David Chandler

List of Publications by Year
in descending order

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222 papers	43,239 citations	2423 97 h-index	1974 206 g-index
225 all docs	225 docs citations	225 times ranked	18705 citing authors

#	Article	IF	Citations
1	Role of Repulsive Forces in Determining the Equilibrium Structure of Simple Liquids. Journal of Chemical Physics, 1971, 54, 5237-5247.	1.2	4,429
2	Interfaces and the driving force of hydrophobic assembly. Nature, 2005, 437, 640-647.	13.7	3,039
3	TRANSITIONPATHSAMPLING: Throwing Ropes Over Rough Mountain Passes, in the Dark. Annual Review of Physical Chemistry, 2002, 53, 291-318.	4.8	1,704
4	Hydrogen-bond kinetics in liquid water. Nature, 1996, 379, 55-57.	13.7	1,619
5	Hydrophobicity at Small and Large Length Scales. Journal of Physical Chemistry B, 1999, 103, 4570-4577.	1.2	1,521
6	Optimized Cluster Expansions for Classical Fluids. II. Theory of Molecular Liquids. Journal of Chemical Physics, 1972, 57, 1930-1937.	1.2	1,292
7	Statistical mechanics of isomerization dynamics in liquids and the transition state approximation. Journal of Chemical Physics, 1978, 68, 2959.	1.2	1,219
8	Exploiting the isomorphism between quantum theory and classical statistical mechanics of polyatomic fluids. Journal of Chemical Physics, 1981, 74, 4078-4095.	1.2	1,077
9	Effect of Environment on Hydrogen Bond Dynamics in Liquid Water. Physical Review Letters, 1996, 76, 928-931.	2.9	974
10	Transition path sampling and the calculation of rate constants. Journal of Chemical Physics, 1998, 108, 1964-1977.	1.2	925
11	Theory of the hydrophobic effect. Journal of Chemical Physics, 1977, 67, 3683-3704.	1.2	797
12	Structure and hydrogen bond dynamics of waterâ€“dimethyl sulfoxide mixtures by computer simulations. Journal of Chemical Physics, 1993, 98, 8160-8173.	1.2	778
13	Autoionization in Liquid Water. Science, 2001, 291, 2121-2124.	6.0	672
14	Relationship between the Hard-Sphere Fluid and Fluids with Realistic Repulsive Forces. Physical Review A, 1971, 4, 1597-1607.	1.0	572
15	Rigorous formulation of quantum transition state theory and its dynamical corrections. Journal of Chemical Physics, 1989, 91, 7749-7760.	1.2	498
16	Optimized Cluster Expansions for Classical Fluids. I. General Theory and Variational Formulation of the Mean Spherical Model and Hard Sphere Percusâ€Yevick Equations. Journal of Chemical Physics, 1972, 57, 1918-1929.	1.2	424
17	Molecular model for aqueous ferrousâ€“ferric electron transfer. Journal of Chemical Physics, 1988, 89, 3248-3257.	1.2	417
18	Dynamics on the Way to Forming Glass: Bubbles in Space-Time. Annual Review of Physical Chemistry, 2010, 61, 191-217.	4.8	405

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19	Vibrational dephasing and frequency shifts of polyatomic molecules in solution. Journal of Chemical Physics, 1982, 76, 2296-2314.	1.2	385
20	Geometrical Explanation and Scaling of Dynamical Heterogeneities in Glass Forming Systems. Physical Review Letters, 2002, 89, 035704.	2.9	383
21	Density functional theory of nonuniform polyatomic systems. I. General formulation. Journal of Chemical Physics, 1986, 85, 5971-5976.	1.2	358
22	Dynamic Pathways for Viral Capsid Assembly. Biophysical Journal, 2006, 91, 42-54.	0.2	349
23	Instantaneous Liquid Interfaces. Journal of Physical Chemistry B, 2010, 114, 1954-1958.	1.2	349
24	Dynamic Order-Disorder in Atomistic Models of Structural Glass Formers. Science, 2009, 323, 1309-1313.	6.0	333
25	Free energy functions in the extended RISM approximation. Molecular Physics, 1985, 55, 621-625.	0.8	331
