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 g-index
344 all docs	344 docs citations	344 times ranked	17376 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.	2.1	25
2	Liquidâ€“liquid criticality in the WAIL water model. Journal of Chemical Physics, 2022, 157, .	1.2	20
3	Thermodynamics of DNA Hybridization from Atomistic Simulations. Journal of Physical Chemistry B, 2021, 125, 771-779.	1.2	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.	2.3	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.	1.2	3
6	Manifestations of metastable criticality in the long-range structure of model water glasses. Nature Communications, 2021, 12, 3398.	5.8	14
7	Effect of configuration-dependent multi-body forces on interconversion kinetics of a chiral tetramer model. Journal of Chemical Physics, 2021, 155, 084105.	1.2	8
8	Thermodynamics and kinetics of crystallization in deeply supercooled Stillingerâ€“Weber silicon. Journal of Chemical Physics, 2021, 155, 194502.	1.2	7
9	Interconversion-controlled liquidâ€“liquid phase separation in a molecular chiral model. Journal of Chemical Physics, 2021, 155, 204502.	1.2	9
10	A Computational Study of RNA Tetraloop Thermodynamics, Including Misfolded States. Journal of Physical Chemistry B, 2021, 125, 13685-13695.	1.2	5
11	Computational investigation of retroâ€isomer equilibrium structures: Intrinsically disordered, foldable, and cyclic peptides. FEBS Letters, 2020, 594, 104-113.	1.3	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.	3.3	112
13	Second critical point in two realistic models of water. Science, 2020, 369, 289-292.	6.0	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.	2.3	4
15	Stability of Protein Structure during Nanocarrier Encapsulation: Insights on Solvent Effects from Simulations and Spectroscopic Analysis. ACS Nano, 2020, 14, 16962-16972.	7.3	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.	1.2	6
17	Insights into Hydrophobic Ion Pairing from Molecular Simulation and Experiment. ACS Nano, 2020, 14, 6097-6106.	7.3	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.	1.2	19
20	A computational investigation of the thermodynamics of the Stillinger-Weber family of models at supercooled conditions. Molecular Physics, 2019, 117, 3254-3268.	0.8	9
21	Computational Investigation of the Effect of Backbone Chiral Inversions on Polypeptide Structure. Biophysical Journal, 2019, 116, 46a.	0.2	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.	1.2	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.	1.2	70
24	Computational Investigation of the Effect of Pressure on Protein Stability. Journal of Physical Chemistry Letters, 2019, 10, 1894-1899.	2.1	11
25	Effect of heterochiral inversions on the structure of a Î²â€hairpin peptide. Proteins: Structure, Function and Bioinformatics, 2019, 87, 569-578.	1.5	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.	1.2	9
27	Low temperature protein refolding suggested by molecular simulation. Journal of Chemical Physics, 2019, 151, 185101.	1.2	13
28	Forward flux sampling calculation of homogeneous nucleation rates from aqueous NaCl solutions. Journal of Chemical Physics, 2018, 148, 044505.	1.2	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.	1.2	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.	1.2	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.	1.2	6
32	Waterâ€™s Thermal Pressure Drives the Temperature Dependence of Hydrophobic Hydration. Journal of Physical Chemistry B, 2018, 122, 3620-3625.	1.2	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.	3.3	40
34	Communication: Nucleation rates of supersaturated aqueous NaCl using a polarizable force field. Journal of Chemical Physics, 2018, 149, 141102.	1.2	16
35	Computational Investigation of the Effect of Backbone Chiral Inversions on Polypeptide Structure. Journal of Physical Chemistry B, 2018, 122, 6357-6363.	1.2	10
36	Advances in Computational Studies of the Liquidâ€“Liquid Transition in Water and Water-Like Models. Chemical Reviews, 2018, 118, 9129-9151.	23.0	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.	2.1	3
38	Structural and dynamic properties of liquid tin from a new modified embedded-atom method force field. Physical Review B, 2017, 95, .	1.1	22
