B J Berne

List of Publications by Year
in descending order

205 papers	25,505 citations	6254 80 h-index	6996 154 g-index
212 all docs	212 docs citations	212 times ranked	14374 citing authors

#	Article	IF	Citations
1	Efficient sampling of puckering states of monosaccharides through replica exchange with solute tempering and bond softening. Journal of Chemical Physics, 2018, 149, 072306.	3.0	12
2	Simulated Force Quench Dynamics Shows GB1 Protein Is Not a Two State Folder. Journal of Physical Chemistry B, 2017, 121, 5162-5173.	2.6	14
3	How and when does an anticancer drug leave its binding site?. Science Advances, 2017, 3, e1700014.	10.3	111
4	Predicting reaction coordinates in energy landscapes with diffusion anisotropy. Journal of Chemical Physics, 2017, 147, 152701.	3.0	37
5	Advancing Drug Discovery through Enhanced Free Energy Calculations. Accounts of Chemical Research, 2017, 50, 1625-1632.	15.6	211
6	How wet should be the reaction coordinate for ligand unbinding?. Journal of Chemical Physics, 2016, 145, 054113.	3.0	31
7	Kramers turnover: From energy diffusion to spatial diffusion using metadynamics. Journal of Chemical Physics, 2016, 144, 134103.	3.0	18
8	Prediction of Proteinâ€“Ligand Binding Poses via a Combination of Induced Fit Docking and Metadynamics Simulations. Journal of Chemical Theory and Computation, 2016, 12, 2990-2998.	5.3	184
9	Spectral gap optimization of order parameters for sampling complex molecular systems. Proceedings of the National Academy of Sciences of the United States of America, 2016, 113, 2839-2844.	7.1	210
10	How a Kinase Inhibitor Withstands Gatekeeper Residue Mutations. Journal of the American Chemical Society, 2016, 138, 4608-4615.	13.7	44
11	Role of water and steric constraints in the kinetics of cavityâ€“ligand unbinding. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, 12015-12019.	7.1	74
12	Role of Desolvation in Thermodynamics and Kinetics of Ligand Binding to a Kinase. Journal of Chemical Theory and Computation, 2014, 10, 5696-5705.	5.3	61
13	Elasticity, structure, and relaxation of extended proteins under force. Proceedings of the National Academy of Sciences of the United States of America, 2013, 110, 3847-3852.	7.1	81
14	When Does Trimethylamine N-Oxide Fold a Polymer Chain and Urea Unfold It?. Journal of Physical Chemistry B, 2013, 117, 8723-8732.	2.6	99
15	How hydrophobic drying forces impact the kinetics of molecular recognition. Proceedings of the National Academy of Sciences of the United States of America, 2013, 110, 13277-13282.	7.1	45
16	Unraveling quantum mechanical effects in water using isotopic fractionation. Proceedings of the National Academy of Sciences of the United States of America, 2012, 109, 7988-7991.	7.1	97
17	Rate limit of protein elastic response is tether dependent. Proceedings of the National Academy of Sciences of the United States of America, 2012, 109, 14416-14421.	7.1	59
18	Are Hydrodynamic Interactions Important in the Kinetics of Hydrophobic Collapse?. Journal of Physical Chemistry B, 2012, 116, 11537-11544.	2.6	29

#	Article	IF	Citations
19	Interplay between Hydrodynamics and the Free Energy Surface in the Assembly of Nanoscale Hydrophobes. Journal of Physical Chemistry B, 2012, 116, 378-389.	2.6	52
20	Structure and Dynamics of Acetonitrile Confined in a Silica Nanopore. Journal of Physical Chemistry C, 2012, 116, 9582-9593.	3.1	38
21	Theory and simulations of quantum glass forming liquids. Journal of Chemical Physics, 2012, 136, 074511.	3.0	34
22	On achieving high accuracy and reliability in the calculation of relative proteinâ€"ligand binding affinities. Proceedings of the National Academy of Sciences of the United States of America, 2012, 109, 1937-1942.	7.1	204
23	Comment on â€œUrea-Mediated Protein Denaturation: A Consensus Viewâ€• Journal of Physical Chemistry B, 2011, 115, 1323-1326.	2.6	35
