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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

206 papers	22,629 citations	78 h-index	147 g-index
212 ext. papers	24,151 ext. citations	5.8 avg, IF	6.91 L-index

#	Paper	IF	Citations
206	Reversible multiple time scale molecular dynamics. <i>Journal of Chemical Physics</i> , 1992 , 97, 1990-2001	3.9	2628
205	Modification of the overlap potential to mimic a linear site-site potential. <i>Journal of Chemical Physics</i> , 1981 , 74, 3316-3319	3.9	1064
204	Dynamical fluctuating charge force fields: Application to liquid water. <i>Journal of Chemical Physics</i> , 1994 , 101, 6141-6156	3.9	1048
203	On the Simulation of Quantum Systems: Path Integral Methods. <i>Annual Review of Physical Chemistry</i> , 1986 , 37, 401-424	15.7	619
202	Replica exchange with solute tempering: a method for sampling biological systems in explicit water. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2005 , 102, 13749-54	11.5	530
201	The free energy landscape for beta hairpin folding in explicit water. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2001 , 98, 14931-6	11.5	458
200	Urea denaturation by stronger dispersion interactions with proteins than water implies a 2-stage unfolding. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2008 , 105, 16928-33	11.5	424
199	Replica exchange with solute scaling: a more efficient version of replica exchange with solute tempering (REST2). <i>Journal of Physical Chemistry B</i> , 2011 , 115, 9431-8	3.4	387
198	On path integral Monte Carlo simulations. <i>Journal of Chemical Physics</i> , 1982 , 76, 5150-5155	3.9	354
197	On the Calculation of Time Correlation Functions. <i>Advances in Chemical Physics</i> , 2007 , 63-227		346
196	Observation of a dewetting transition in the collapse of the melittin tetramer. <i>Nature</i> , 2005 , 437, 159-62	50.4	333
195	Quantum and classical relaxation rates from classical simulations. <i>Journal of Chemical Physics</i> , 1994 , 100, 8359-8366	3.9	328
194	Can a continuum solvent model reproduce the free energy landscape of a beta -hairpin folding in water?. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2002 , 99, 12777-82	11.5	308
193	On the Calculation of Diffusion Coefficients in Confined Fluids and Interfaces with an Application to the Liquid-Vapor Interface of Water. <i>Journal of Physical Chemistry B</i> , 2004 , 108, 6595-6602	3.4	281
192	Development of a polarizable force field for proteins via ab initio quantum chemistry: first generation model and gas phase tests. <i>Journal of Computational Chemistry</i> , 2002 , 23, 1515-31	3.5	276
191	A Monte Carlo simulation of the hydrophobic interaction. <i>Journal of Chemical Physics</i> , 1979 , 71, 2975	3.9	263
190	Urea's action on hydrophobic interactions. <i>Journal of the American Chemical Society</i> , 2009 , 131, 1535-41	16.4	261

189	Combined fluctuating charge and polarizable dipole models: Application to a five-site water potential function. <i>Journal of Chemical Physics</i> , 2001 , 115, 2237-2251	3.9	256
188	Computer Simulation of Hydrophobic Hydration Forces on Stacked Plates at Short Range. <i>The Journal of Physical Chemistry</i> , 1995 , 99, 2893-2899		256
187	Computer Simulation of a Green Chemistry Room-Temperature Ionic Solvent. <i>Journal of Physical Chemistry B</i> , 2002 , 106, 12017-12021	3.4	253
186	Dewetting-induced collapse of hydrophobic particles. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2003 , 100, 11953-8	11.5	245
185	Effects of Polarizability on the Hydration of the Chloride Ion. <i>The Journal of Physical Chemistry</i> , 1996 , 100, 11934-11943		242
184	Fluctuating Charge, Polarizable Dipole, and Combined Models: Parameterization from ab Initio Quantum Chemistry. <i>Journal of Physical Chemistry B</i> , 1999 , 103, 4730-4737	3.4	239
183	Parametrizing a polarizable force field from ab initio data. I. The fluctuating point charge model. <i>Journal of Chemical Physics</i> , 1999 , 110, 741-754	3.9	225
182	Development of an Accurate and Robust Polarizable Molecular Mechanics Force Field from ab Initio Quantum Chemistry. <i>Journal of Physical Chemistry A</i> , 2004 , 108, 621-627	2.8	209
