Pablo Debenedetti

List of Articles by Year
in descending order

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290 peer-reviewed articles	25,168 peer-reviewed citations	6040 79 peer-reviewed h-index	302050 4.71 score
321 documents	28348 doc citations	6980 83 h-index	21663 citing authors

#	Article	IF	Citations
1	On the Possibility of Chiral Symmetry Breaking in Liquid Hydrogen Peroxide. Journal of Physical Chemistry B, 2025, 129, 5335-5342.	2.0	0
2	Computational investigation of water glasses using machine-learning potentials. Proceedings of the National Academy of Sciences of the United States of America, 2025, 122, .	5.2	7
3	A first-principles machine-learning force field for heterogeneous ice nucleation on microcline feldspar. Faraday Discussions, 2024, 249, 98-113.	2.6	34
4	Free-energy landscape and spinodals for the liquid–liquid transition of the TIP4P/2005 and TIP4P/Ice models of water. Journal of Chemical Physics, 2024, 160, .	2.2	18
5	Anneke Levelt Sengers: An international authority in the thermodynamics of fluids and a passionate advocate for women in science. Proceedings of the National Academy of Sciences of the United States of America, 2024, 121, .	5.2	1
6	Formation of dissipative structures in microscopic models of mixtures with species interconversion. Proceedings of the National Academy of Sciences of the United States of America, 2023, 120, .	5.2	15
7	Critical behavior in a chiral molecular model. Journal of Chemical Physics, 2023, 159, .	2.2	10
8	Autobiography of Pablo G. Debenedetti. Journal of Physical Chemistry B, 2023, 127, 8079-8085.	2.0	0
9	Melting curves of ice polymorphs in the vicinity of the liquid–liquid critical point. Journal of Chemical Physics, 2023, 159, .	2.2	6
10	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.	2.9	55
11	Liquid–liquid criticality in the WAIL water model. Journal of Chemical Physics, 2022, 157, .	2.2	42
12	Homogeneous ice nucleation in an ab initio machine-learning model of water. Proceedings of the National Academy of Sciences of the United States of America, 2022, 119, .	5.2	95
13	Fluid–fluid phase transitions in a chiral molecular model. Journal of Chemical Physics, 2022, 157, .	2.2	7
14	Crystal Prediction via Genetic Algorithms in a Model Chiral System. Journal of Physical Chemistry B, 2022, 126, 7771-7780.	2.0	1
15	Liquid-Liquid Transition in Water from First Principles. Physical Review Letters, 2022, 129, .	5.8	73
16	Thermodynamics of DNA Hybridization from Atomistic Simulations. Journal of Physical Chemistry B, 2021, 125, 771-779.	2.0	30
17	Phase Equilibrium of Water with Hexagonal and Cubic Ice Using the SCAN Functional. Journal of Chemical Theory and Computation, 2021, 17, 3065-3077.	3.6	78
18	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.	2.0	10

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19	Manifestations of metastable criticality in the long-range structure of model water glasses. Nature Communications, 2021, 12, .	10.8	29
20	Effect of configuration-dependent multi-body forces on interconversion kinetics of a chiral tetramer model. Journal of Chemical Physics, 2021, 155, .	2.2	11
21	Thermodynamics and kinetics of crystallization in deeply supercooled Stillinger–Weber silicon. Journal of Chemical Physics, 2021, 155, 194502.	2.2	11
22	Interconversion-controlled liquid–liquid phase separation in a molecular chiral model. Journal of Chemical Physics, 2021, 155, .	2.2	14
23	A Computational Study of RNA Tetraloop Thermodynamics, Including Misfolded States. Journal of Physical Chemistry B, 2021, 125, 13685-13695.	2.0	29
24	Computational investigation of retro-isomer equilibrium structures: Intrinsically disordered, foldable, and cyclic peptides. FEBS Letters, 2020, 594, 104-113.	1.8	7
25	Signatures of a liquid–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.	5.2	171
26	Genetic Algorithm Approach for the Optimization of Protein Antifreeze Activity Using Molecular Simulations. Journal of Chemical Theory and Computation, 2020, 16, 7866-7873.	3.6	18
27	Stability of Protein Structure during Nanocarrier Encapsulation: Insights on Solvent Effects from Simulations and Spectroscopic Analysis. ACS Nano, 2020, 14, 16962-16972.	11.5	5
28	The Handedness of DNA Assembly around Carbon Nanotubes Is Determined by the Chirality of DNA. Journal of Physical Chemistry B, 2020, 124, 5362-5369.	2.0	10
29	Insights into Hydrophobic Ion Pairing from Molecular Simulation and Experiment. ACS Nano, 2020, 14, 6097-6106.	11.5	43
30	Water's two-critical-point scenario in the Ising paradigm. Journal of Chemical Physics, 2019, 150, .	2.2	26
31	A computational investigation of the thermodynamics of the Stillinger-Weber family of models at supercooled conditions. Molecular Physics, 2019, 117, 3254-3268.	1.1	9
32	Thermodynamic analysis of the stability of planar interfaces between coexisting phases and its application to supercooled water. Journal of Chemical Physics, 2019, 150, .	2.2	14
33	Nucleation in aqueous NaCl solutions shifts from 1-step to 2-step mechanism on crossing the spinodal. Journal of Chemical Physics, 2019, 150, .	2.2	92
34	Computational Investigation of the Effect of Pressure on Protein Stability. Journal of Physical Chemistry Letters, 2019, 10, 1894-1899.	2.9	15
35	Effect of heterochiral inversions on the structure of a β-hairpin peptide. Proteins: Structure, Function and Bioinformatics, 2019, 87, 569-578.	1.9	11
36	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, .	2.2	11