24	Efficient multiple time scale molecular dynamics: Using colored noise thermostats to stabilize resonances. Journal of Chemical Physics, 2011, 134, 014103.	3.0	61
25	Replica Exchange with Solute Scaling: A More Efficient Version of Replica Exchange with Solute Tempering (REST2). Journal of Physical Chemistry B, 2011, 115, 9431-9438.	2.6	595
26	Ligand binding to protein-binding pockets with wet and dry regions. Proceedings of the National Academy of Sciences of the United States of America, 2011, 108, 1326-1330.	7.1	178
27	Dewetting transitions in protein cavities. Proteins: Structure, Function and Bioinformatics, 2010, 78, 1856-1869.	2.6	64
28	Waterâ€™s role in the force-induced unfolding of ubiquitin. Proceedings of the National Academy of Sciences of the United States of America, 2010, 107, 19284-19289.	7.1	37
29	Probing static disorder in Arrhenius kinetics by single-molecule force spectroscopy. Proceedings of the National Academy of Sciences of the United States of America, 2010, 107, 11336-11340.	7.1	65
30	First passage time distribution in stochastic processes with moving and static absorbing boundaries with application to biological rupture experiments. Journal of Chemical Physics, 2010, 133, 034105.	3.0	30
31	Thermal and Structural Stability of Adsorbed Proteins. Biophysical Journal, 2010, 99, 1157-1165.	0.5	32
32	Competition of Electrostatic and Hydrophobic Interactions between Small Hydrophobes and Model Enclosures. Journal of Physical Chemistry B, 2010, 114, 7294-7301.	2.6	32
33	A Displaced-Solvent Functional Analysis of Model Hydrophobic Enclosures. Journal of Chemical Theory and Computation, 2010, 6, 2924-2934.	5.3	31
34	Molecular Dynamics with Multiple Time Scales: How to Avoid Pitfalls. Journal of Chemical Theory and Computation, 2010, 6, 1798-1804.	5.3	57
35	Hydrophobic interactions in model enclosures from small to large length scales: non-additivity in explicit and implicit solvent models. Faraday Discussions, 2010, 146, 247.	3.2	31
36	Single homopolypeptide chains collapse into mechanically rigid conformations. Proceedings of the National Academy of Sciences of the United States of America, 2009, 106, 12605-12610.	7.1	84

#	Article	IF	Citations
37	Solvent Effects on the Self-Assembly of 1-Bromoeicosane on Graphite. Part I. Scanning Tunneling Microscopy. Journal of Physical Chemistry C, 2009, 113, 3631-3640.	3.1	23
38	Hydrophobic Interactions and Dewetting between Plates with Hydrophobic and Hydrophilic Domains. Journal of Physical Chemistry C, 2009, 113, 5244-5253.	3.1	104
39	Solvent Effects on the Self-Assembly of 1-Bromoeicosane on Graphite. Part II. Theory. Journal of Physical Chemistry C, 2009, 113, 3641-3649.	3.1	9
40	Thermodynamic Properties of Liquid Water: An Application of a Nonparametric Approach to Computing the Entropy of a Neat Fluid. Journal of Chemical Theory and Computation, 2009, 5, 1462-1473.	5.3	47
41	Ureaâ€™s Action on Hydrophobic Interactions. Journal of the American Chemical Society, 2009, 131, 1535-1541.	13.7	288
42	Role of Water in Mediating the Assembly of Alzheimer Amyloid-Î² AÎ²16âˆ’22 Protofilaments. Journal of the American Chemical Society, 2008, 130, 11066-11072.	13.7	208
43	Massively parallel molecular dynamics simulations of lysozyme unfolding. IBM Journal of Research and Development, 2008, 52, 19-30.	3.1	22
44	Chain-Length Effects on the Self-Assembly of Short 1-Bromoalkane and n-Alkane Monolayers on Graphite. Journal of Physical Chemistry C, 2008, 112, 18067-18075.	3.1	36
45	Dissecting Entropic Coiling and Poor Solvent Effects in Protein Collapse. Journal of the American Chemical Society, 2008, 130, 11578-11579.	13.7	31
46	Scanning Tunneling Microscopy Images of Alkane Derivatives on Graphite: Role of Electronic Effects. Nano Letters, 2008, 8, 3160-3165.	9.1	86
