 66, 056703.	0.8	209
21	Phase Transitions Induced by Nanoconfinement in Liquid Water. <i>Physical Review Letters</i> , 2009, 102, 050603.	2.9	208
22	Solute-solvent interactions in infinitely dilute supercritical mixtures: A molecular dynamics investigation. <i>Journal of Chemical Physics</i> , 1989, 91, 7075-7084.	1.2	201
23	Direct calculation of ice homogeneous nucleation rate for a molecular model of water. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2015, 112, 10582-10588.	3.3	199
24	Precipitation of Proteins in Supercritical Carbon Dioxide. <i>Journal of Pharmaceutical Sciences</i> , 1996, 85, 586-594.	1.6	185
25	Formation of bioerodible polymeric microspheres and microparticles by rapid expansion of supercritical solutions. <i>Biotechnology Progress</i> , 1991, 7, 403-411.	1.3	182
26	Second critical point in two realistic models of water. <i>Science</i> , 2020, 369, 289-292.	6.0	176
27	Atomistic Simulation of Aging and Rejuvenation in Glasses. <i>Physical Review Letters</i> , 2000, 84, 1471-1474.	2.9	175
28	Clustering in dilute, binary supercritical mixtures: A fluctuation analysis. <i>Chemical Engineering Science</i> , 1987, 42, 2203-2212.	1.9	166
29	A computational study of hydration, solution structure, and dynamics in dilute carbohydrate solutions. <i>Journal of Chemical Physics</i> , 2005, 122, 204511.	1.2	166
30	Rapid expansion of supercritical solutions (ress): fundamentals and applications. <i>Fluid Phase Equilibria</i> , 1993, 82, 311-321.	1.4	162
31	A single-bond approach to orientation-dependent interactions and its implications for liquid water. <i>Journal of Chemical Physics</i> , 1999, 111, 2647-2656.	1.2	157
32	Homogeneous Nucleation of Methane Hydrate in Microsecond Molecular Dynamics Simulations. <i>Journal of Physical Chemistry Letters</i> , 2012, 3, 2942-2947.	2.1	156
33	Effect of Temperature on the Structure and Phase Behavior of Water Confined by Hydrophobic, Hydrophilic, and Heterogeneous Surfaces. <i>Journal of Physical Chemistry B</i> , 2009, 113, 13723-13734.	1.2	155
34	Advances in Computational Studies of the Liquid-Liquid Transition in Water and Water-Like Models. <i>Chemical Reviews</i> , 2018, 118, 9129-9151.	23.0	152
35	Evaporation rate of water in hydrophobic confinement. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2012, 109, 4365-4370.	3.3	150
36	Attractive, weakly attractive, and repulsive near-critical systems. <i>Journal of Chemical Physics</i> , 1989, 90, 4528-4536.	1.2	148

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37	Structural precursor to freezing in the hard-disk and hard-sphere systems. <i>Physical Review E</i> , 1998, 58, 3083-3088.	0.8	147
38	Statistical geometry of particle packings. Algorithm for exact determination of connectivity, volume, and surface areas of void space in monodisperse and polydisperse sphere packings. <i>Physical Review E</i> , 1997, 56, 5524-5532.	0.8	145
39	Two-state thermodynamics and the possibility of a liquid-liquid phase transition in supercooled TIP4P/2005 water. <i>Journal of Chemical Physics</i> , 2016, 144, 144504.	1.2	145
40	Liquid-liquid transition in ST2 water. <i>Journal of Chemical Physics</i> , 2012, 137, 214505.	1.2	144
41	Diffusion and mass transfer in supercritical fluids. <i>AIChE Journal</i> , 1986, 32, 2034-2046.	1.8	143
42	Homogeneous nucleation in supercritical fluids. <i>AIChE Journal</i> , 1990, 36, 1289-1298.	1.8	143
43	Thermodynamic implications of confinement for a waterlike fluid. <i>Journal of Chemical Physics</i> , 2001, 114, 2401-2418.	1.2	143
44	Effect of Surface Polarity on the Structure and Dynamics of Water in Nanoscale Confinement. <i>Journal of Physical Chemistry B</i> , 2009, 113, 1438-1446.	1.2	143