181	Electronic properties of CdSe nanocrystals in the absence and presence of a dielectric medium. <i>Journal of Chemical Physics</i> , 1999 , 110, 5355-5369	3.9	209
180	Effect of ions on the hydrophobic interaction between two plates. <i>Journal of the American Chemical Society</i> , 2007 , 129, 4678-86	16.4	208
179	Hydrogen-Bond Kinetics in the Solvation Shell of a Polypeptide. <i>Journal of Physical Chemistry B</i> , 2001 , 105, 11929-11932	3.4	206
178	Dynamical Fluctuating Charge Force Fields: The Aqueous Solvation of Amides. <i>Journal of the American Chemical Society</i> , 1996 , 118, 672-679	16.4	199
177	Novel methods of sampling phase space in the simulation of biological systems. <i>Current Opinion in Structural Biology</i> , 1997 , 7, 181-9	8.1	196
176	Can Water Polarizability Be Ignored in Hydrogen Bond Kinetics?. <i>Journal of Physical Chemistry B</i> , 2002 , 106, 2054-2060	3.4	183
175	Role of water in mediating the assembly of Alzheimer amyloid-beta Abeta16-22 protofilaments. <i>Journal of the American Chemical Society</i> , 2008 , 130, 11066-72	16.4	180
174	Blue Gene: A vision for protein science using a petaflop supercomputer. <i>IBM Systems Journal</i> , 2001 , 40, 310-327		175
173	Ligand binding to protein-binding pockets with wet and dry regions. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2011 , 108, 1326-30	11.5	156
172	On achieving high accuracy and reliability in the calculation of relative protein-ligand binding affinities. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2012 , 109, 1937-42	11.5	151

171	Vibrational relaxation in simple fluids: Comparison of theory and simulation. <i>Journal of Chemical Physics</i> , 1993 , 98, 7301-7318	3.9	148
170	Quantum effects in liquid water: Path-integral simulations of a flexible and polarizable ab initio model. <i>Journal of Chemical Physics</i> , 2001 , 115, 7622-7628	3.9	147
169	Path integral Monte Carlo studies of the behavior of excess electrons in simple fluids. <i>Journal of Chemical Physics</i> , 1987 , 86, 5689-5702	3.9	138
168	Spectral gap optimization of order parameters for sampling complex molecular systems. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2016 , 113, 2839-44	11.5	135
167	Hydrophobic hydration around a pair of apolar species in water. <i>Journal of Chemical Physics</i> , 1979 , 71, 2982	3.9	135
166	Effective potentials for liquid water using polarizable and nonpolarizable models. <i>The Journal of Physical Chemistry</i> , 1993 , 97, 13841-13851		134
165	Molecular Dynamics Study of the Dependence of Water Solvation Free Energy on Solute Curvature and Surface Area. <i>The Journal of Physical Chemistry</i> , 1995 , 99, 2885-2892		129
164	Advancing Drug Discovery through Enhanced Free Energy Calculations. <i>Accounts of Chemical Research</i> , 2017 , 50, 1625-1632	24.3	126
163	Constructing ab initio force fields for molecular dynamics simulations. <i>Journal of Chemical Physics</i> , 1998 , 108, 4739-4755	3.9	126
162	Time-Correlation Functions, Memory Functions, and Molecular Dynamics. <i>Physical Review A</i> , 1970 , 2, 975-996	2.6	126
161	Prediction of Protein-Ligand Binding Poses via a Combination of Induced Fit Docking and Metadynamics Simulations. <i>Journal of Chemical Theory and Computation</i> , 2016 , 12, 2990-8	6.4	120
160	The Aqueous Solvation of Water: A Comparison of Continuum Methods with Molecular Dynamics. <i>Journal of the American Chemical Society</i> , 1994 , 116, 3949-3954	16.4	118
159	Intramolecular rate process: Isomerization dynamics and the transition to chaos. <i>Journal of Chemical Physics</i> , 1981 , 75, 3495-3510	3.9	116
158	Surface Curvature Effects in the Aqueous Ionic Solvation of the Chloride Ion. <i>Journal of Physical Chemistry A</i> , 1999 , 103, 10300-10307	2.8	112
157	Localization of an excess electron in water clusters. <i>Journal of Chemical Physics</i> , 1986 , 85, 1583-1591	3.9	111
156	Calculating the hopping rate for self-diffusion on rough potential energy surfaces: Cage correlations. <i>Journal of Chemical Physics</i> , 1997 , 107, 6867-6876	3.9	110