47	Temperature Dependence of Dimerization and Dewetting of Large-Scale Hydrophobes: A Molecular Dynamics Study. Journal of Physical Chemistry B, 2008, 112, 8634-8644.	2.6	83
48	Urea denaturation by stronger dispersion interactions with proteins than water implies a 2-stage unfolding. Proceedings of the National Academy of Sciences of the United States of America, 2008, 105, 16928-16933.	7.1	470
49	Destruction of long-range interactions by a single mutation in lysozyme. Proceedings of the National Academy of Sciences of the United States of America, 2007, 104, 5824-5829.	7.1	71
50	On the Calculation of Time Correlation Functions. Advances in Chemical Physics, 2007, , 63-227.	0.3	415
51	Signatures of hydrophobic collapse in extended proteins captured with force spectroscopy. Proceedings of the National Academy of Sciences of the United States of America, 2007, 104, 7916-7921.	7.1	99
52	Serial Replica Exchange. Journal of Physical Chemistry B, 2007, 111, 1416-1423.	2.6	35
53	Molecular Dynamics Simulation Studies of Self-Assembly of Racemic (R)/(S)-2-Bromohexadecanoic Acid on a Graphite Surface:â€‰ Enantio-pure or Enantio-mixed Domains?. Journal of Physical Chemistry C, 2007, 111, 18243-18250.	3.1	10
54	Replica Exchange with Solute Tempering:Â Efficiency in Large Scale Systems. Journal of Physical Chemistry B, 2007, 111, 5405-5410.	2.6	103

#	Article	IF	Citations
55	Effect of Ions on the Hydrophobic Interaction between Two Plates. Journal of the American Chemical Society, 2007, 129, 4678-4686.	13.7	223
56	Hydrophobic Aided Replica Exchange:Â an Efficient Algorithm for Protein Folding in Explicit Solventâ€. Journal of Physical Chemistry B, 2006, 110, 19018-19022.	2.6	74
57	Aggregation and Dispersion of Small Hydrophobic Particles in Aqueous Electrolyte Solutions. Journal of Physical Chemistry B, 2006, 110, 22736-22741.	2.6	92
58	Dynamics of Water Confined in the Interdomain Region of a Multidomain Proteinâ€. Journal of Physical Chemistry B, 2006, 110, 3704-3711.	2.6	93
59	Elastic Bag Model for Molecular Dynamics Simulations of Solvated Systems:Â Application to Liquid Water and Solvated Peptides. Journal of Physical Chemistry B, 2006, 110, 13256-13263.	2.6	10
60	Replica exchange with solute tempering: A method for sampling biological systems in explicit water. Proceedings of the National Academy of Sciences of the United States of America, 2005, 102, 13749-13754.	7.1	634
61	Observation of a dewetting transition in the collapse of the melittin tetramer. Nature, 2005, 437, 159-162.	27.8	362
62	Transport properties of normal liquid helium: Comparison of various methodologies. Journal of Chemical Physics, 2005, 123, 184506.	3.0	18
63	Ultra-high vacuum scanning tunneling microscopy and theoretical studies of 1-halohexane monolayers on graphite. Proceedings of the National Academy of Sciences of the United States of America, 2005, 102, 5315-5322.	7.1	37
64	Polarizable molecules in the vibrational spectroscopy of water. Proceedings of the National Academy of Sciences of the United States of America, 2005, 102, 11611-11616.	7.1	77
65	Elastic Bag Model for Molecular Dynamics Simulations of Solvated Systems:Â Application to Liquid Argon. Journal of Physical Chemistry B, 2005, 109, 463-470.	2.6	14
66	Structure and Dynamics of the Solvation of Bovine Pancreatic Trypsin Inhibitor in Explicit Water:â€‰ A Comparative Study of the Effects of Solvent and Protein Polarizability. Journal of Physical Chemistry B, 2005, 109, 16529-16538.	2.6	55
67	Efficient Simulation Method for Polarizable Protein Force Fields:â€‰ Application to the Simulation of BPTI in Liquid Water. Journal of Chemical Theory and Computation, 2005, 1, 169-180.	5.3	68
68	Hydrogen-Bond Dynamics in the Airâˆ’Water Interface. Journal of Physical Chemistry B, 2005, 109, 2949-2955.	2.6	121