45	Systematic determination of order parameters for chain dynamics using diffusion maps. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2010, 107, 13597-13602.	3.3	142
46	Nonlinear dimensionality reduction in molecular simulation: The diffusion map approach. <i>Chemical Physics Letters</i> , 2011, 509, 1-11.	1.2	141
47	Low-temperature fluid-phase behavior of ST2 water. <i>Journal of Chemical Physics</i> , 2009, 131, 104508.	1.2	139
48	Precipitation of poly(l-lactic acid) and composite poly(l-lactic acid)-pyrene particles by rapid expansion of supercritical solutions. <i>Journal of Supercritical Fluids</i> , 1994, 7, 9-29.	1.6	136
49	A computational investigation of thermodynamics, structure, dynamics and solvation behavior in modified water models. <i>Journal of Chemical Physics</i> , 2008, 128, 124511.	1.2	134
50	The Kauzmann Paradox Revisited. <i>Journal of Physical Chemistry B</i> , 2001, 105, 11809-11816.	1.2	131
51	Solubility and Molecular Conformations of <i>n</i> -Alkane Chains in Water. <i>Journal of Physical Chemistry B</i> , 2009, 113, 6405-6414.	1.2	131
52	Application of supercritical fluids for the production of sustained delivery devices. <i>Journal of Controlled Release</i> , 1993, 24, 27-44.	4.8	128
53	Structure and Dynamics in Concentrated, Amorphous Carbohydrate-Water Systems by Molecular Dynamics Simulation. <i>Journal of Physical Chemistry B</i> , 1999, 103, 7308-7318.	1.2	128
54	An improved Monte Carlo method for direct calculation of the density of states. <i>Journal of Chemical Physics</i> , 2003, 119, 9406-9411.	1.2	128

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55	Quantification of order in the Lennard-Jones system. <i>Journal of Chemical Physics</i> , 2003, 118, 2256-2263.	1.2	124
56	Polyamorphism and density anomalies in network-forming fluids: Zeroth- and first-order approximations. <i>Journal of Chemical Physics</i> , 1996, 105, 658-672.	1.2	122
57	Computational Studies of Pressure, Temperature, and Surface Effects on the Structure and Thermodynamics of Confined Water. <i>Annual Review of Physical Chemistry</i> , 2012, 63, 179-200.	4.8	120
58	Singularity-free interpretation of the thermodynamics of supercooled water. II. Thermal and volumetric behavior. <i>Journal of Chemical Physics</i> , 1998, 109, 626-633.	1.2	119
59	A simple molecular thermodynamic theory of hydrophobic hydration. <i>Journal of Chemical Physics</i> , 2002, 116, 2907-2921.	1.2	118
60	Liquid-Liquid Immiscibility in Pure Fluids: Polyamorphism in Simulations of a Network-Forming Fluid. <i>Physical Review Letters</i> , 1996, 77, 4386-4389.	2.9	117
61	Numerical modeling of mass transfer in the supercritical antisolvent process: miscible conditions. <i>Journal of Supercritical Fluids</i> , 2000, 18, 11-24.	1.6	114
62	Free volume in the hard sphere liquid. <i>Molecular Physics</i> , 1998, 95, 289-297.	0.8	112
63	Signatures of a liquid-liquid transition in an ab initio deep neural network model for water. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2020, 117, 26040-26046.	3.3	112
64	Numerical modeling of mass transfer in the supercritical antisolvent process. <i>Journal of Supercritical Fluids</i> , 1999, 16, 167-181.	1.6	111
65	Structure of the first- and second-neighbor shells of simulated water: Quantitative relation to translational and orientational order. <i>Physical Review E</i> , 2007, 76, 051201.	0.8	109
66	Molecular Dynamics Study of Carbon Dioxide Hydrate Dissociation. <i>Journal of Physical Chemistry A</i> , 2011, 115, 6102-6111.	1.1	107
67	Two-structure thermodynamics for the TIP4P/2005 model of water covering supercooled and deeply stretched regions. <i>Journal of Chemical Physics</i> , 2017, 146, 034502.	1.2	107