39	Molecular modeling and structural characterization of a high glycineâ€“tyrosine hair keratin associated protein. Physical Chemistry Chemical Physics, 2017, 19, 8575-8583.	1.3	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.	3.3	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.	3.3	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.	1.2	107
43	Thermodynamic Anomalies in Stretched Water. Langmuir, 2017, 33, 11771-11778.	1.6	27
44	Effects of disulfide bridges and backbone connectivity on water sorption by protein matrices. Scientific Reports, 2017, 7, 7957.	1.6	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.	1.6	7
46	Perspective: Surface freezing in water: A nexus of experiments and simulations. Journal of Chemical Physics, 2017, 147, 060901.	1.2	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.	0.7	14
48	Chemical physics of water. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, 13325-13326.	3.3	13
49	Communication: Relationship between local structure and the stability of water in hydrophobic confinement. Journal of Chemical Physics, 2017, 147, 241102.	1.2	13
50	Water anomalous thermodynamics, attraction, repulsion, and hydrophobic hydration. Journal of Chemical Physics, 2016, 144, 164501.	1.2	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.	1.2	80
52	Molecular model for chirality phenomena. Journal of Chemical Physics, 2016, 145, 154503.	1.2	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.	1.2	145
54	A cavitation transition in the energy landscape of simple cohesive liquids and glasses. Journal of Chemical Physics, 2016, 145, 211905.	1.2	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.	3.3	48
56	Computational investigation of dynamical transitions in Trp-cage miniprotein powders. Scientific Reports, 2016, 6, 25612.	1.6	15
57	Density and bond-orientational relaxations in supercooled water. Molecular Physics, 2016, 114, 2580-2585.	0.8	14
58	Concentration Fluctuations and Capacitive Response in Dense Ionic Solutions. Journal of Physical Chemistry Letters, 2016, 7, 2333-2338.	2.1	60
59	Formation of cyclopentane methane binary clathrate hydrate in brine solutions. Chemical Engineering Science, 2016, 141, 125-132.	1.9	61
60	Palmer et al. reply. Nature, 2016, 531, E2-E3.	13.7	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.	1.3	28
62	Thermodynamic and kinetic anisotropies in octane thin films. Journal of Chemical Physics, 2015, 143, 214501.	1.2	18
63	Liquid li structure and dynamics: A comparison between OFDFT and second nearestâ€neighbor embeddedâ€atom method. AICHE Journal, 2015, 61, 2841-2853.	1.8	24
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.	1.2	9
65	Recent advances in molecular simulation: A chemical engineering perspective. AICHE Journal, 2015, 61, 370-383.	1.8	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.	2.1	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.	3.3	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.	3.3	95
69	Systematic characterization of protein folding pathways using diffusion maps: Application to Trp-cage miniprotein. Journal of Chemical Physics, 2015, 142, 085101.	1.2	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.	1.2	27
71	The effect of substrate on thermodynamic and kinetic anisotropies in atomic thin films. Journal of Chemical Physics, 2014, 141, 024506.	1.2	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.	1.2	25

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73	Two-state thermodynamics of the ST2 model for supercooled water. Journal of Chemical Physics, 2014, 140, 104502.	1.2	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.	1.3	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.	1.2	11
76	Formation kinetics of cyclopentaneâ€“methane binary clathrate hydrate. Chemical Engineering Science, 2014, 119, 147-157.	1.9	37
77	Molecular Dynamics Simulations of Water Permeation across Nafion Membrane Interfaces. Journal of Physical Chemistry B, 2014, 118, 8798-8807.	1.2	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.	1.2	37
79	Metastable liquidâ€“liquid transition in a molecular model of water. Nature, 2014, 510, 385-388.	13.7	431