26	Rough hard sphere theory of the selfâ€diffusion constant for molecular liquids. Journal of Chemical Physics, 1975, 62, 1358-1363.	1.2	329
27	Hydrophobicity: Two faces of water. Nature, 2002, 417, 491-491.	13.7	321
28	Efficient transition path sampling: Application to Lennard-Jones cluster rearrangements. Journal of Chemical Physics, 1998, 108, 9236-9245.	1.2	313
29	Kinetic Pathways of Ion Pair Dissociation in Water. Journal of Physical Chemistry B, 1999, 103, 3706-3710.	1.2	310
30	The Hydrophobic Effect and the Influence of Soluteâ^'Solvent Attractions. Journal of Physical Chemistry B, 2002, 106, 2047-2053.	1.2	307
31	The putative liquid-liquid transition is a liquid-solid transition in atomistic models of water. Journal of Chemical Physics, 2011, 135, 134503.	1.2	300
32	Trajectory analysis of a kinetic theory for isomerization dynamics in condensed phases. Journal of Chemical Physics, 1979, 70, 4056-4066.	1.2	294
33	On the calculation of reaction rate constants in the transition path ensemble. Journal of Chemical Physics, 1999, 110, 6617-6625.	1.2	292
34	Coarse-grained microscopic model of glass formers. Proceedings of the National Academy of Sciences of the United States of America, 2003, 100, 9710-9714.	3.3	291
35	Statistical mechanics of chemical equilibria and intramolecular structures of nonrigid molecules in condensed phases. Journal of Chemical Physics, 1976, 65, 2925-2940.	1.2	286
36	Theory of intermolecular pair correlations for molecular liquids. Applications to the liquids carbon tetrachloride, carbon disulfide, carbon diselenide, and benzene. Journal of Chemical Physics, 1974, 61, 5228-5241.	1.2	284

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37	Sampling ensembles of deterministic transition pathways. Faraday Discussions, 1998, 110, 421-436.	1.6	282
38	Drying-induced hydrophobic polymer collapse. Proceedings of the National Academy of Sciences of the United States of America, 2002, 99, 6539-6543.	3.3	258
39	Fluctuations of Water near Extended Hydrophobic and Hydrophilic Surfaces. Journal of Physical Chemistry B, 2010, 114, 1632-1637.	1.2	254
40	Hydration of metal surfaces can be dynamically heterogeneous and hydrophobic. Proceedings of the National Academy of Sciences of the United States of America, 2013, 110, 4200-4205.	3.3	242
41	Excess electrons in simple fluids. I. General equilibrium theory for classical hard sphere solvents. Journal of Chemical Physics, 1984, 81, 1975-1982.	1.2	240
42	Scaling of Hydrophobic Solvation Free Energiesâ€. Journal of Physical Chemistry B, 2001, 105, 6704-6709.	1.2	238
43	Roles of Repulsive and Attractive Forces in Liquids : The Equilibrium Theory of Classical Fluids. Advances in Chemical Physics, 2007, , 105-156.	0.3	231
44	Density functional theory of nonuniform polyatomic systems. II. Rational closures for integral equations. Journal of Chemical Physics, 1986, 85, 5977-5982.	1.2	223
45	Micelle Formation and the Hydrophobic Effect. Journal of Physical Chemistry B, 2004, 108, 6778-6781.	1.2	223
46	Roles of Repulsive and Attractive Forces in Liquids: The Optimized Random Phase Approximation. Journal of Chemical Physics, 1972, 56, 3812-3823.	1.2	214
47	New type of cluster theory for molecular fluids: Interaction site cluster expansion. Journal of Chemical Physics, 1975, 62, 4308-4324.	1.2	212
48	Convenient and accurate discretized path integral methods for equilibrium quantum mechanical calculations. Journal of Chemical Physics, 1981, 75, 1347-1364.	1.2	209