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37	Low temperature protein refolding suggested by molecular simulation. Journal of Chemical Physics, 2019, 151, .	2.2	14
38	Forward flux sampling calculation of homogeneous nucleation rates from aqueous NaCl solutions. Journal of Chemical Physics, 2018, 148, .	2.2	61
39	A Computational Study of the Ionic Liquid-Induced Destabilization of the Miniprotein Trp-Cage. Journal of Physical Chemistry B, 2018, 122, 5707-5715.	2.0	10
40	Cavitation transition in the energy landscape: Distinct tensile yielding behavior in strongly and weakly attractive systems. Journal of Chemical Physics, 2018, 148, .	2.2	8
41	Water's Thermal Pressure Drives the Temperature Dependence of Hydrophobic Hydration. Journal of Physical Chemistry B, 2018, 122, 3620-3625.	2.0	9
42	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.	5.2	55
43	Communication: Nucleation rates of supersaturated aqueous NaCl using a polarizable force field. Journal of Chemical Physics, 2018, 149, .	2.2	23
44	Computational Investigation of the Effect of Backbone Chiral Inversions on Polypeptide Structure. Journal of Physical Chemistry B, 2018, 122, 6357-6363.	2.0	11
45	Advances in Computational Studies of the Liquid–Liquid Transition in Water and Water-Like Models. Chemical Reviews, 2018, 118, 9129-9151.	42.5	190
46	Microscopic Origin of Hysteresis in Water Sorption on Protein Matrices. Journal of Physical Chemistry Letters, 2017, 8, 1185-1190.	2.9	3
47	Structural and dynamic properties of liquid tin from a new modified embedded-atom method force field. Physical Review B, 2017, 95, .	2.4	33
48	Molecular modeling and structural characterization of a high glycine–tyrosine hair keratin associated protein. Physical Chemistry Chemical Physics, 2017, 19, 8575-8583.	2.0	22
49	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, .	5.2	62
50	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.	5.2	76
51	Two-structure thermodynamics for the TIP4P/2005 model of water covering supercooled and deeply stretched regions. Journal of Chemical Physics, 2017, 146, .	2.2	147
52	Thermodynamic Anomalies in Stretched Water. Langmuir, 2017, 33, 11771-11778.	3.0	32
53	Effects of disulfide bridges and backbone connectivity on water sorption by protein matrices. Scientific Reports, 2017, 7, .	2.7	6
54	Characterization of the liquid Li-solid Mo (1 1 0) interface from classical molecular dynamics for plasma-facing applications. Nuclear Fusion, 2017, 57, 116036.	2.9	10