69	Multiple â€œtime stepâ€•Monte Carlo simulations: Application to charged systems with Ewald summation. Journal of Chemical Physics, 2004, 121, 44.	3.0	15
70	Reply to the Comment on â€œDo Molecules as Small as Neopentane Induce a Hydrophobic Response Similar to that of Large Hydrophobic Surfaces?. Journal of Physical Chemistry B, 2004, 108, 9373-9374.	2.6	0
71	Comment on â€œCan a Continuum Solvent Model Reproduce the Free Energy Landscape of a Î²-Hairpin Folding in Water?â€•The Poissonâˆ’Boltzmann Equation. Journal of Physical Chemistry B, 2004, 108, 7528-7530.	2.6	34
72	Development of an Accurate and Robust Polarizable Molecular Mechanics Force Field from ab Initio Quantum Chemistry. Journal of Physical Chemistry A, 2004, 108, 621-627.	2.5	221

#	Article	IF	Citations
73	On the Calculation of Diffusion Coefficients in Confined Fluids and Interfaces with an Application to the Liquidâˆ'Vapor Interface of Water. Journal of Physical Chemistry B, 2004, 108, 6595-6602.	2.6	337
74	Do Molecules as Small as Neopentane Induce a Hydrophobic Response Similar to That of Large Hydrophobic Surfaces?. Journal of Physical Chemistry B, 2003, 107, 11742-11748.	2.6	66
75	Quantum path minimization: An efficient method for global optimization. Journal of Chemical Physics, 2003, 118, 2999-3005.	3.0	28
76	Dewetting-induced collapse of hydrophobic particles. Proceedings of the National Academy of Sciences of the United States of America, 2003, 100, 11953-11958.	7.1	264
77	Can a continuum solvent model reproduce the free energy landscape of a Â-hairpin folding in water?. Proceedings of the National Academy of Sciences of the United States of America, 2002, 99, 12777-12782.	7.1	326
78	The calculation of transport properties in quantum liquids using the maximum entropy numerical analytic continuation method: Application to liquid para-hydrogen. Proceedings of the National Academy of Sciences of the United States of America, 2002, 99, 1129-1133.	7.1	89
79	Computer Simulation of a â€œGreen Chemistryâ€•Room-Temperature Ionic Solvent. Journal of Physical Chemistry B, 2002, 106, 12017-12021.	2.6	268
80	Helix Unfolding and Intramolecular Hydrogen Bond Dynamics in Small Î±-Helices in Explicit Solvent. Journal of Physical Chemistry B, 2002, 106, 10748-10752.	2.6	33
81	Multiple â€œtime stepâ€•Monte Carlo. Journal of Chemical Physics, 2002, 117, 8203-8207.	3.0	47
82	Can Water Polarizability Be Ignored in Hydrogen Bond Kinetics?. Journal of Physical Chemistry B, 2002, 106, 2054-2060.	2.6	195
83	Development of a polarizable force field for proteins via ab initio quantum chemistry: First generation model and gas phase tests. Journal of Computational Chemistry, 2002, 23, 1515-1531.	3.3	296
84	Blue Gene: A vision for protein science using a petaflop supercomputer. IBM Systems Journal, 2001, 40, 310-327.	3.0	211
85	Hydrogen-Bond Kinetics in the Solvation Shell of a Polypeptide. Journal of Physical Chemistry B, 2001, 105, 11929-11932.	2.6	225
86	Quantum Rate Constants from Short-Time Dynamics:Â An Analytic Continuation Approachâ€. Journal of Physical Chemistry A, 2001, 105, 2824-2833.	2.5	50
87	Quantum Thermal Annealing with Renormalization:Â Application to a Frustrated Model Protein. Journal of Physical Chemistry A, 2001, 105, 459-464.	2.5	23
88	The free energy landscape for Â hairpin folding in explicit water. Proceedings of the National Academy of Sciences of the United States of America, 2001, 98, 14931-14936.	7.1	499
89	Efficient multiple time step method for use with Ewald and particle mesh Ewald for large biomolecular systems. Journal of Chemical Physics, 2001, 115, 2348-2358.	3.0	121
90	Quantum effects in liquid water: Path-integral simulations of a flexible and polarizable ab initio model. Journal of Chemical Physics, 2001, 115, 7622-7628.	3.0	157