155	Hydrogen-bond dynamics in the air-water interface. <i>Journal of Physical Chemistry B</i> , 2005 , 109, 2949-55	3.4	110
154	Dynamic friction on rigid and flexible bonds. <i>Journal of Chemical Physics</i> , 1990 , 93, 5084-5095	3.9	108

153	Path integral Monte Carlo study of the hydrated electron. <i>Journal of Chemical Physics</i> , 1987 , 86, 6404-6418	3.9	107
152	A path integral Monte Carlo study of liquid neon and the quantum effective pair potential. <i>Journal of Chemical Physics</i> , 1984 , 81, 2523-2527	3.9	107
151	Behavior of the hydrated electron at different temperatures: structure and absorption spectrum. <i>The Journal of Physical Chemistry</i> , 1988 , 92, 1721-1730		106
150	Efficient multiple time step method for use with Ewald and particle mesh Ewald for large biomolecular systems. <i>Journal of Chemical Physics</i> , 2001 , 115, 2348-2358	3.9	104
149	Nonergodicity in path integral molecular dynamics. <i>Journal of Chemical Physics</i> , 1984 , 81, 3641-3643	3.9	100
148	Large scale simulation of macromolecules in solution: Combining the periodic fast multipole method with multiple time step integrators. <i>Journal of Chemical Physics</i> , 1997 , 106, 9835-9849	3.9	98
147	Computer simulation of the nucleation and thermodynamics of microclusters. <i>Journal of Chemical Physics</i> , 1978 , 68, 1325-1336	3.9	98
146	Replica exchange with solute tempering: efficiency in large scale systems. <i>Journal of Physical Chemistry B</i> , 2007 , 111, 5405-10	3.4	95
145	Hydrophobic Interactions and Dewetting between Plates with Hydrophobic and Hydrophilic Domains. <i>Journal of Physical Chemistry C</i> , 2009 , 113, 5244-5253	3.8	93
144	Can imaginary instantaneous normal mode frequencies predict barriers to self-diffusion?. <i>Journal of Chemical Physics</i> , 1997 , 107, 4618-4627	3.9	91
143	Solvation energies and electronic spectra in polar, polarizable media: Simulation tests of dielectric continuum theory. <i>Journal of Chemical Physics</i> , 1996 , 104, 1293-1308	3.9	90
142	Vibrational energy relaxation in the condensed phases: Quantum vs classical bath for multiphonon processes. <i>Journal of Chemical Physics</i> , 1997 , 107, 6050-6061	3.9	89
141	Unraveling quantum mechanical effects in water using isotopic fractionation. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2012 , 109, 7988-91	11.5	88
140	Dynamics of water confined in the interdomain region of a multidomain protein. <i>Journal of Physical Chemistry B</i> , 2006 , 110, 3704-11	3.4	88
139	The calculation of transport properties in quantum liquids using the maximum entropy numerical analytic continuation method: application to liquid para-hydrogen. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2002 , 99, 1129-33	11.5	88
138	Molecular dynamics with multiple time scales: The selection of efficient reference system propagators. <i>Journal of Chemical Physics</i> , 1996 , 105, 1426-1436	3.9	88
137	Signatures of hydrophobic collapse in extended proteins captured with force spectroscopy. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2007 , 104, 7916-21	11.5	87
136	Free Energy of the Hydrophobic Interaction from Molecular Dynamics Simulations: The Effects of Solute and Solvent Polarizability. <i>Journal of Physical Chemistry B</i> , 1997 , 101, 10488-10493	3.4	86

135	Aggregation and dispersion of small hydrophobic particles in aqueous electrolyte solutions. <i>Journal of Physical Chemistry B</i> , 2006 , 110, 22736-41	3.4	84
134	Effect of pressure on hydrogen bonding in glycerol: A molecular dynamics investigation. <i>Journal of Chemical Physics</i> , 1997 , 107, 4350-4357	3.9	83
133	Smart walking: A new method for Boltzmann sampling of protein conformations. <i>Journal of Chemical Physics</i> , 1997 , 107, 9185-9196	3.9	83
132	When does trimethylamine N-oxide fold a polymer chain and urea unfold it?. <i>Journal of Physical Chemistry B</i> , 2013 , 117, 8723-32	3.4	82
131	On the calculation of dynamical properties of solvated electrons by maximum entropy analytic continuation of path integral Monte Carlo data. <i>Journal of Chemical Physics</i> , 1996 , 105, 7064-7078	3.9	82