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55	Perspective: Surface freezing in water: A nexus of experiments and simulations. Journal of Chemical Physics, 2017, 147, .	2.2	25
56	A free energy study of the liquid-liquid phase transition of the Jagla two-scale potential. Journal of Chemical Sciences, 2017, 129, 801-823.	1.2	16
57	Chemical physics of water. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, 13325-13326.	5.2	14
58	Communication: Relationship between local structure and the stability of water in hydrophobic confinement. Journal of Chemical Physics, 2017, 147, .	2.2	15
59	Water anomalous thermodynamics, attraction, repulsion, and hydrophobic hydration. Journal of Chemical Physics, 2016, 144, .	2.2	17
60	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, .	2.2	98
61	Molecular model for chirality phenomena. Journal of Chemical Physics, 2016, 145, .	2.2	25
62	Two-state thermodynamics and the possibility of a liquid-liquid phase transition in supercooled TIP4P/2005 water. Journal of Chemical Physics, 2016, 144, .	2.2	177
63	A cavitation transition in the energy landscape of simple cohesive liquids and glasses. Journal of Chemical Physics, 2016, 145, .	2.2	11
64	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.	5.2	66
65	Computational investigation of dynamical transitions in Trp-cage miniprotein powders. Scientific Reports, 2016, 6, .	2.7	16
66	Density and bond-orientational relaxations in supercooled water. Molecular Physics, 2016, 114, 2580-2585.	1.1	15
67	Concentration Fluctuations and Capacitive Response in Dense Ionic Solutions. Journal of Physical Chemistry Letters, 2016, 7, 2333-2338.	2.9	72
68	Formation of cyclopentane methane binary clathrate hydrate in brine solutions. Chemical Engineering Science, 2016, 141, 125-132.	3.8	72
69	Palmer et al. reply. Nature, 2016, 531, E2-E3.	30.7	17
70	Computational investigation of structure, dynamics and nucleation kinetics of a family of modified Stillinger–Weber model fluids in bulk and free-standing thin films. Physical Chemistry Chemical Physics, 2016, 18, 4102-4111.	2.0	30
71	Thermodynamic and kinetic anisotropies in octane thin films. Journal of Chemical Physics, 2015, 143, .	2.2	22
72	Liquid li structure and dynamics: A comparison between OFDFT and second nearest-neighbor embedded-atom method. AICHE Journal, 2015, 61, 2841-2853.	3.3	27

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73	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.	2.0	9
74	Recent advances in molecular simulation: A chemical engineering perspective. AICHE Journal, 2015, 61, 370-383.	3.3	55
75	Anomalous Capacitance Maximum of the Glassy Carbon–Ionic Liquid Interface through Dilution with Organic Solvents. Journal of Physical Chemistry Letters, 2015, 6, 2644-2648.	2.9	78
76	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.	5.2	241
77	Pathways to dewetting in hydrophobic confinement. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, 8181-8186.	5.2	108
78	Systematic characterization of protein folding pathways using diffusion maps: Application to Trp-cage miniprotein. Journal of Chemical Physics, 2015, 142, .	2.2	59
79	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.	2.0	35
80	The liquid–liquid transition in supercooled ST2 water: a comparison between umbrella sampling and well-tempered metadynamics. Faraday Discussions, 2014, 167, 77.	2.6	95
81	The effect of substrate on thermodynamic and kinetic anisotropies in atomic thin films. Journal of Chemical Physics, 2014, 141, .	2.2	37
82	The role of material flexibility on the drying transition of water between hydrophobic objects: A thermodynamic analysis. Journal of Chemical Physics, 2014, 141, .	2.2	25
83	Two-state thermodynamics of the ST2 model for supercooled water. Journal of Chemical Physics, 2014, 140, .	2.2	117
84	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.	2.0	77
85	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.	2.0	12
86	Formation kinetics of cyclopentane–methane binary clathrate hydrate. Chemical Engineering Science, 2014, 119, 147-157.	3.8	45
87	Molecular Dynamics Simulations of Water Permeation across Nafion Membrane Interfaces. Journal of Physical Chemistry B, 2014, 118, 8798-8807.	2.0	33
88	Computational Study of the Stability of the Miniprotein Trp-Cage, the GB1 β-Hairpin, and the AK16 Peptide, under Negative Pressure. Journal of Physical Chemistry B, 2014, 118, 7761-7769.	2.0	40
89	Metastable liquid–liquid transition in a molecular model of water. Nature, 2014, 510, 385-388.	30.7	514
90	Simulations of vapor–liquid phase equilibrium and interfacial tension in the CO2–H2O–NaCl system. AICHE Journal, 2013, 59, 3514-3522.	3.3	60