80	Simulations of vaporâ€“liquid phase equilibrium and interfacial tension in the CO₂â€“H₂Oâ€“NaCl system. AICHE Journal, 2013, 59, 3514-3522.	1.8	43
81	Molecular Dynamics Simulations of Water Sorption in a Perfluorosulfonic Acid Membrane. Journal of Physical Chemistry B, 2013, 117, 12649-12660.	1.2	40
82	A computational investigation of attrition-enhanced chiral symmetry breaking in conglomerate crystals. Journal of Chemical Physics, 2013, 139, 174503.	1.2	27
83	The liquidâ€“liquid transition in supercooled ST2 water: a comparison between umbrella sampling and well-tempered metadynamics. Faraday Discussions, 2013, 167, 77.	1.6	85
84	Glass Transition Thermodynamics and Kinetics. Annual Review of Condensed Matter Physics, 2013, 4, 263-285.	5.2	217
85	Creation and Persistence of Chiral Asymmetry in a Microscopically Reversible Molecular Model. Journal of Physical Chemistry B, 2013, 117, 602-614.	1.2	10
86	Stretched to the limit. Nature Physics, 2013, 9, 7-8.	6.5	12
87	Temperature and length scale dependence of solvophobic solvation in a single-site water-like liquid. Journal of Chemical Physics, 2013, 138, 064506.	1.2	15
88	Relaxation processes in liquids: Variations on a theme by Stokes and Einstein. Journal of Chemical Physics, 2013, 138, 12A526.	1.2	83
89	A Coarse-Grained Protein Model in a Water-like Solvent. Scientific Reports, 2013, 3, 1841.	1.6	12
90	Modeling simple amphiphilic solutes in a Jagla solvent. Journal of Chemical Physics, 2012, 136, 044511.	1.2	18

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91	Molecular modeling of mechanical stresses on proteins in glassy matrices: Formalism. Journal of Chemical Physics, 2012, 137, 035103.	1.2	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.	1.2	40
93	Thermal Stability of Hydrophobic Helical Oligomers: A Lattice Simulation Study in Explicit Water. Journal of Physical Chemistry B, 2012, 116, 9963-9970.	1.2	0
94	Free Energy Barriers to Evaporation of Water in Hydrophobic Confinement. Journal of Physical Chemistry B, 2012, 116, 13282-13289.	1.2	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.	3.3	150
96	Massively parallel chemical potential calculation on graphics processing units. Computer Physics Communications, 2012, 183, 2054-2062.	3.0	25
97	Phase Behavior of a Lattice Hydrophobic Oligomer in Explicit Water. Journal of Physical Chemistry B, 2012, 116, 9540-9548.	1.2	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.	1.2	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.	4.8	120
100	Liquid-liquid transition in ST2 water. Journal of Chemical Physics, 2012, 137, 214505.	1.2	144
101	Computer Simulation of Water Sorption on Flexible Protein Crystals. Journal of Physical Chemistry Letters, 2012, 3, 2713-2718.	2.1	16
102	Homogeneous Nucleation of Methane Hydrate in Microsecond Molecular Dynamics Simulations. Journal of Physical Chemistry Letters, 2012, 3, 2942-2947.	2.1	156
103	Hydrogen bond strength and network structure effects on hydration of non-polar molecules. Physical Chemistry Chemical Physics, 2011, 13, 2748-2757.	1.3	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.	1.3	60
105	Dissecting the Energetics of Hydrophobic Hydration of Polypeptides. Journal of Physical Chemistry B, 2011, 115, 14859-14865.	1.2	34
106	Tribute to H. Eugene Stanley. Journal of Physical Chemistry B, 2011, 115, 13963-13964.	1.2	0
107	Evaporation Length Scales of Confined Water and Some Common Organic Liquids. Journal of Physical Chemistry Letters, 2011, 2, 1000-1003.	2.1	48
108	Properties of model atomic free-standing thin films. Journal of Chemical Physics, 2011, 134, 114524.	1.2	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.	1.2	34
110	Molecular Dynamics Study of Carbon Dioxide Hydrate Dissociation. Journal of Physical Chemistry A, 2011, 115, 6102-6111.	1.1	107
111	Monte Carlo Simulations of High-Pressure Phase Equilibria of CO₂â€“H₂O Mixtures. Journal of Physical Chemistry B, 2011, 115, 6629-6635.	1.2	45
112	Waterlike glass polyamorphism in a monoatomic isotropic Jagla model. Journal of Chemical Physics, 2011, 134, 064507.	1.2	46
113	Physics and chemistry of water and ice. Physical Chemistry Chemical Physics, 2011, 13, 19660.	1.3	12
114	Structure and Energetics of Thin Film Water. Journal of Physical Chemistry C, 2011, 115, 4624-4635.	1.5	33