130	Vibronic spectra in condensed matter: A comparison of exact quantum mechanical and various semiclassical treatments for harmonic baths. <i>Journal of Chemical Physics</i> , 1998 , 108, 1407-1422	3.9	81
129	Single homopolypeptide chains collapse into mechanically rigid conformations. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2009 , 106, 12605-10	11.5	78
128	Scanning tunneling microscopy images of alkane derivatives on graphite: role of electronic effects. <i>Nano Letters</i> , 2008 , 8, 3160-5	11.5	77
127	Temperature dependence of dimerization and dewetting of large-scale hydrophobes: a molecular dynamics study. <i>Journal of Physical Chemistry B</i> , 2008 , 112, 8634-44	3.4	77
126	Polarizable molecules in the vibrational spectroscopy of water. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2005 , 102, 11611-6	11.5	74
125	The absorption spectrum of the solvated electron in fluid helium by maximum entropy inversion of imaginary time correlation functions from path integral Monte Carlo simulations. <i>Journal of Chemical Physics</i> , 1994 , 101, 9909-9918	3.9	72
124	Hydrophobic aided replica exchange: an efficient algorithm for protein folding in explicit solvent. <i>Journal of Physical Chemistry B</i> , 2006 , 110, 19018-22	3.4	71
123	Molecular Reorientation in Liquids and Gases. <i>Journal of Chemical Physics</i> , 1968 , 49, 3125-3129	3.9	71
122	How and when does an anticancer drug leave its binding site?. <i>Science Advances</i> , 2017 , 3, e1700014	14.3	69
121	Quantum mechanical canonical rate theory: A new approach based on the reactive flux and numerical analytic continuation methods. <i>Journal of Chemical Physics</i> , 2000 , 112, 2605-2614	3.9	69
120	Direct Observation of Stretched-Exponential Relaxation in Low-Temperature Lennard-Jones Systems Using the Cage Correlation Function. <i>Physical Review Letters</i> , 1999 , 82, 3649-3652	7.4	69
119	Molecular Dynamics Calculation of the Effect of Solvent Polarizability on the Hydrophobic Interaction. <i>Journal of the American Chemical Society</i> , 1995 , 117, 7172-7179	16.4	69
118	On the Adequacy of Mixed Quantum-Classical Dynamics in Condensed Phase Systems. <i>Journal of Physical Chemistry B</i> , 1999 , 103, 10978-10991	3.4	68

117	Theory of correlated hops in surface diffusion. <i>Physical Review Letters</i> , 1993 , 70, 3299-3302	7.4	68
116	On the use of semiclassical dynamics in determining electronic spectra of Br ₂ in an Ar matrix. <i>Journal of Chemical Physics</i> , 1985 , 83, 230-238	3.9	67
115	Destruction of long-range interactions by a single mutation in lysozyme. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2007 , 104, 5824-9	11.5	66
114	Topics in Time-Dependent Statistical Mechanics. <i>Annual Review of Physical Chemistry</i> , 1971 , 22, 563-596	15.7	66
113	Efficient Simulation Method for Polarizable Protein Force Fields: Application to the Simulation of BPTI in Liquid Water. <i>Journal of Chemical Theory and Computation</i> , 2005 , 1, 169-80	6.4	65
112	Global Optimization: Quantum Thermal Annealing with Path Integral Monte Carlo. <i>Journal of Physical Chemistry A</i> , 2000 , 104, 86-95	2.8	65
111	A Born-Oppenheimer approximation for path integrals with an application to electron solvation in polarizable fluids. <i>Journal of Chemical Physics</i> , 1993 , 99, 2902-2916	3.9	65
110	Elasticity, structure, and relaxation of extended proteins under force. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2013 , 110, 3847-52	11.5	63
109	Solvation and reorganization energies in polarizable molecular and continuum solvents. <i>Journal of Chemical Physics</i> , 1997 , 106, 2372-2387	3.9	63
108	Do Molecules as Small as Neopentane Induce a Hydrophobic Response Similar to That of Large Hydrophobic Surfaces?. <i>Journal of Physical Chemistry B</i> , 2003 , 107, 11742-11748	3.4	62
107	On the force bias Monte Carlo simulation of simple liquids. <i>Journal of Chemical Physics</i> , 1979 , 71, 129-133	3.9	62
106	Density dependence of excess electronic ground-state energies in simple atomic fluids. <i>Journal of Chemical Physics</i> , 1992 , 97, 2002-2021	3.9	61
105	Role of water and steric constraints in the kinetics of cavity-ligand unbinding. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2015 , 112, 12015-9	11.5	60