#	Article	IF	Citations
91	Combined fluctuating charge and polarizable dipole models: Application to a five-site water potential function. Journal of Chemical Physics, 2001, 115, 2237-2251.	3.0	267
92	Quantum time correlation functions from complex time Monte Carlo simulations: A maximum entropy approach. Journal of Chemical Physics, 2001, 114, 1075-1088.	3.0	48
93	Perspective on "Statistical mechanics of isomerization dynamics in liquids and the transition state approximation". Theoretical Chemistry Accounts, 2000, 103, 335-336.	1.4	1
94	Multicanonical jump walk annealing: An efficient method for geometric optimization. Journal of Chemical Physics, 2000, 112, 2701-2708.	3.0	29
95	Quantum mechanical canonical rate theory: A new approach based on the reactive flux and numerical analytic continuation methods. Journal of Chemical Physics, 2000, 112, 2605-2614.	3.0	72
96	Catalytic tempering: A method for sampling rough energy landscapes by Monte Carlo. Proceedings of the National Academy of Sciences of the United States of America, 2000, 97, 11164-11169.	7.1	24
97	Rabani, Gezelter, and Berne Reply:. Physical Review Letters, 2000, 85, 467-467.	7.8	7
98	Global Optimization:Â Quantum Thermal Annealing with Path Integral Monte Carlo. Journal of Physical Chemistry A, 2000, 104, 86-95.	2.5	68
99	Multicanonical jump walking: A method for efficiently sampling rough energy landscapes. Journal of Chemical Physics, 1999, 110, 10299-10306.	3.0	40
100	Real time quantum correlation functions. I. Centroid molecular dynamics of anharmonic systems. Journal of Chemical Physics, 1999, 111, 9140-9146.	3.0	31
101	The dependence of the rate constant for isomerization on the competition between intramolecular vibrational relaxation and energy transfer to the bath: A stochastic model. Journal of Chemical Physics, 1999, 110, 1053-1060.	3.0	8
102	Path-integral diffusion Monte Carlo: Calculation of observables of many-body systems in the ground state. Journal of Chemical Physics, 1999, 110, 6143-6153.	3.0	20
103	Calculating the hopping rate for diffusion in molecular liquids: CS2. Journal of Chemical Physics, 1999, 110, 3444-3452.	3.0	26
104	Direct Observation of Stretched-Exponential Relaxation in Low-Temperature Lennard-Jones Systems Using the Cage Correlation Function. Physical Review Letters, 1999, 82, 3649-3652.	7.8	73
105	Second-Order Reentrant Phase Transition in the Quantum Anisotropic Planar Rotor Model. Physical Review Letters, 1999, 83, 4606-4609.	7.8	14
106	Electronic properties of CdSe nanocrystals in the absence and presence of a dielectric medium. Journal of Chemical Physics, 1999, 110, 5355-5369.	3.0	235
107	Real time quantum correlation functions. II. Maximum entropy numerical analytic continuation of path integral Monte Carlo and centroid molecular dynamics data. Journal of Chemical Physics, 1999, 111, 9147-9156.	3.0	52
108	Nonradiative relaxation processes in condensed phases: Quantum versus classical baths. Journal of Chemical Physics, 1999, 110, 5238-5248.	3.0	64

#	Article	IF	Citations
109	Parametrizing a polarizable force field from ab initio data. I. The fluctuating point charge model. Journal of Chemical Physics, 1999, 110, 741-754.	3.0	251
110	Classical Approximation to Nonradiative Electronic Relaxation in Condensed Phase Systems. Journal of Physical Chemistry A, 1999, 103, 9539-9544.	2.5	39
111	Fluctuating Charge, Polarizable Dipole, and Combined Models:â€‰ Parameterization from ab Initio Quantum Chemistry. Journal of Physical Chemistry B, 1999, 103, 4730-4737.	2.6	250
112	On the Adequacy of Mixed Quantum-Classical Dynamics in Condensed Phase Systems. Journal of Physical Chemistry B, 1999, 103, 10978-10991.	2.6	72
113	Surface Curvature Effects in the Aqueous Ionic Solvation of the Chloride Ion. Journal of Physical Chemistry A, 1999, 103, 10300-10307.	2.5	117