115	Nonlinear dimensionality reduction in molecular simulation: The diffusion map approach. Chemical Physics Letters, 2011, 509, 1-11.	1.2	141
116	Integrating diffusion maps with umbrella sampling: Application to alanine dipeptide. Journal of Chemical Physics, 2011, 134, 135103.	1.2	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.	3.3	142
119	An Experimental and Computational Investigation of Spontaneous Lasso Formation in Microcin J25. Biophysical Journal, 2010, 99, 3056-3065.	0.2	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.	1.2	29
121	Chiral symmetry breaking in a microscopic model with asymmetric autocatalysis and inhibition. Journal of Chemical Physics, 2010, 133, 224502.	1.2	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.	3.3	106
123	Low-temperature fluid-phase behavior of ST2 water. Journal of Chemical Physics, 2009, 131, 104508.	1.2	139
124	Hydrate Molecular Ballet. Science, 2009, 326, 1070-1071.	6.0	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.	3.3	28
126	Phase Transitions Induced by Nanoconfinement in Liquid Water. Physical Review Letters, 2009, 102, 050603.	2.9	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.	1.2	143
128	Evolution from Surface-Influenced to Bulk-Like Dynamics in Nanoscopically Confined Water. Journal of Physical Chemistry B, 2009, 113, 7973-7976.	1.2	97
129	Structural and mechanical properties of glassy water in nanoscale confinement. Faraday Discussions, 2009, 141, 359-376.	1.6	49
130	Structureâ€“energy relations in hen egg white lysozyme observed during refolding from a quenched unfolded state. Chemical Communications, 2009, , 4441.	2.2	10
131	Solubility and Molecular Conformations of n-Alkane Chains in Water. Journal of Physical Chemistry B, 2009, 113, 6405-6414.	1.2	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.	1.2	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.	3.3	242
134	The effect of sequence on the conformational stability of a model heteropolymer in explicit water. Journal of Chemical Physics, 2008, 128, 175102.	1.2	15
135	A computational investigation of thermodynamics, structure, dynamics and solvation behavior in modified water models. Journal of Chemical Physics, 2008, 128, 124511.	1.2	134
136	Lindemann measures for the solid-liquid phase transition. Journal of Chemical Physics, 2007, 126, 204508.	1.2	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.	3.3	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.	0.8	109
139	Hydration Behavior under Confinement by Nanoscale Surfaces with Patterned Hydrophobicity and Hydrophilicity. Journal of Physical Chemistry C, 2007, 111, 1323-1332.	1.5	224
140	Effect of Surface Polarity on Water Contact Angle and Interfacial Hydration Structure. Journal of Physical Chemistry B, 2007, 111, 9581-9587.	1.2	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.	1.1	6
142	A Water-Explicit Lattice Model of Heat-, Cold-, and Pressure-Induced Protein Unfolding. Biophysical Journal, 2007, 93, 4116-4127.	0.2	42
143	Stability of proteins in the presence of carbohydrates; experiments and modeling using scaled particle theory. Biophysical Chemistry, 2007, 127, 51-63.	1.5	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.	1.2	55
146	Scaled particle theory for hard sphere pairs. I. Mathematical structure. Journal of Chemical Physics, 2006, 125, 204504.	1.2	17
147	In Honor of Eduardo Glandt. Industrial & Engineering Chemistry Research, 2006, 45, 5419-5420.	1.8	0
148	When a phase is born. Nature, 2006, 441, 168-169.	13.7	36
149	A conformal solution theory for the energy landscape and glass transition of mixtures. Fluid Phase Equilibria, 2006, 241, 147-154.	1.4	17
150	Accurate prediction of clathrate hydrate phase equilibria below 300 K from a simple model. Journal of Petroleum Science and Engineering, 2006, 51, 45-53.	2.1	25
151	Solid-State Stabilization of Î±-Chymotrypsin and Catalase with Carbohydrates. Industrial & Engineering Chemistry Research, 2006, 45, 5134-5147.	1.8	32
152	Family of tunable spherically symmetric potentials that span the range from hard spheres to waterlike behavior. Physical Review E, 2006, 73, 051204.	0.8	106