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91	Molecular Dynamics Simulations of Water Sorption in a Perfluorosulfonic Acid Membrane. Journal of Physical Chemistry B, 2013, 117, 12649-12660.	2.0	45
92	A computational investigation of attrition-enhanced chiral symmetry breaking in conglomerate crystals. Journal of Chemical Physics, 2013, 139, .	2.2	31
93	Glass Transition Thermodynamics and Kinetics. Annual Review of Condensed Matter Physics, 2013, 4, 263-285.	18.0	261
94	Creation and Persistence of Chiral Asymmetry in a Microscopically Reversible Molecular Model. Journal of Physical Chemistry B, 2013, 117, 602-614.	2.0	11
95	Temperature and length scale dependence of solvophobic solvation in a single-site water-like liquid. Journal of Chemical Physics, 2013, 138, .	2.2	16
96	Relaxation processes in liquids: Variations on a theme by Stokes and Einstein. Journal of Chemical Physics, 2013, 138, .	2.2	102
97	A Coarse-Grained Protein Model in a Water-like Solvent. Scientific Reports, 2013, 3, .	2.7	14
98	Modeling simple amphiphilic solutes in a Jagla solvent. Journal of Chemical Physics, 2012, 136, .	2.2	19
99	Molecular modeling of mechanical stresses on proteins in glassy matrices: Formalism. Journal of Chemical Physics, 2012, 137, .	2.2	18
100	A computational investigation of the phase behavior and capillary sublimation of water confined between nanoscale hydrophobic plates. Journal of Chemical Physics, 2012, 137, .	2.2	41
101	Thermal Stability of Hydrophobic Helical Oligomers: A Lattice Simulation Study in Explicit Water. Journal of Physical Chemistry B, 2012, 116, 9963-9970.	2.0	0
102	Free Energy Barriers to Evaporation of Water in Hydrophobic Confinement. Journal of Physical Chemistry B, 2012, 116, 13282-13289.	2.0	65
103	Evaporation rate of water in hydrophobic confinement. Proceedings of the National Academy of Sciences of the United States of America, 2012, 109, 4365-4370.	5.2	169
104	Massively parallel chemical potential calculation on graphics processing units. Computer Physics Communications, 2012, 183, 2054-2062.	2.8	27
105	Phase Behavior of a Lattice Hydrophobic Oligomer in Explicit Water. Journal of Physical Chemistry B, 2012, 116, 9540-9548.	2.0	3
106	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.	2.0	62
107	Liquid-liquid transition in ST2 water. Journal of Chemical Physics, 2012, 137, .	2.2	153
108	Computer Simulation of Water Sorption on Flexible Protein Crystals. Journal of Physical Chemistry Letters, 2012, 3, 2713-2718.	2.9	19

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109	Homogeneous Nucleation of Methane Hydrate in Microsecond Molecular Dynamics Simulations. Journal of Physical Chemistry Letters, 2012, 3, 2942-2947.	2.9	181
110	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.	2.0	68
111	Dissecting the Energetics of Hydrophobic Hydration of Polypeptides. Journal of Physical Chemistry B, 2011, 115, 14859-14865.	2.0	36
112	Tribute to H. Eugene Stanley. Journal of Physical Chemistry B, 2011, 115, 13963-13964.	2.0	0
113	Evaporation Length Scales of Confined Water and Some Common Organic Liquids. Journal of Physical Chemistry Letters, 2011, 2, 1000-1003.	2.9	50
114	Properties of model atomic free-standing thin films. Journal of Chemical Physics, 2011, 134, .	2.2	41
115	Structure, dynamics, and thermodynamics of a family of potentials with tunable softness. Journal of Chemical Physics, 2011, 135, .	2.2	38
116	Molecular Dynamics Study of Carbon Dioxide Hydrate Dissociation. Journal of Physical Chemistry A, 2011, 115, 6102-6111.	1.8	134
117	Monte Carlo Simulations of High-Pressure Phase Equilibria of CO2–H2O Mixtures. Journal of Physical Chemistry B, 2011, 115, 6629-6635.	2.0	57
118	Waterlike glass polyamorphism in a monoatomic isotropic Jagla model. Journal of Chemical Physics, 2011, 134, .	2.2	51
119	Structure and Energetics of Thin Film Water. Journal of Physical Chemistry C, 2011, 115, 4624-4635.	2.3	35
120	Nonlinear dimensionality reduction in molecular simulation: The diffusion map approach. Chemical Physics Letters, 2011, 509, 1-11.	2.0	165
121	Integrating diffusion maps with umbrella sampling: Application to alanine dipeptide. Journal of Chemical Physics, 2011, 134, .	2.2	77
122	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.	5.2	162
123	An Experimental and Computational Investigation of Spontaneous Lasso Formation in Microcin J25. Biophysical Journal, 2010, 99, 3056-3065.	1.5	72
124	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, .	2.2	32
125	Chiral symmetry breaking in a microscopic model with asymmetric autocatalysis and inhibition. Journal of Chemical Physics, 2010, 133, .	2.2	21
126	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.	5.2	116