49	Corresponding States of Structural Glass Formers. Journal of Physical Chemistry B, 2009, 113, 5563-5567.	1.2	207
50	Excitation lines and the breakdown of Stokes-Einstein relations in supercooled liquids. Physical Review E, 2004, 69, 061205.	0.8	200
51	The Electric Double Layer Has a Life of Its Own. Journal of Physical Chemistry C, 2014, 118, 18291-18298.	1.5	195
52	Sitting at the Edge: How Biomolecules use Hydrophobicity to Tune Their Interactions and Function. Journal of Physical Chemistry B, 2012, 116, 2498-2503.	1.2	191
53	Solution of a new integral equation for pair correlation functions in molecular liquids. Journal of Chemical Physics, 1973, 59, 6587-6595.	1.2	188
54	The putative liquid-liquid transition is a liquid-solid transition in atomistic models of water. II. Journal of Chemical Physics, 2013, 138, 214504.	1.2	181

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55	Space-time thermodynamics of the glass transition. Proceedings of the National Academy of Sciences of the United States of America, 2005, 102, 10837-10840.	3.3	180
56	Gaussian field model of fluids with an application to polymeric fluids. Physical Review E, 1993, 48, 2898-2905.	0.8	179
57	Computer simulation of photochemically induced electron transfer. Chemical Physics Letters, 1989, 157, 501-504.	1.2	178
58	Perturbation Theory of the Thermodynamic Properties of Simple Liquids. Journal of Chemical Physics, 1971, 55, 5422-5423.	1.2	175
59	Staging: A sampling technique for the Monte Carlo evaluation of path integrals. Physical Review B, 1985, 31, 4234-4244.	1.1	172
60	Equilibrium Structure of Simple Liquids. Physical Review Letters, 1970, 25, 149-152.	2.9	169
61	New and proper integral equations for site-site equilibrium correlations in molecular fluids. Molecular Physics, 1982, 46, 1335-1345.	0.8	169
62	A molecular dynamics and Monte Carlo study of solvent effects on the conformational equilibrium	1.2	167
63	Semiclassical study of electronically nonadiabatic dynamics in the condensed-phase: Spin-boson problem with Debye spectral density. Journal of Chemical Physics, 1999, 110, 4828-4840.	1.2	159
64	Statistical mechanics of small chain molecules in liquids. I. Effects of liquid packing on conformational structures. Journal of Chemical Physics, 1978, 68, 4202-4212.	1.2	157
65	Solvent coarse-graining and the string method applied to the hydrophobic collapse of a hydrated chain. Proceedings of the National Academy of Sciences of the United States of America, 2007, 104, 14559-14564.	3.3	155
66	Molecular Explanation for Why Talc Surfaces Can Be Both Hydrophilic and Hydrophobic. Journal of the American Chemical Society, 2011, 133, 20521-20527.	6.6	152
67	Excitations Are Localized and Relaxation Is Hierarchical in Glass-Forming Liquids. Physical Review X, 2011, 1, .	2.8	151
68	Derivation of an integral equation for pair correlation functions in molecular fluids. Journal of Chemical Physics, 1973, 59, 2742-2746.	1.2	140
69	Extended surfaces modulate hydrophobic interactions of neighboring solutes. Proceedings of the National Academy of Sciences of the United States of America, 2011, 108, 17678-17683.	3.3	140
70	Isomerization dynamics in liquids by molecular dynamics. Chemical Physics Letters, 1980, 75, 162-168.	1.2	139
71	Effects of soluteâ€“solvent attractive forces on hydrophobic correlations. Journal of Chemical Physics, 1980, 73, 3434-3441.	1.2	138
72	Excess electrons in simple fluids. II. Numerical results for the hard sphere solvent. Journal of Chemical Physics, 1984, 81, 5109-5116.	1.2	137