114	Energy Dissipation in Nonlinear Systems Coupled to a Bath:Â On the Use of Perturbative Maps. Journal of Physical Chemistry A, 1998, 102, 9380-9389.	2.5	2
115	A comparison of exact quantum mechanical and various semiclassical treatments for the vibronic absorption spectrum: The case of fast vibrational relaxation. Journal of Chemical Physics, 1998, 109, 6376-6381.	3.0	38
116	Constructing ab initio force fields for molecular dynamics simulations. Journal of Chemical Physics, 1998, 108, 4739-4755.	3.0	133
117	Vibronic spectra in condensed matter: A comparison of exact quantum mechanical and various semiclassical treatments for harmonic baths. Journal of Chemical Physics, 1998, 108, 1407-1422.	3.0	86
118	On the application of numerical analytic continuation methods to the study of quantum mechanical vibrational relaxation processes. Journal of Chemical Physics, 1998, 109, 7745-7755.	3.0	45
119	Response to â€œComment on a critique of the instantaneous normal mode (INM) approach to diffusionâ€• [J. Chem. Phys. 109, 4693 (1998)]. Journal of Chemical Physics, 1998, 109, 4695-4696.	3.0	20
120	Can imaginary instantaneous normal mode frequencies predict barriers to self-diffusion?. Journal of Chemical Physics, 1997, 107, 4618-4627.	3.0	99
121	Large scale simulation of macromolecules in solution: Combining the periodic fast multipole method with multiple time step integrators. Journal of Chemical Physics, 1997, 106, 9835-9849.	3.0	108
122	The simulation of electronic absorption spectrum of a chromophore coupled to a condensed phase environment: Maximum entropy versus singular value decomposition approaches. Journal of Chemical Physics, 1997, 107, 9312-9318.	3.0	40
123	Effect of pressure on hydrogen bonding in glycerol: A molecular dynamics investigation. Journal of Chemical Physics, 1997, 107, 4350-4357.	3.0	94
124	Circumventing the pathological behavior of path-integral Monte Carlo for systems with Coulomb potentials. Journal of Chemical Physics, 1997, 107, 571-575.	3.0	22
125	Calculating the hopping rate for self-diffusion on rough potential energy surfaces: Cage correlations. Journal of Chemical Physics, 1997, 107, 6867-6876.	3.0	118
126	Solvation and reorganization energies in polarizable molecular and continuum solvents. Journal of Chemical Physics, 1997, 106, 2372-2387.	3.0	70

#	Article	IF	Citations
127	Vibrational energy relaxation in the condensed phases: Quantum vs classical bath for multiphonon processes. Journal of Chemical Physics, 1997, 107, 6050-6061.	3.0	94
128	Smart walking: A new method for Boltzmann sampling of protein conformations. Journal of Chemical Physics, 1997, 107, 9185-9196.	3.0	87
129	Free Energy of the Hydrophobic Interaction from Molecular Dynamics Simulations:â€‰ The Effects of Solute and Solvent Polarizability. Journal of Physical Chemistry B, 1997, 101, 10488-10493.	2.6	89
130	Novel methods of sampling phase space in the simulation of biological systems. Current Opinion in Structural Biology, 1997, 7, 181-189.	5.7	206
131	Dynamical Fluctuating Charge Force Fields: The Aqueous Solvation of Amides. Journal of the American Chemical Society, 1996, 118, 672-679.	13.7	223
132	Molecular dynamics with multiple time scales: The selection of efficient reference system propagators. Journal of Chemical Physics, 1996, 105, 1426-1436.	3.0	121
133	Inferring the hydrophobic interaction from the properties of neat water.. Proceedings of the National Academy of Sciences of the United States of America, 1996, 93, 8800-8803.	7.1	50
134	Path-Integral Monte Carlo Scheme for Rigid Tops: Application to the Quantum Rotator Phase Transition in Solid Methane. Physical Review Letters, 1996, 77, 2638-2641.	7.8	29
135	Molecular dynamics for nonequilibrium systems in which there are a small number of very hot particles in a cold bath: Reference system propagator methods. Journal of Chemical Physics, 1996, 105, 235-239.	3.0	4