104	Dewetting transitions in protein cavities. <i>Proteins: Structure, Function and Bioinformatics</i> , 2010 , 78, 1856-69	4.9	60
103	Nonradiative relaxation processes in condensed phases: Quantum versus classical baths. <i>Journal of Chemical Physics</i> , 1999 , 110, 5238-5248	3.9	60
102	Time correlation functions in quantum systems. <i>Journal of Chemical Physics</i> , 1984 , 81, 2512-2513	3.9	58
101	Probing static disorder in Arrhenius kinetics by single-molecule force spectroscopy. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2010 , 107, 11336-40	11.5	57
100	Low-temperature variational approximation for the Feynman quantum propagator and its application to the simulation of quantum systems. <i>Journal of Chemical Physics</i> , 1990 , 92, 7531-7539	3.9	56

99	Efficient multiple time scale molecular dynamics: Using colored noise thermostats to stabilize resonances. <i>Journal of Chemical Physics</i> , 2011 , 134, 014103	3.9	54
98	A new quantum propagator for hard sphere and cavity systems. <i>Journal of Chemical Physics</i> , 1992 , 97, 2382-2385	3.9	54
97	Hydrophobic effect on chain folding. The trans to gauche isomerization of n-butane in water. <i>Journal of the American Chemical Society</i> , 1982 , 104, 7647-7649	16.4	54
96	Structure and dynamics of the solvation of bovine pancreatic trypsin inhibitor in explicit water: a comparative study of the effects of solvent and protein polarizability. <i>Journal of Physical Chemistry B</i> , 2005 , 109, 16529-38	3.4	51
95	Laser Light Scattering from Liquids. <i>Annual Review of Physical Chemistry</i> , 1974 , 25, 233-253	15.7	49
94	Rate limit of protein elastic response is tether dependent. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2012 , 109, 14416-21	11.5	48
93	Quantum Rate Constants from Short-Time Dynamics: An Analytic Continuation Approach \square <i>Journal of Physical Chemistry A</i> , 2001 , 105, 2824-2833	2.8	48
92	Inferring the hydrophobic interaction from the properties of neat water. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 1996 , 93, 8800-3	11.5	48
91	Interplay between hydrodynamics and the free energy surface in the assembly of nanoscale hydrophobes. <i>Journal of Physical Chemistry B</i> , 2012 , 116, 378-89	3.4	46
90	Molecular Dynamics with Multiple Time Scales: How to Avoid Pitfalls. <i>Journal of Chemical Theory and Computation</i> , 2010 , 6, 1798-804	6.4	46
89	Light Scattering as a Probe of Fast Reaction Kinetics. <i>Journal of Chemical Physics</i> , 1967 , 47, 3675-3676	3.9	46
88	Quantum time correlation functions from complex time Monte Carlo simulations: A maximum entropy approach. <i>Journal of Chemical Physics</i> , 2001 , 114, 1075-1088	3.9	45
87	Real time quantum correlation functions. II. Maximum entropy numerical analytic continuation of path integral Monte Carlo and centroid molecular dynamics data. <i>Journal of Chemical Physics</i> , 1999 , 111, 9147-9156	3.9	45
86	Method for accelerating chain folding and mixing. <i>Journal of Chemical Physics</i> , 1993 , 99, 6071-6077	3.9	45
85	Role of Desolvation in Thermodynamics and Kinetics of Ligand Binding to a Kinase. <i>Journal of Chemical Theory and Computation</i> , 2014 , 10, 5696-5705	6.4	44
84	The energy relaxation of a nonlinear oscillator coupled to a linear bath. <i>Journal of Chemical Physics</i> , 1996 , 104, 1111-1119	3.9	44
83	Many-body dispersion forces of polarizable clusters and liquids. <i>Journal of Chemical Physics</i> , 1992 , 97, 8628-8636	3.9	44
82	On the application of numerical analytic continuation methods to the study of quantum mechanical vibrational relaxation processes. <i>Journal of Chemical Physics</i> , 1998 , 109, 7745-7755	3.9	43

81	Computer simulation of solid C60 using multiple time-step algorithms. <i>Journal of Chemical Physics</i> , 1994 , 101, 2421-2431	3.9	43
80	Impulsive stochastic models of molecular relaxation and isomerization reactions. <i>Journal of Chemical Physics</i> , 1980 , 73, 4314-4320	3.9	43
79	Multiple time step Monte Carlo. <i>Journal of Chemical Physics</i> , 2002 , 117, 8203-8207	3.9	41