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73	Translational and rotational diffusion in liquids. I. Translational singleâ€particle correlation functions. Journal of Chemical Physics, 1974, 60, 3500-3507.	1.2	136
74	Optimized Cluster Expansions for Classical Fluids. III. Applications to Ionic Solutions and Simple Liquids. Journal of Chemical Physics, 1972, 57, 2626-2631.	1.2	132
75	Translational and rotational diffusion in liquids. II. Orientational singleâ€particle correlation functions. Journal of Chemical Physics, 1974, 60, 3508-3512.	1.2	129
76	Charge Fluctuations in Nanoscale Capacitors. Physical Review Letters, 2013, 111, 106102.	2.9	129
77	A Coarse-Grained Model of Water Confined in a Hydrophobic Tube. Journal of Physical Chemistry B, 2003, 107, 1189-1193.	1.2	124
78	Dynamics of Nucleation in the Ising Modelâ€. Journal of Physical Chemistry B, 2004, 108, 19681-19686.	1.2	120
79	Water at an electrochemical interfaceâ€”a simulation study. Faraday Discussions, 2009, 141, 423-441.	1.6	120
80	Transition path sampling of cavitation between molecular scale solvophobic surfaces. Journal of Chemical Physics, 2000, 113, 8154-8160.	1.2	119
81	Atomistic understanding of kinetic pathways for single base-pair binding and unbinding in DNA. Proceedings of the National Academy of Sciences of the United States of America, 2003, 100, 13922-13927.	3.3	117
82	Combined neutron diffraction and computer simulation study of liquid dimethyl sulphoxide. Journal of Chemical Physics, 1993, 99, 6836-6847.	1.2	116
83	Electrostatic analogy for surfactant assemblies. The Journal of Physical Chemistry, 1992, 96, 4077-4083.	2.9	114
84	Coherent-incoherent transition and relaxation in condensed-phase tunneling systems. Physical Review A, 1991, 44, 2352-2369.	1.0	112
85	Free energies of electron transfer. The Journal of Physical Chemistry, 1992, 96, 1748-1753.	2.9	112
86	Mode Expansion in Equilibrium Statistical Mechanics. III. Optimized Convergence and Application to Ionic Solution Theory. Journal of Chemical Physics, 1971, 55, 1497-1504.	1.2	111
87	Cluster diagrammatic analysis of the RISM equation. Molecular Physics, 1976, 31, 1213-1223.	0.8	111
88	The dielectric constant and related equilibrium properties of molecular fluids: Interaction site cluster theory analysis. Journal of Chemical Physics, 1977, 67, 1113.	1.2	111
89	Time correlation function and path integral analysis of quantum rate constants. The Journal of Physical Chemistry, 1989, 93, 7009-7015.	2.9	111
90	Perturbation Theory for Repulsive Forces in Classical Fluids: Selected Applications. Journal of Chemical Physics, 1972, 56, 4989-4994.	1.2	110

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91	Water Evaporation: A Transition Path Sampling Study. Journal of Physical Chemistry B, 2013, 117, 1419-1428.	1.2	108
92	The molecular structure of the interface between water and a hydrophobic substrate is liquid-vapor like. Journal of Chemical Physics, 2014, 141, 18C519.	1.2	106
93	Mode Expansion in Equilibrium Statistical Mechanics. I. General Theory and Application to the Classical Electron Gas. Journal of Chemical Physics, 1970, 53, 547-554.	1.2	105
94	Dielectric solvation dynamics of molecules of arbitrary shape and charge distribution. Journal of Chemical Physics, 1998, 108, 2594-2600.	1.2	105
95	Interaction site cluster series for the Helmholtz free energy and variational principle for chemical equilibria and intramolecular structures. Journal of Chemical Physics, 1977, 66, 147-151.	1.2	104