68	Family of tunable spherically symmetric potentials that span the range from hard spheres to waterlike behavior. <i>Physical Review E</i> , 2006, 73, 051204.	0.8	106
69	Enhanced surface hydrophobicity by coupling of surface polarity and topography. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2009, 106, 15181-15185.	3.3	106
70	Effects of process conditions on crystals obtained from supercritical mixtures. <i>AIChE Journal</i> , 1989, 35, 325-328.	1.8	104
71	The Equation of State of an Energy Landscape. <i>Journal of Physical Chemistry B</i> , 1999, 103, 7390-7397.	1.2	103
72	Cooperative Origin of Low-Density Domains in Liquid Water. <i>Physical Review Letters</i> , 2002, 89, 215503.	2.9	103

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73	Differential Scanning Calorimetry Studies of Clathrate Hydrate Formation. <i>Journal of Physical Chemistry B</i> , 2004, 108, 16717-16722.	1.2	102
74	Spinodal curve of some supercooled liquids. <i>The Journal of Physical Chemistry</i> , 1991, 95, 4540-4551.	2.9	101
75	Influence of solute-solvent asymmetry upon the behavior of dilute supercritical mixtures. <i>The Journal of Physical Chemistry</i> , 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. <i>The Journal of Physical Chemistry</i> , 1995, 99, 3781-3792.	2.9	98
77	Mathematical modeling of aerosol formation by rapid expansion of supercritical solutions in a converging nozzle. <i>Journal of Aerosol Science</i> , 1993, 24, 445-469.	1.8	97
78	Evolution from Surface-Influenced to Bulk-Like Dynamics in Nanoscopically Confined Water. <i>Journal of Physical Chemistry B</i> , 2009, 113, 7973-7976.	1.2	97
79	Mathematical modeling of nucleation and growth of particles formed by the rapid expansion of a supercritical solution under subsonic conditions. <i>Journal of Supercritical Fluids</i> , 2002, 23, 65-80.	1.6	96
80	Two-state thermodynamics of the ST2 model for supercooled water. <i>Journal of Chemical Physics</i> , 2014, 140, 104502.	1.2	96
81	Pathways to dewetting in hydrophobic confinement. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2015, 112, 8181-8186.	3.3	95
82	Constraints, metastability, and inherent structures in liquids. <i>Physical Review E</i> , 1997, 55, 5522-5534.	0.8	94
83	Water-like solvation thermodynamics in a spherically symmetric solvent model with two characteristic lengths. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2007, 104, 20177-20182.	3.3	93
84	Computational Investigation of Order, Structure, and Dynamics in Modified Water Models. <i>Journal of Physical Chemistry B</i> , 2005, 109, 6527-6534.	1.2	88
85	The liquid-liquid transition in supercooled ST2 water: a comparison between umbrella sampling and well-tempered metadynamics. <i>Faraday Discussions</i> , 2013, 167, 77.	1.6	85
86	Statistical geometry of particle packings. II. Weak spots in liquids. <i>Physical Review E</i> , 1997, 56, 5533-5543.	0.8	83
87	Lindemann measures for the solid-liquid phase transition. <i>Journal of Chemical Physics</i> , 2007, 126, 204508.	1.2	83
88	Relaxation processes in liquids: Variations on a theme by Stokes and Einstein. <i>Journal of Chemical Physics</i> , 2013, 138, 12A526.	1.2	83
89	Engineering pharmaceutical stability with amorphous solids. <i>AIChE Journal</i> , 2002, 48, 1140-1144.	1.8	82
90	Supercritical antisolvent process for substituted para-linked aromatic polyamides: phase equilibrium and morphology study. <i>Macromolecules</i> , 1993, 26, 6207-6210.	2.2	81

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91	A computational study of homogeneous liquid-vapor nucleation in the Lennard-Jones fluid. <i>Journal of Chemical Physics</i> , 1999, 111, 3581-3589.	1.2	81