78	The simulation of electronic absorption spectrum of a chromophore coupled to a condensed phase environment: Maximum entropy versus singular value decomposition approaches. <i>Journal of Chemical Physics</i> , 1997 , 107, 9312-9318	3.9	39
77	Thermodynamic properties of liquid water: an application of a nonparametric approach to computing the entropy of a neat fluid. <i>Journal of Chemical Theory and Computation</i> , 2009 , 5, 1462-1473	6.4	38
76	Monte Carlo methods for accelerating barrier crossing: Anti-force-bias and variable step algorithms. <i>Journal of Chemical Physics</i> , 1990 , 92, 1980-1985	3.9	38
75	A comparison of exact quantum mechanical and various semiclassical treatments for the vibronic absorption spectrum: The case of fast vibrational relaxation. <i>Journal of Chemical Physics</i> , 1998 , 109, 6376-6381	3.9	37
74	Multicanonical jump walking: A method for efficiently sampling rough energy landscapes. <i>Journal of Chemical Physics</i> , 1999 , 110, 10299-10306	3.9	37
73	Structure of a liquid-vapor interface in the presence of a hard wall in the transition region. <i>Journal of Chemical Physics</i> , 1979 , 71, 3802-3806	3.9	37
72	How hydrophobic drying forces impact the kinetics of molecular recognition. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2013 , 110, 13277-82	11.5	36
71	Ultra-high vacuum scanning tunneling microscopy and theoretical studies of 1-halohexane monolayers on graphite. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2005 , 102, 5315-22	11.5	36
70	Classical Approximation to Nonradiative Electronic Relaxation in Condensed Phase Systems. <i>Journal of Physical Chemistry A</i> , 1999 , 103, 9539-9544	2.8	36
69	Theory and simulation of polar and nonpolar polarizable fluids. <i>Journal of Chemical Physics</i> , 1993 , 99, 6998-7011	3.9	36
68	Chain-Length Effects on the Self-Assembly of Short 1-Bromoalkane and n-Alkane Monolayers on Graphite. <i>Journal of Physical Chemistry C</i> , 2008 , 112, 18067-18075	3.8	34
67	Structure and Dynamics of Acetonitrile Confined in a Silica Nanopore. <i>Journal of Physical Chemistry C</i> , 2012 , 116, 9582-9593	3.8	33
66	Water's role in the force-induced unfolding of ubiquitin. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2010 , 107, 19284-9	11.5	33
65	Comment on "urea-mediated protein denaturation: a consensus view". <i>Journal of Physical Chemistry B</i> , 2011 , 115, 1323-6; discussion 1327-8	3.4	33
64	Excess electronic states in fluid helium. <i>Journal of Chemical Physics</i> , 1988 , 89, 2128-2137	3.9	33

63	Helix Unfolding and Intramolecular Hydrogen Bond Dynamics in Small α -Helices in Explicit Solvent. <i>Journal of Physical Chemistry B</i> , 2002 , 106, 10748-10752	3.4	32
62	Serial replica exchange. <i>Journal of Physical Chemistry B</i> , 2007 , 111, 1416-23	3.4	31
61	Comment on "Can a Continuum Solvent Model Reproduce the Free Energy Landscape of a α -Hairpin Folding in Water?" The Poisson-Boltzmann Equation. <i>Journal of Physical Chemistry B</i> , 2004 , 108, 7528-7530	3.4	31
60	Real time quantum correlation functions. I. Centroid molecular dynamics of anharmonic systems. <i>Journal of Chemical Physics</i> , 1999 , 111, 9140-9146	3.9	30
59	Competition of electrostatic and hydrophobic interactions between small hydrophobes and model enclosures. <i>Journal of Physical Chemistry B</i> , 2010 , 114, 7294-301	3.4	28
58	Dissecting entropic coiling and poor solvent effects in protein collapse. <i>Journal of the American Chemical Society</i> , 2008 , 130, 11578-9	16.4	28
57	Are hydrodynamic interactions important in the kinetics of hydrophobic collapse?. <i>Journal of Physical Chemistry B</i> , 2012 , 116, 11537-44	3.4	27
56	Thermal and structural stability of adsorbed proteins. <i>Biophysical Journal</i> , 2010 , 99, 1157-65	2.9	27
55	A displaced-solvent functional analysis of model hydrophobic enclosures. <i>Journal of Chemical Theory and Computation</i> , 2010 , 6, 2924-2934	6.4	27
54	Hydrophobic interactions in model enclosures from small to large length scales: non-additivity in explicit and implicit solvent models. <i>Faraday Discussions</i> , 2010 , 146, 247-62; discussion 283-98, 395-401	3.6	27