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127	Low-temperature fluid-phase behavior of ST2 water. Journal of Chemical Physics, 2009, 131, .	2.2	147
128	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.	5.2	31
129	Phase Transitions Induced by Nanoconfinement in Liquid Water. Physical Review Letters, 2009, 102, .	5.8	236
130	Effect of Surface Polarity on the Structure and Dynamics of Water in Nanoscale Confinement. Journal of Physical Chemistry B, 2009, 113, 1438-1446.	2.0	160
131	Evolution from Surface-Influenced to Bulk-Like Dynamics in Nanoscopically Confined Water. Journal of Physical Chemistry B, 2009, 113, 7973-7976.	2.0	106
132	Structure–energy relations in hen egg white lysozyme observed during refolding from a quenched unfolded state. Chemical Communications, 2009, , 4441.	2.4	10
133	Solubility and Molecular Conformations of n-Alkane Chains in Water. Journal of Physical Chemistry B, 2009, 113, 6405-6414.	2.0	143
134	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.	2.0	168
135	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.	5.2	256
136	The effect of sequence on the conformational stability of a model heteropolymer in explicit water. Journal of Chemical Physics, 2008, 128, .	2.2	15
137	A computational investigation of thermodynamics, structure, dynamics and solvation behavior in modified water models. Journal of Chemical Physics, 2008, 128, .	2.2	177
138	Structural and mechanical properties of glassy water in nanoscale confinement. Faraday Discussions, 2008, 141, 359-376.	2.6	53
139	Lindemann measures for the solid-liquid phase transition. Journal of Chemical Physics, 2007, 126, 204508.	2.2	100
140	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.	5.2	94
141	Structure of the first- and second-neighbor shells of simulated water: Quantitative relation to translational and orientational order. Physical Review E, 2007, 76, .	1.5	122
142	Hydration Behavior under Confinement by Nanoscale Surfaces with Patterned Hydrophobicity and Hydrophilicity. Journal of Physical Chemistry C, 2007, 111, 1323-1332.	2.3	239
143	Effect of Surface Polarity on Water Contact Angle and Interfacial Hydration Structure. Journal of Physical Chemistry B, 2007, 111, 9581-9587.	2.0	494
144	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.	1.8	6

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145	A Water-Explicit Lattice Model of Heat-, Cold-, and Pressure-Induced Protein Unfolding. Biophysical Journal, 2007, 93, 4116-4127.	1.5	44
146	Stability of proteins in the presence of carbohydrates; experiments and modeling using scaled particle theory. Biophysical Chemistry, 2007, 127, 51-63.	1.4	32
147	Computational characterization of the sequence landscape in simple protein alphabets. Proteins: Structure, Function and Bioinformatics, 2006, 62, 232-243.	1.9	11
148	Fluid-phase behavior of binary mixtures in which one component can have two critical points. Journal of Chemical Physics, 2006, 124, 154503.	2.2	58
149	Scaled particle theory for hard sphere pairs. I. Mathematical structure. Journal of Chemical Physics, 2006, 125, 204504.	2.2	18
150	In Honor of Eduardo Glandt. Industrial & Engineering Chemistry Research, 2006, 45, 5419-5420.	2.9	0
151	A conformal solution theory for the energy landscape and glass transition of mixtures. Fluid Phase Equilibria, 2006, 241, 147-154.	2.1	17
152	Accurate prediction of clathrate hydrate phase equilibria below 300 K from a simple model. Journal of Petroleum Science and Engineering, 2006, 51, 45-53.	3.7	26
153	Solid-State Stabilization of α-Chymotrypsin and Catalase with Carbohydrates. Industrial & Engineering Chemistry Research, 2006, 45, 5134-5147.	2.9	33
154	Family of tunable spherically symmetric potentials that span the range from hard spheres to waterlike behavior. Physical Review E, 2006, 73, .	1.5	111
155	Computational probes of molecular motion in the Lewis-Wahnström model for ortho-terphenyl. Journal of Chemical Physics, 2006, 125, 174507.	2.2	65
156	Scaled particle theory for hard sphere pairs. II. Numerical analysis. Journal of Chemical Physics, 2006, 125, 204505.	2.2	14
157	Effect of pressure on the phase behavior and structure of water confined between nanoscale hydrophobic and hydrophilic plates. Physical Review E, 2006, 73, .	1.5	346
158	Structure, dynamics and thermodynamics in complex systems: Theoretical challenges and opportunities. AICHE Journal, 2005, 51, 2391-2395.	3.3	12
159	Dynamic heterogeneity and non-Gaussian behaviour in a model supercooled liquid. Journal of Physics Condensed Matter, 2005, 17, S4035-S4046.	1.6	64
160	Structural order in glassy water. Physical Review E, 2005, 71, .	1.5	53
161	Effects of nonpolar solutes on the thermodynamic response functions of aqueous mixtures. Journal of Chemical Physics, 2005, 123, 164503.	2.2	30
162	A computational study of hydration, solution structure, and dynamics in dilute carbohydrate solutions. Journal of Chemical Physics, 2005, 122, 204511.	2.2	179