136	Solvation energies and electronic spectra in polar, polarizable media: Simulation tests of dielectric continuum theory. Journal of Chemical Physics, 1996, 104, 1293-1308.	3.0	96
137	The energy relaxation of a nonlinear oscillator coupled to a linear bath. Journal of Chemical Physics, 1996, 104, 1111-1119.	3.0	49
138	On the calculation of dynamical properties of solvated electrons by maximum entropy analytic continuation of path integral Monte Carlo data. Journal of Chemical Physics, 1996, 105, 7064-7078.	3.0	85
139	Effects of Polarizability on the Hydration of the Chloride Ion. The Journal of Physical Chemistry, 1996, 100, 11934-11943.	2.9	258
140	A scaling and mapping theory for excess electrons in simple fluids. Journal of Chemical Physics, 1995, 102, 432-436.	3.0	34
141	Activated rate processes: The reactive flux method for oneâ€dimensional surface diffusion. Journal of Chemical Physics, 1995, 102, 4037-4055.	3.0	27
142	The energyâ€dependent transmission coefficient and the energy distribution of classical particles escaping from a metastable well. Journal of Chemical Physics, 1995, 102, 7953-7965.	3.0	13
143	Molecular Dynamics Study of the Dependence of Water Solvation Free Energy on Solute Curvature and Surface Area. The Journal of Physical Chemistry, 1995, 99, 2885-2892.	2.9	140
144	Computer Simulation of Hydrophobic Hydration Forces on Stacked Plates at Short Range. The Journal of Physical Chemistry, 1995, 99, 2893-2899.	2.9	279

#	Article	IF	Citations
145	Molecular Dynamics Calculation of the Effect of Solvent Polarizability on the Hydrophobic Interaction. Journal of the American Chemical Society, 1995, 117, 7172-7179.	13.7	77
146	Hydrodynamic calculation of the frequency dependent friction on the bond of a diatomic molecule. Journal of Chemical Physics, 1995, 103, 1160-1174.	3.0	13
147	Computer simulation of solid C60 using multiple timeâ€step algorithms. Journal of Chemical Physics, 1994, 101, 2421-2431.	3.0	47
148	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. Journal of Chemical Physics, 1994, 101, 9909-9918.	3.0	78
149	Dynamical fluctuating charge force fields: Application to liquid water. Journal of Chemical Physics, 1994, 101, 6141-6156.	3.0	1,133
150	Quantum and classical relaxation rates from classical simulations. Journal of Chemical Physics, 1994, 100, 8359-8366.	3.0	358
151	The Aqueous Solvation of Water: A Comparison of Continuum Methods with Molecular Dynamics. Journal of the American Chemical Society, 1994, 116, 3949-3954.	13.7	135
152	Multiple Time Scales in Molecular Dynamics: Applications to Vibrational Relaxation. Jerusalem Symposia on Quantum Chemistry and Biochemistry, 1994, , 471-494.	0.2	0
153	Theory and simulation of polar and nonpolar polarizable fluids. Journal of Chemical Physics, 1993, 99, 6998-7011.	3.0	40
154	Effective potentials for liquid water using polarizable and nonpolarizable models. The Journal of Physical Chemistry, 1993, 97, 13841-13851.	2.9	140
155	Reply to Comment on: Reversible multiple time scale molecular dynamics. Journal of Chemical Physics, 1993, 99, 2278-2279.	3.0	29
156	Vibrational relaxation in simple fluids: Comparison of theory and simulation. Journal of Chemical Physics, 1993, 98, 7301-7318.	3.0	160
157	Theory of polarizable liquid crystals: Optical birefringence. Journal of Chemical Physics, 1993, 99, 2213-2220.	3.0	11
158	Method for accelerating chain folding and mixing. Journal of Chemical Physics, 1993, 99, 6071-6077.	3.0	52
159	Theory of correlated hops in surface diffusion. Physical Review Letters, 1993, 70, 3299-3302.	7.8	68
160	A Bornâ€"Oppenheimer approximation for path integrals with an application to electron solvation in polarizable fluids. Journal of Chemical Physics, 1993, 99, 2902-2916.	3.0	69