96	Cavity formation and the drying transition in the Lennard-Jones fluid. Physical Review E, 2000, 61, 1501-1506.	0.8	103
97	Applications of the RISM equation to diatomic fluids: the liquids nitrogen, oxygen and bromine. Chemical Physics, 1976, 14, 213-228.	0.9	102
98	Corresponding States of Structural Glass Formers. II. Journal of Physical Chemistry B, 2010, 114, 17113-17119.	1.2	98
99	Reference interaction site model polaron theory of the hydrated electron. Journal of Chemical Physics, 1991, 95, 4444-4453.	1.2	96
100	Oil on troubled waters. Nature, 2007, 445, 831-832.	13.7	95
101	Quantum theory of polarization in liquids: Exact solution of the mean spherical and related approximations. Journal of Chemical Physics, 1982, 76, 1128-1135.	1.2	94
102	Dynamical exchanges in facilitated models of supercooled liquids. Journal of Chemical Physics, 2005, 123, 084509.	1.2	93
103	Gaussian Field Model of Dielectric Solvation Dynamics. The Journal of Physical Chemistry, 1996, 100, 11954-11959.	2.9	91
104	Phase diagram of supercooled water confined to hydrophilic nanopores. Journal of Chemical Physics, 2012, 137, 044509.	1.2	91
105	Quantifying Density Fluctuations in Volumes of All Shapes and Sizes Using Indirect Umbrella Sampling. Journal of Statistical Physics, 2011, 145, 265-275.	0.5	90
106	Effective adiabatic approximation for a two level system coupled to a bath. Journal of Chemical Physics, 1985, 82, 3400-3404.	1.2	88
107	Roles of classical dynamics and quantum dynamics on activated processes occurring in liquids. Journal of Statistical Physics, 1986, 42, 49-67.	0.5	88
108	Importance sampling and theory of nonequilibrium solvation dynamics in water. Journal of Chemical Physics, 2000, 113, 9759-9765.	1.2	88

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109	Lengthscale dependence of dynamic four-point susceptibilities in glass formers. Physical Review E, 2006, 74, 051501.	0.8	85
110	Decoupling of exchange and persistence times in atomistic models of glass formers. Journal of Chemical Physics, 2007, 127, 211101.	1.2	84
111	Stochastic molecular dynamics study of transâ€“gauche isomerization processes in simple chain molecules. Journal of Chemical Physics, 1980, 73, 3688-3694.	1.2	83
112	Heterogeneity and growing length scales in the dynamics of kinetically constrained lattice gases in two dimensions. Physical Review E, 2005, 72, 041106.	0.8	83
113	Solving the sign problem in quantum Monte Carlo dynamics. Physical Review A, 1990, 41, 5709-5712.	1.0	82
114	Hydrophobic solvation of nonspherical solutes. Journal of Chemical Physics, 1980, 73, 3430-3433.	1.2	81
115	Electronic States of a Topologically Disordered System: Exact Solution of the Mean Spherical Model for Liquids. Physical Review Letters, 1982, 49, 1100-1103.	2.9	80
116	Comparative study of theory and simulation calculations for excess electrons in simple fluids. Journal of Chemical Physics, 1987, 87, 4088-4092.	1.2	79
117	Efficient transition path sampling for nonequilibrium stochastic dynamics. Physical Review E, 2001, 64, 026109.	0.8	79
118	Filaggrin inhibits generation of CD1a neolipid antigens by house dust miteâ€derived phospholipase. Science Translational Medicine, 2016, 8, 325ra18.	5.8	77
119	An improved coarse-grained model of solvation and the hydrophobic effect. Journal of Chemical Physics, 2011, 134, 074109.	1.2	76
120	Stochastic molecular dynamics study of cyclohexane isomerization. The Journal of Physical Chemistry, 1988, 92, 3261-3267.	2.9	74
121	A density functional treatment of the hard dumbbell freezing transition. Journal of Chemical Physics, 1987, 87, 4853-4858.	1.2	73