53	Quantum path minimization: An efficient method for global optimization. <i>Journal of Chemical Physics</i> , 2003 , 118, 2999-3005	3.9	27
52	Multicanonical jump walk annealing: An efficient method for geometric optimization. <i>Journal of Chemical Physics</i> , 2000 , 112, 2701-2708	3.9	27
51	Activated rate processes: The reactive flux method for one-dimensional surface diffusion. <i>Journal of Chemical Physics</i> , 1995 , 102, 4037-4055	3.9	27
50	Path-Integral Monte Carlo Scheme for Rigid Tops: Application to the Quantum Rotator Phase Transition in Solid Methane. <i>Physical Review Letters</i> , 1996 , 77, 2638-2641	7.4	27
49	Reply to Comment on: Reversible multiple time scale molecular dynamics. <i>Journal of Chemical Physics</i> , 1993 , 99, 2278-2279	3.9	27
48	Predicting reaction coordinates in energy landscapes with diffusion anisotropy. <i>Journal of Chemical Physics</i> , 2017 , 147, 152701	3.9	26
47	How a Kinase Inhibitor Withstands Gatekeeper Residue Mutations. <i>Journal of the American Chemical Society</i> , 2016 , 138, 4608-15	16.4	26
46	Theory and simulations of quantum glass forming liquids. <i>Journal of Chemical Physics</i> , 2012 , 136, 074511	3.9	25

45	First passage time distribution in stochastic processes with moving and static absorbing boundaries with application to biological rupture experiments. <i>Journal of Chemical Physics</i> , 2010 , 133, 034105	3.9	24
44	Evaluation of microcanonical rate constants for bimolecular reactions by path integral techniques. <i>Journal of Chemical Physics</i> , 1985 , 83, 2972-2975	3.9	24
43	Calculating the hopping rate for diffusion in molecular liquids: CS ₂ . <i>Journal of Chemical Physics</i> , 1999 , 110, 3444-3452	3.9	23
42	Solvent Effects on the Self-Assembly of 1-Bromoeicosane on Graphite. Part I. Scanning Tunneling Microscopy. <i>Journal of Physical Chemistry C</i> , 2009 , 113, 3631-3640	3.8	22
41	How wet should be the reaction coordinate for ligand unbinding?. <i>Journal of Chemical Physics</i> , 2016 , 145, 054113	3.9	22
40	Circumventing the pathological behavior of path-integral Monte Carlo for systems with Coulomb potentials. <i>Journal of Chemical Physics</i> , 1997 , 107, 571-575	3.9	21
39	Catalytic tempering: A method for sampling rough energy landscapes by Monte Carlo. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2000 , 97, 11164-9	11.5	21
38	Quantum Thermal Annealing with Renormalization: Application to a Frustrated Model Protein. <i>Journal of Physical Chemistry A</i> , 2001 , 105, 459-464	2.8	21
37	Transport properties of normal liquid helium: comparison of various methodologies. <i>Journal of Chemical Physics</i> , 2005 , 123, 184506	3.9	18
36	Path-integral diffusion Monte Carlo: Calculation of observables of many-body systems in the ground state. <i>Journal of Chemical Physics</i> , 1999 , 110, 6143-6153	3.9	18
35	Response to Comment on a critique of the instantaneous normal mode (INM) approach to diffusion[J. Chem. Phys. 109, 4693 (1998)]. <i>Journal of Chemical Physics</i> , 1998 , 109, 4695-4696	3.9	17
34	Kramers turnover: From energy diffusion to spatial diffusion using metadynamics. <i>Journal of Chemical Physics</i> , 2016 , 144, 134103	3.9	17
33	Multiple "time step" Monte Carlo simulations: application to charged systems with Ewald summation. <i>Journal of Chemical Physics</i> , 2004 , 121, 44-50	3.9	14
32	Elastic bag model for molecular dynamics simulations of solvated systems: application to liquid argon. <i>Journal of Physical Chemistry B</i> , 2005 , 109, 463-70	3.4	13
31	The energy-dependent transmission coefficient and the energy distribution of classical particles escaping from a metastable well. <i>Journal of Chemical Physics</i> , 1995 , 102, 7953-7965	3.9	13
30	Nucleation in finite systems: Theory and computer simulation. <i>Astrophysics and Space Science</i> , 1979 , 65, 39-46	1.6	13
29	Simulated Force Quench Dynamics Shows GB1 Protein Is Not a Two State Folder. <i>Journal of Physical Chemistry B</i> , 2017 , 121, 5162-5173	3.4	12
28	Characterization of heterogeneous solutions using laser light scattering: study of the tubulin system. <i>Biochemistry</i> , 1977 , 16, 5776-81	3.2	12