92	On the calculation of solubilities via direct coexistence simulations: Investigation of NaCl aqueous solutions and Lennard-Jones binary mixtures. <i>Journal of Chemical Physics</i> , 2016, 145, 154111.	1.2	80
93	The molecular basis of temperature effects in supercritical extraction. <i>AIChE Journal</i> , 1988, 34, 645-657.	1.8	77
94	Density-functional study of homogeneous bubble nucleation in the stretched Lennard-Jones fluid. <i>Journal of Chemical Physics</i> , 2001, 114, 4149-4159.	1.2	75
95	Reversible work of formation of an embryo of a new phase within a uniform macroscopic mother phase. <i>Journal of Chemical Physics</i> , 1998, 108, 5498-5505.	1.2	70
96	Energy landscape diversity and supercooled liquid properties. <i>Journal of Chemical Physics</i> , 2002, 116, 3353-3361.	1.2	70
97	Nucleation in aqueous NaCl solutions shifts from 1-step to 2-step mechanism on crossing the spinodal. <i>Journal of Chemical Physics</i> , 2019, 150, 124502.	1.2	70
98	Anomalous Capacitance Maximum of the Glassy Carbon-Ionic Liquid Interface through Dilution with Organic Solvents. <i>Journal of Physical Chemistry Letters</i> , 2015, 6, 2644-2648.	2.1	69
99	Secondary Structure Characterization of Microparticulate Insulin Powders. <i>Journal of Pharmaceutical Sciences</i> , 1994, 83, 1651-1656.	1.6	67
100	Suppression of sub-surface freezing in free-standing thin films of a coarse-grained model of water. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 25916-25927.	1.3	65
101	Integrating diffusion maps with umbrella sampling: Application to alanine dipeptide. <i>Journal of Chemical Physics</i> , 2011, 134, 135103.	1.2	64
102	Free Energy Barriers to Evaporation of Water in Hydrophobic Confinement. <i>Journal of Physical Chemistry B</i> , 2012, 116, 13282-13289.	1.2	62
103	Formation of cyclopentane methane binary clathrate hydrate in brine solutions. <i>Chemical Engineering Science</i> , 2016, 141, 125-132.	1.9	61
104	Estimation of the Characteristic Time Scales in the Supercritical Antisolvent Process. <i>Industrial & Engineering Chemistry Research</i> , 2003, 42, 3156-3162.	1.8	60
105	Non-monotonic dependence of water reorientation dynamics on surface hydrophilicity: competing effects of the hydration structure and hydrogen-bond strength. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 19911.	1.3	60
106	Concentration Fluctuations and Capacitive Response in Dense Ionic Solutions. <i>Journal of Physical Chemistry Letters</i> , 2016, 7, 2333-2338.	2.1	60
107	Liquid Structure, Thermodynamics, and Mixing Behavior of Saturated Hydrocarbon Polymers. 1. Cohesive Energy Density and Internal Pressure. <i>Macromolecules</i> , 1998, 31, 6991-6997.	2.2	59
108	Theory of supercooled liquids and glasses: Energy landscape and statistical geometry perspectives. <i>Advances in Chemical Engineering</i> , 2001, 28, 21-79.	0.5	58

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109	An Experimental and Computational Investigation of Spontaneous Lasso Formation in Microcin J25. <i>Biophysical Journal</i> , 2010, 99, 3056-3065.	0.2	58
110	Computational investigation of surface freezing in a molecular model of water. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2017, 114, 3316-3321.	3.3	58
111	Comment on "The putative liquid-liquid transition is a liquid-solid transition in atomistic models of water" [I and II: <i>J. Chem. Phys.</i> 135, 134503 (2011); <i>J. Chem. Phys.</i> 138, 214504 (2013)]. <i>Journal of Chemical Physics</i> , 2018, 148, 137101.	1.2	58
112	Applications of Supercritical Fluids in the Controlled Release of Drugs. <i>ACS Symposium Series</i> , 1992, , 238-257.	0.5	57
113	A kinetic theory of homogeneous bubble nucleation. <i>Journal of Chemical Physics</i> , 2003, 118, 768-783.	1.2	57