122	The Role of Solvent Fluctuations in Hydrophobic Assemblyâ€. Journal of Physical Chemistry B, 2008, 112, 6187-6192.	1.2	72
123	Theory of amorphous ices. Proceedings of the National Academy of Sciences of the United States of America, 2014, 111, 9413-9418.	3.3	72
124	Finite-temperature critical point of a glass transition. Proceedings of the National Academy of Sciences of the United States of America, 2010, 107, 12793-12798.	3.3	70
125	Equilibrium structure and molecular motion in liquids. Accounts of Chemical Research, 1974, 7, 246-251.	7.6	66
126	Statistical mechanics of small chain molecules in liquids. II. Intermolecular pair correlations for liquidnâ€butane. Journal of Chemical Physics, 1978, 68, 4213-4217.	1.2	65

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127	Transition pathways in a many-body system: Application to hydrogen-bond breaking in water. Journal of Chemical Physics, 1998, 109, 1125-1133.	1.2	65
128	Simulation of an excess electron in a hard sphere fluid. Journal of Chemical Physics, 1985, 83, 3042-3049.	1.2	63
129	Monte Carlo study of polymers in equilibrium with random obstacles. Journal of Chemical Physics, 1992, 96, 835-841.	1.2	63
130	Mode Expansion in Equilibrium Statistical Mechanics. II. A Rapidly Convergent Theory of Ionic Solutions. Journal of Chemical Physics, 1971, 54, 26-33.	1.2	61
131	Classical diffusion in strong random media. Journal of Statistical Physics, 1994, 76, 911-927.	0.5	61
132	Chemical dynamics of the protonated water trimer analyzed by transition path sampling. Physical Chemistry Chemical Physics, 1999, 1, 1317-1322.	1.3	61
133	Model of a fluid at small and large length scales and the hydrophobic effect. Physical Review E, 2001, 65, 011201.	0.8	61
134	Premelting, fluctuations, and coarse-graining of water-ice interfaces. Journal of Chemical Physics, 2014, 141, 18C505.	1.2	61
135	Space-time thermodynamics and subsystem observables in a kinetically constrained model of glassy materials. Journal of Chemical Physics, 2006, 125, 184509.	1.2	60
136	Comparisons of Monte Carlo and RISM calculations of pair correlation functions. Journal of Chemical Physics, 1977, 66, 5231-5234.	1.2	59
137	Negative differential mobility of weakly driven particles in models of glass formers. Physical Review E, 2008, 78, 011506.	0.8	58
138	Constrained dynamics of localized excitations causes a non-equilibrium phase transition in an atomistic model of glass formers. Journal of Chemical Physics, 2012, 136, 184509.	1.2	58
139	Pre-transition effects mediate forces of assembly between transmembrane proteins. ELife, 2016, 5, e13150.	2.8	56
140	Quantum theory of solvent effects on electronic spectra: Predictions of the exact solution of the mean spherical model. Journal of Chemical Physics, 1983, 78, 4118-4125.	1.2	55
141	Ab initio analysis of proton transfer dynamics in (H2O)3H+. Chemical Physics Letters, 2000, 321, 225-230.	1.2	54
142	Transition path sampling: throwing ropes over mountains in the dark. Journal of Physics Condensed Matter, 2000, 12, A147-A152.	0.7	52
143	Elastic energy storage in ?-sheets with application to F1-ATPase. European Biophysics Journal, 2003, 32, 676-683.	1.2	52
144	Fluctuation-dissipation ratios in the dynamics of self-assembly. Physical Review E, 2007, 76, 021119.	0.8	49

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145	Excess electrons in simple fluids. IV. Real time behavior. Journal of Chemical Physics, 1987, 87, 6671-6681.	1.2	48