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163	Computational Investigation of Order, Structure, and Dynamics in Modified Water Models†. Journal of Physical Chemistry B, 2005, 109, 6527-6534.	2.0	90
164	Novel Computational Probes of Diffusive Motion. Journal of Physical Chemistry B, 2005, 109, 21329-21333.	2.0	1
165	Alternative View of Self-Diffusion and Shear Viscosity†. Journal of Physical Chemistry B, 2005, 109, 6604-6609.	2.0	21
166	Saddles in the Energy Landscape: Extensivity and Thermodynamic Formalism. Physical Review Letters, 2004, 92, .	5.8	25
167	Flat-Histogram Dynamics and Optimization in Density of States Simulations of Fluids†. Journal of Physical Chemistry B, 2004, 108, 19748-19755.	2.0	35
168	A Calorimetric and Spectroscopic Study of DNA at Low Hydration. Journal of Physical Chemistry B, 2004, 108, 3098-3106.	2.0	55
169	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.	11.7	32
170	Differential Scanning Calorimetry Studies of Clathrate Hydrate Formation. Journal of Physical Chemistry B, 2004, 108, 16717-16722.	2.0	112
171	Thermodynamics and the glass transition in model energy landscapes. Physical Review E, 2004, 69, .	1.5	20
172	Inherent-Structure View of Self-Diffusion in Liquids. Journal of Physical Chemistry B, 2004, 108, 6772-6777.	2.0	21
173	Phase transitions, Kauzmann curves, and inverse melting. Biophysical Chemistry, 2003, 105, 211-220.	1.4	51
174	Quantification of order in the Lennard-Jones system. Journal of Chemical Physics, 2003, 118, 2256-2263.	2.2	140
175	Estimation of the Characteristic Time Scales in the Supercritical Antisolvent Process. Industrial & Engineering Chemistry Research, 2003, 42, 3156-3162.	2.9	60
176	Supercooled and glassy water. Journal of Physics Condensed Matter, 2003, 15, R1669-R1726.	1.6	1,027
177	Model Energy Landscapes. Journal of Physical Chemistry B, 2003, 107, 14434-14442.	2.0	43
178	A Theoretical Study of the Interfacial Properties of Supercooled Water. Industrial & Engineering Chemistry Research, 2003, 42, 6396-6405.	2.9	15
179	A kinetic theory of homogeneous bubble nucleation. Journal of Chemical Physics, 2003, 118, 768-783.	2.2	67
180	Energy landscapes, ideal glasses, and their equation of state. Journal of Chemical Physics, 2003, 118, 8821-8830.	2.2	57

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181	A statistical mechanical model for inverse melting. Journal of Chemical Physics, 2003, 119, 4582-4591.	2.2	37
182	An improved Monte Carlo method for direct calculation of the density of states. Journal of Chemical Physics, 2003, 119, 9406-9411.	2.2	136
183	Supercooled and Glassy Water. Physics Today, 2003, 56, 40-46.	0.2	507
184	Generalization of the Wang-Landau method for off-lattice simulations. Physical Review E, 2002, 66, .	1.5	211
185	Cooperative Origin of Low-Density Domains in Liquid Water. Physical Review Letters, 2002, 89, .	5.8	108
186	Energy landscape diversity and supercooled liquid properties. Journal of Chemical Physics, 2002, 116, 3353-3361.	2.2	76
187	A simple molecular thermodynamic theory of hydrophobic hydration. Journal of Chemical Physics, 2002, 116, 2907-2921.	2.2	123
188	Molecular structural order and anomalies in liquid silica. Physical Review E, 2002, 66, .	1.5	224
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