114	The distribution of tetravalent network glasses. <i>Molecular Physics</i> , 1996, 88, 1293-1316.	0.8	56
115	Effect of material flexibility on the thermodynamics and kinetics of hydrophobically induced evaporation of water. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2017, 114, E2548-E2555.	3.3	56
116	Fluid-phase behavior of binary mixtures in which one component can have two critical points. <i>Journal of Chemical Physics</i> , 2006, 124, 154503.	1.2	55
117	Computational probes of molecular motion in the Lewis-Wahnström model for ortho-terphenyl. <i>Journal of Chemical Physics</i> , 2006, 125, 174507.	1.2	55
118	Molecular dynamics study of solute-solute microstructure in attractive and repulsive supercritical mixtures. <i>Industrial & Engineering Chemistry Research</i> , 1992, 31, 1391-1397.	1.8	54
119	One substance, two liquids?. <i>Nature</i> , 1998, 392, 127-128.	13.7	54
120	Dynamic heterogeneity and non-Gaussian behaviour in a model supercooled liquid. <i>Journal of Physics Condensed Matter</i> , 2005, 17, S4035-S4046.	0.7	54
121	Energy landscapes, ideal glasses, and their equation of state. <i>Journal of Chemical Physics</i> , 2003, 118, 8821-8830.	1.2	53
122	Recent advances in molecular simulation: A chemical engineering perspective. <i>AIChE Journal</i> , 2015, 61, 370-383.	1.8	53
123	Systematic characterization of protein folding pathways using diffusion maps: Application to Trp-cage miniprotein. <i>Journal of Chemical Physics</i> , 2015, 142, 085101.	1.2	53
124	Cross-flow, solid-state electrochemical reactors: a steady state analysis. <i>Industrial & Engineering Chemistry Fundamentals</i> , 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. <i>Journal of Physical Chemistry B</i> , 2012, 116, 8095-8104.	1.2	52
126	Potential energy landscape signatures of slow dynamics in glass forming liquids. <i>Physica A: Statistical Mechanics and Its Applications</i> , 1999, 270, 301-308.	1.2	50

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127	A Calorimetric and Spectroscopic Study of DNA at Low Hydration. <i>Journal of Physical Chemistry B</i> , 2004, 108, 3098-3106.	1.2	50
128	Structural and mechanical properties of glassy water in nanoscale confinement. <i>Faraday Discussions</i> , 2009, 141, 359-376.	1.6	49
129	A computational study of metastability in vapor-liquid equilibrium. <i>Chemical Engineering Science</i> , 1994, 49, 2717-2734.	1.9	48
130	Structural order in glassy water. <i>Physical Review E</i> , 2005, 71, 061505.	0.8	48
131	Evaporation Length Scales of Confined Water and Some Common Organic Liquids. <i>Journal of Physical Chemistry Letters</i> , 2011, 2, 1000-1003.	2.1	48
132	Computational investigation of cold denaturation in the Trp-cage miniprotein. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2016, 113, 8991-8996.	3.3	48
133	Infinite dilution fugacity coefficients and the general behavior of dilute binary systems. <i>AIChE Journal</i> , 1986, 32, 1253-1262.	1.8	47
134	On the nature of the tensile instability in metastable liquids and its relationship to density anomalies. <i>Journal of Chemical Physics</i> , 1986, 84, 3339-3345.	1.2	47
135	Disproportionation of toluene over ZSM-5 under near-critical conditions. <i>AIChE Journal</i> , 1988, 34, 1211-1214.	1.8	47
136	Phase transitions, Kauzmann curves, and inverse melting. <i>Biophysical Chemistry</i> , 2003, 105, 211-220.	1.5	47
137	Forward flux sampling calculation of homogeneous nucleation rates from aqueous NaCl solutions. <i>Journal of Chemical Physics</i> , 2018, 148, 044505.	1.2	47
138	On the use of the Verlet neighbor list in molecular dynamics. <i>Computer Physics Communications</i> , 1990, 60, 215-224.	3.0	46