146	Molecular dynamics study of cyclohexane interconversion. Chemical Physics, 1990, 149, 11-20.	0.9	48
147	The conformational states of Mgï¿½ATP in water. European Biophysics Journal, 2004, 33, 29-37.	1.2	48
148	Preparation and Relaxation of Very Stable Glassy States of a Simulated Liquid. Physical Review Letters, 2011, 107, 275702.	2.9	48
149	Quantum theory for free energies of electron transfer. Journal of Chemical Physics, 1992, 97, 4958-4963.	1.2	46
150	Gaussian statistics of the hard-sphere fluid. Physical Review E, 1997, 56, 4217-4221.	0.8	46
151	Pathâ€integral calculation of the tunnel splitting in aqueous ferrousâ€“ferric electron transfer. Journal of Chemical Physics, 1991, 95, 889-894.	1.2	45
152	Computer simulation of a quantum particle in a quenched disordered system: Direct observation of Lifshitz traps. Physical Review B, 1985, 32, 545-547.	1.1	44
153	Density-functional theory for the freezing of water. Physical Review Letters, 1987, 59, 1698-1701.	2.9	44
154	Theory of percolation in fluids of long molecules. Journal of Statistical Physics, 1991, 63, 837-856.	0.5	44
155	Optimized cluster theory, the Lennard-Jones fluid, and the liquid-gas phase transition. Physical Review A, 1974, 9, 1688-1697.	1.0	43
156	Excess electrons in simple fluids. III. Role of solvent polarization. Journal of Chemical Physics, 1986, 84, 398-403.	1.2	43
157	The Unbinding of ATP from F1-ATPase. Biophysical Journal, 2003, 85, 695-706.	0.2	43
158	Hydrophobic interactions and osmotic second virial coefficients for methanol in water. Journal of Solution Chemistry, 1980, 9, 1-17.	0.6	41
159	Diffusion of ionic penetrants in charged disordered media. Journal of Chemical Physics, 1994, 100, 1528-1541.	1.2	41
160	Characterizing heterogeneous dynamics at hydrated electrode surfaces. Journal of Chemical Physics, 2013, 138, 184702.	1.2	40
161	Water Exchange at a Hydrated Platinum Electrode is Rare and Collective. Journal of Physical Chemistry C, 2015, 119, 24016-24024.	1.5	40
162	Comment on the role of constraints on the conformational structure of n-butane in liquid solvents. Journal of Chemical Physics, 1979, 71, 5386.	1.2	39

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163	Calculation of the dielectric constant of polyatomic fluids with the interaction site formalism. Molecular Physics, 1982, 47, 871-879.	0.8	39
164	Umbrella sampling molecular dynamics study of the dielectric constant of water. Molecular Physics, 1993, 78, 1155-1165.	0.8	39
165	Phase diagram for excess electrons in simple fluids. Physical Review E, 1994, 49, 2851-2865.	0.8	39
166	Stochastic transition pathways in the aqueous sodium chloride dissociation process. Chemical Physics Letters, 2000, 328, 169-176.	1.2	39
167	Quantum theory of solvation. The Journal of Physical Chemistry, 1984, 88, 3400-3407.	2.9	38
168	Two simulation studies of chemical dynamics in liquids. Faraday Discussions of the Chemical Society, 1988, 85, 329.	2.2	38
169	Coarse-grained modeling of the interface between water and heterogeneous surfaces. Faraday Discussions, 2009, 141, 209-220.	1.6	38
170	Corresponding states for mesostructure and dynamics of supercooled water. Faraday Discussions, 2013, 167, 485.	1.6	38
171	The Cooling Rate- and Volatility-Dependent Glass-Forming Properties of Organic Aerosols Measured by Broadband Dielectric Spectroscopy. Environmental Science & Technology, 2019, 53, 12366-12378.	4.6	37
172	Dynamical Aspects of Isomerization and Melting Transitions in [H2O]8â€. Journal of Physical Chemistry A, 2001, 105, 2646-2651.	1.1	36