27	Second-Order Reentrant Phase Transition in the Quantum Anisotropic Planar Rotor Model. <i>Physical Review Letters</i> , 1999 , 83, 4606-4609	7.4	11
26	Massively parallel molecular dynamics simulations of lysozyme unfolding. <i>IBM Journal of Research and Development</i> , 2008 , 52, 19-30	2.5	10
25	Path-integral Monte Carlo simulations of electron localization in water clusters. <i>Journal of Statistical Physics</i> , 1986 , 43, 973-984	1.5	10
24	Efficient sampling of puckering states of monosaccharides through replica exchange with solute tempering and bond softening. <i>Journal of Chemical Physics</i> , 2018 , 149, 072306	3.9	9
23	Molecular Dynamics Simulation Studies of Self-Assembly of Racemic (R)/(S)-2-Bromohexadecanoic Acid on a Graphite Surface: Enantio-pure or Enantio-mixed Domains?. <i>Journal of Physical Chemistry C</i> , 2007 , 111, 18243-18250	3.8	9
22	Elastic bag model for molecular dynamics simulations of solvated systems: application to liquid water and solvated peptides. <i>Journal of Physical Chemistry B</i> , 2006 , 110, 13256-63	3.4	9
21	Hydrodynamic calculation of the frequency dependent friction on the bond of a diatomic molecule. <i>Journal of Chemical Physics</i> , 1995 , 103, 1160-1174	3.9	9
20	Theory of polarizable liquid crystals: Optical birefringence. <i>Journal of Chemical Physics</i> , 1993 , 99, 2213-2220	3.9	9
19	Solvent Effects on the Self-Assembly of 1-Bromoeicosane on Graphite. Part II. Theory. <i>Journal of Physical Chemistry C</i> , 2009 , 113, 3641-3649	3.8	8
18	The dependence of the rate constant for isomerization on the competition between intramolecular vibrational relaxation and energy transfer to the bath: A stochastic model. <i>Journal of Chemical Physics</i> , 1999 , 110, 1053-1060	3.9	8
17	Rabani, gezelter, and berne reply:. <i>Physical Review Letters</i> , 2000 , 85, 467	7.4	7
16	Radial correlations in associated liquids. <i>Journal of Chemical Physics</i> , 1979 , 71, 3889-3891	3.9	7
15	Monte Carlo Simulation of Water. <i>ACS Symposium Series</i> , 1978 , 29-31	0.4	6
14	On the effects of translation-rotation coupling on hydrodynamic diffusion tensors. <i>Journal of Chemical Physics</i> , 1977 , 67, 5971-5972	3.9	5
13	Determination of the Mean Force of Two Noble Gas Atoms Dissolved in Water. <i>ACS Symposium Series</i> , 1978 , 32-34	0.4	5
12	Comments on the Coupling between Linear and Angular Momentum of Structured Molecules. <i>Journal of Chemical Physics</i> , 1970 , 52, 5193-5194	3.9	5
11	Dispersion of the Electrically Induced Refractive-Index Anisotropy in Nonpolar Liquids as a Probe of Reaction Kinetics. <i>Journal of Chemical Physics</i> , 1970 , 52, 1259-1261	3.9	4
10	A scaling and mapping theory for excess electrons in simple fluids. <i>Journal of Chemical Physics</i> , 1995 , 102, 432-436	3.9	3

9	The Theory of Multi-Barrier Crossing 1995 , 67-92		3
8	Molecular dynamics for nonequilibrium systems in which there are a small number of very hot particles in a cold bath: Reference system propagator methods. <i>Journal of Chemical Physics</i> , 1996 , 105, 235-239	3.9	2
7	Perspective on Statistical mechanics of isomerization dynamics in liquids and the transition state approximation <i>Theoretical Chemistry Accounts</i> , 2000 , 103, 335-336	1.9	1
6	Energy Dissipation in Nonlinear Systems Coupled to a Bath: On the Use of Perturbative Maps. <i>Journal of Physical Chemistry A</i> , 1998 , 102, 9380-9389	2.8	1
5	Fluctuations in lattice Monte Carlo simulations. <i>Physical Review D</i> , 1984 , 30, 1791-1794	4.9	1
4	Reply to the Comment on Do Molecules as Small as Neopentane Induce a Hydrophobic Response Similar to that of Large Hydrophobic Surfaces?. <i>Journal of Physical Chemistry B</i> , 2004 , 108, 9373-9374	3.4	
3	Comment on A statistical theory of rate constants in nonergodic systems <i>Journal of Chemical Physics</i> , 1982 , 76, 5187-5188	3.9	
2	Multiple Time Scales in Molecular Dynamics: Applications to Vibrational Relaxation. <i>Jerusalem Symposia on Quantum Chemistry and Biochemistry</i> , 1994 , 471-494		
1	Computer Experiments on Heterogeneous Systems. <i>Topics in Current Physics</i> , 1982 , 99-127		