139	Waterlike glass polyamorphism in a monoatomic isotropic Jagla model. <i>Journal of Chemical Physics</i> , 2011, 134, 064507.	1.2	46
140	Monte Carlo Simulations of High-Pressure Phase Equilibria of CO ₂ -H ₂ O Mixtures. <i>Journal of Physical Chemistry B</i> , 2011, 115, 6629-6635.	1.2	45
141	<i>Supercritical Fluids: Fundamentals and Applications</i> . , 1994, , 30-35.		45
142	Protein purification with vapor-phase carbon dioxide. , 1999, 62, 247-258.		44
143	Local Density Augmentation in Supercritical Solutions. <i>ACS Symposium Series</i> , 1992, , 60-72.	0.5	43
144	Simulations of vapor-liquid phase equilibrium and interfacial tension in the CO ₂ -H ₂ O-NaCl system. <i>AIChE Journal</i> , 2013, 59, 3514-3522.	1.8	43

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145	A Water-Explicit Lattice Model of Heat-, Cold-, and Pressure-Induced Protein Unfolding. <i>Biophysical Journal</i> , 2007, 93, 4116-4127.	0.2	42
146	Loss of tensile strength in liquids without property discontinuities: A thermodynamic analysis. <i>Journal of Chemical Physics</i> , 1987, 86, 2229-2235.	1.2	41
147	Integral equation study of microstructure and solvation in model attractive and repulsive supercritical mixtures. <i>Industrial & Engineering Chemistry Research</i> , 1993, 32, 2118-2128.	1.8	41
148	Model Energy Landscapes. <i>Journal of Physical Chemistry B</i> , 2003, 107, 14434-14442.	1.2	40
149	A computational investigation of the phase behavior and capillary sublimation of water confined between nanoscale hydrophobic plates. <i>Journal of Chemical Physics</i> , 2012, 137, 144501.	1.2	40
150	Molecular Dynamics Simulations of Water Sorption in a Perfluorosulfonic Acid Membrane. <i>Journal of Physical Chemistry B</i> , 2013, 117, 12649-12660.	1.2	40
151	Combined molecular dynamics and neural network method for predicting protein antifreeze activity. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2018, 115, 13252-13257.	3.3	40
152	Steady-state analysis of high temperature fuel cells. <i>Chemical Engineering Science</i> , 1983, 38, 1817-1829.	1.9	39
153	Stability and tensile strength of liquids exhibiting density maxima. <i>AIChE Journal</i> , 1988, 34, 447-455.	1.8	38
154	Clustering in supercritical mixtures: Theory, applications and simulations. <i>Fluid Phase Equilibria</i> , 1989, 52, 347-356.	1.4	38
155	Solids Formation After the Expansion of Supercritical Mixtures. <i>ACS Symposium Series</i> , 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. <i>Macromolecules</i> , 1998, 31, 6998-7002.	2.2	38
157	Properties of model atomic free-standing thin films. <i>Journal of Chemical Physics</i> , 2011, 134, 114524.	1.2	38
158	Formation kinetics of cyclopentane-methane binary clathrate hydrate. <i>Chemical Engineering Science</i> , 2014, 119, 147-157.	1.9	37
159	Computational Study of the Stability of the Miniprotein Trp-Cage, the GB1 $\hat{1}^2$ -Hairpin, and the AK16 Peptide, under Negative Pressure. <i>Journal of Physical Chemistry B</i> , 2014, 118, 7761-7769.	1.2	37
160	Phase Equilibrium of Water with Hexagonal and Cubic Ice Using the SCAN Functional. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 3065-3077.	2.3	37
161	Statistical geometry of cavities in a metastable confined fluid. <i>Physical Review E</i> , 2000, 62, 538-544.	0.8	36
162	A statistical mechanical model for inverse melting. <i>Journal of Chemical Physics</i> , 2003, 119, 4582-4591.	1.2	36

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163	When a phase is born. <i>Nature</i> , 2006, 441, 168-169.	13.7	36
164	Distinguishing Vibrational and Structural Equilibration Contributions to Thermal Expansion. <i>Journal of Physical Chemistry B</i> , 1999, 103, 4052-4059.	1.2	35
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