153	Computational probes of molecular motion in the Lewis-WahnstrÃ¶m model for ortho-terphenyl. Journal of Chemical Physics, 2006, 125, 174507.	1.2	55
154	Scaled particle theory for hard sphere pairs. II. Numerical analysis. Journal of Chemical Physics, 2006, 125, 204505.	1.2	13
155	Effect of pressure on the phase behavior and structure of water confined between nanoscale hydrophobic and hydrophilic plates. Physical Review E, 2006, 73, 041604.	0.8	319
156	Culmination of the 50th year and some changes for the 51st year. AICHE Journal, 2005, 51, 1836-1838.	1.8	0
157	Preface to perspectives. AICHE Journal, 2005, 51, 2370-2370.	1.8	0
158	Structure, dynamics and thermodynamics in complex systems: Theoretical challenges and opportunities. AICHE Journal, 2005, 51, 2391-2395.	1.8	12
159	Preface to perspectives. AICHE Journal, 2005, 51, 3082-3082.	1.8	0
160	Computational characterization of the sequence landscape in simple protein alphabets. Proteins: Structure, Function and Bioinformatics, 2005, 62, 232-243.	1.5	11
161	Dynamic heterogeneity and non-Gaussian behaviour in a model supercooled liquid. Journal of Physics Condensed Matter, 2005, 17, S4035-S4046.	0.7	54
162	Generating inherent structures of liquids: Comparison of local minimization algorithms. Journal of Chemical Physics, 2005, 123, 206101.	1.2	13

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163	Structural order in glassy water. Physical Review E, 2005, 71, 061505.	0.8	48
164	Reply to â€œComment on Test of nonequilibrium thermodynamics in glassy systems: The soft-sphere caseâ€• Physical Review E, 2005, 71, .	0.8	2
165	Effects of nonpolar solutes on the thermodynamic response functions of aqueous mixtures. Journal of Chemical Physics, 2005, 123, 164503.	1.2	28
166	A computational study of hydration, solution structure, and dynamics in dilute carbohydrate solutions. Journal of Chemical Physics, 2005, 122, 204511.	1.2	166
167	Computational Investigation of Order, Structure, and Dynamics in Modified Water Modelsâ€. Journal of Physical Chemistry B, 2005, 109, 6527-6534.	1.2	88
168	Novel Computational Probes of Diffusive Motion. Journal of Physical Chemistry B, 2005, 109, 21329-21333.	1.2	1
169	Alternative View of Self-Diffusion and Shear Viscosityâ€. Journal of Physical Chemistry B, 2005, 109, 6604-6609.	1.2	20
170	Reply to Comment on ÂSupercooled and glassy waterÂ. Journal of Physics Condensed Matter, 2004, 16, 6815-6817.	0.7	13
171	Saddles in the Energy Landscape: Extensivity and Thermodynamic Formalism. Physical Review Letters, 2004, 92, 035506.	2.9	25
172	Flat-Histogram Dynamics and Optimization in Density of States Simulations of Fluidsâ€. Journal of Physical Chemistry B, 2004, 108, 19748-19755.	1.2	34
173	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.	1.0	28
174	A Calorimetric and Spectroscopic Study of DNA at Low Hydration. Journal of Physical Chemistry B, 2004, 108, 3098-3106.	1.2	50
175	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.	6.6	31
176	Frank H. Stillinger, Theoretical Chemist:Â A Tribute. Journal of Physical Chemistry B, 2004, 108, 19569-19570.	1.2	2
177	Differential Scanning Calorimetry Studies of Clathrate Hydrate Formation. Journal of Physical Chemistry B, 2004, 108, 16717-16722.	1.2	102
178	Thermodynamics and the glass transition in model energy landscapes. Physical Review E, 2004, 69, 051102.	0.8	20
179	Inherent-Structure View of Self-Diffusion in Liquids. Journal of Physical Chemistry B, 2004, 108, 6772-6777.	1.2	21
180	Recent Developments in the Theory of Amorphous Aqueous Systems. ChemInform, 2003, 34, no.	0.1	0

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181	Phase transitions, Kauzmann curves, and inverse melting. Biophysical Chemistry, 2003, 105, 211-220.	1.5	47
182	Quantification of order in the Lennard-Jones system. Journal of Chemical Physics, 2003, 118, 2256-2263.	1.2	124
183	Estimation of the Characteristic Time Scales in the Supercritical Antisolvent Process. Industrial & Engineering Chemistry Research, 2003, 42, 3156-3162.	1.8	60
184	Supercooled and glassy water. Journal of Physics Condensed Matter, 2003, 15, R1669-R1726.	0.7	956
185	Model Energy Landscapes. Journal of Physical Chemistry B, 2003, 107, 14434-14442.	1.2	40
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