173	Neutron Scattering and Monte Carlo Determination of the Variation of the Critical Nucleus Size with Quench Depthâ€. Journal of Physical Chemistry B, 2006, 110, 3692-3696.	1.2	35
174	Barrier crossings: classical theory of rare but important events. , 1998, , .		32
175	Time scales of supercooled water and implications for reversible polyamorphism. Molecular Physics, 2015, 113, 2799-2804.	0.8	31
176	Effective intramolecular potentials for molecular bromine in argon. Comparison of theory with simulation. Journal of Chemical Physics, 1980, 72, 4045-4048.	1.2	30
177	Quantitative molecular interpretation of mesoscopic correlations in bicontinuous microemulsions. Physical Review E, 1995, 52, 6497-6507.	0.8	27
178	Charge-frustrated model of bicontinuous phases. Physical Review E, 1994, 49, 4268-4275.	0.8	26
179	RISM calculation of the structure of liquid chloroform. Molecular Physics, 1979, 37, 299-301.	0.8	25
180	Gridâ€'Flux Method for Learning the Solvent Contribution to the Mechanisms of Reactions. Journal of Physical Chemistry B, 2003, 107, 2796-2801.	1.2	25

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181	Applicability of Dynamic Facilitation Theory to Binary Hard Disk Systems. Physical Review Letters, 2016, 117, 145701.	2.9	25
182	Constrained impulsive molecular dynamics. Molecular Physics, 1981, 42, 1233-1143.	0.8	23
183	Electron transfer in water and other polar environments, how it happens. , 1998, , .		22
184	Segue between Favorable and Unfavorable Solvation. Journal of Physical Chemistry B, 2007, 111, 9025-9030.	1.2	22
185	Catastrophe in the Randomâ€Phase Approximation: Critique of a Theory of Phase Transitions. Journal of Chemical Physics, 1971, 55, 1645-1654.	1.2	21
186	[3] Theoretical and computational studies of hydrophobic interactions. Methods in Enzymology, 1986, 127, 48-63.	0.4	21
187	RISM calculation of the activation barrier for isomerization of solvated cyclohexane. The Journal of Physical Chemistry, 1986, 90, 6015-6017.	2.9	21
188	Optimized cluster theory correction to the van der Waals model of mixtures. Journal of Chemical Physics, 1974, 61, 932-935.	1.2	18
189	Calculation of orientational pair correlation factors with the interaction site formalism. Journal of Chemical Physics, 1984, 80, 4484-4487.	1.2	18
190	Comment on â€œa new rism integral equation for solvent polymersâ€• Chemical Physics Letters, 1987, 140, 108-110.	1.2	18
191	Thermodynamics of coarse-grained models of supercooled liquids. Journal of Chemical Physics, 2005, 123, 044511.	1.2	18
192	Finding transition pathways: throwing ropes over rough mountain passes, in the dark. , 1998, , .		17
193	Liquids: Condensed, disordered, and sometimes complex. Proceedings of the National Academy of Sciences of the United States of America, 2009, 106, 15111-15112.	3.3	17
194	Dynamics with the effective adiabatic theory: The Bloch equations. Journal of Chemical Physics, 1988, 89, 452-458.	1.2	16
195	Statistics of simple chains in a sea of blockers. Journal of Chemical Physics, 1995, 102, 1405-1415.	1.2	16
196	Decoupling of Self-Diffusion and Structural Relaxation during a Fragile-to-Strong Crossover in a Kinetically Constrained Lattice Gas. ChemPhysChem, 2005, 6, 1783-1785.	1.0	16
197	Comment on the structure of a simple liquid solvent near a nâ€butane solute molecule. Journal of Chemical Physics, 1980, 73, 1002-1003.	1.2	15
198	Theory of orientational pair correlations in molecular fluids. The Journal of Physical Chemistry, 1983, 87, 2060-2064.	2.9	15

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