161	Manyâ€body dispersion forces of polarizable clusters and liquids. Journal of Chemical Physics, 1992, 97, 8628-8636.	3.0	48
162	A new quantum propagator for hard sphere and cavity systems. Journal of Chemical Physics, 1992, 97, 2382-2385.	3.0	58

#	Article	IF	Citations
163	Density dependence of excess electronic groundâ€state energies in simple atomic fluids. Journal of Chemical Physics, 1992, 97, 2002-2021.	3.0	65
164	Reversible multiple time scale molecular dynamics. Journal of Chemical Physics, 1992, 97, 1990-2001.	3.0	3,008
165	Monte Carlo methods for accelerating barrier crossing: Antiâ€forceâ€bias and variable step algorithms. Journal of Chemical Physics, 1990, 92, 1980-1985.	3.0	44
166	Dynamic friction on rigid and flexible bonds. Journal of Chemical Physics, 1990, 93, 5084-5095.	3.0	115
167	Lowâ€temperature variational approximation for the Feynman quantum propagator and its application to the simulation of quantum systems. Journal of Chemical Physics, 1990, 92, 7531-7539.	3.0	60
168	Excess electronic states in fluid helium. Journal of Chemical Physics, 1988, 89, 2128-2137.	3.0	34
169	Behavior of the hydrated electron at different temperatures: structure and absorption spectrum. The Journal of Physical Chemistry, 1988, 92, 1721-1730.	2.9	110
170	Path integral Monte Carlo studies of the behavior of excess electrons in simple fluids. Journal of Chemical Physics, 1987, 86, 5689-5702.	3.0	179
171	Path integral Monte Carlo study of the hydrated electron. Journal of Chemical Physics, 1987, 86, 6404-6418.	3.0	116
172	On the Simulation of Quantum Systems: Path Integral Methods. Annual Review of Physical Chemistry, 1986, 37, 401-424.	10.8	653
173	Path-integral Monte Carlo simulations of electron localization in water clusters. Journal of Statistical Physics, 1986, 43, 973-984.	1.2	11
174	Localization of an excess electron in water clusters. Journal of Chemical Physics, 1986, 85, 1583-1591.	3.0	120
175	Evaluation of microcanonical rate constants for bimolecular reactions by path integral techniques. Journal of Chemical Physics, 1985, 83, 2972-2975.	3.0	25
176	On the use of semiclassical dynamics in determining electronic spectra of Br2in an Ar matrix. Journal of Chemical Physics, 1985, 83, 230-238.	3.0	71
177	Nonergodicity in path integral molecular dynamics. Journal of Chemical Physics, 1984, 81, 3641-3643.	3.0	105
178	Fluctuations in lattice Monte Carlo simulations. Physical Review D, 1984, 30, 1791-1794.	4.7	1
179	A path integral Monte Carlo study of liquid neon and the quantum effective pair potential. Journal of Chemical Physics, 1984, 81, 2523-2527.	3.0	116
180	Time correlation functions in quantum systems. Journal of Chemical Physics, 1984, 81, 2512-2513.	3.0	61

#	Article	IF	Citations
181	On path integral Monte Carlo simulations. Journal of Chemical Physics, 1982, 76, 5150-5155.	3.0	386
182	Comment on â€˜â€˜A statistical theory of rate constants in nonergodic systemsâ€™â€™. Journal of Chemical Physics, 1982, 76, 5187-5188.	3.0	0
183	Hydrophobic effect on chain folding. The trans to gauche isomerization of n-butane in water. Journal of the American Chemical Society, 1982, 104, 7647-7649.	13.7	60
184	Computer Experiments on Heterogeneous Systems. Topics in Current Physics, 1982, , 99-127.	0.5	0
185	Modification of the overlap potential to mimic a linear siteâ€“site potential. Journal of Chemical Physics, 1981, 74, 3316-3319.	3.0	1,180
186	Intramolecular rate process: Isomerization dynamics and the transition to chaos. Journal of Chemical Physics, 1981, 75, 3495-3510.	3.0	126
187	Impulsive stochastic models of molecular relaxation and isomerization reactions. Journal of Chemical Physics, 1980, 73, 4314-4320.	3.0	44
188	Structure of a liquidâ€“vapor interface in the presence of a hard wall in the transition region. Journal of Chemical Physics, 1979, 71, 3802-3806.	3.0	38
189	A Monte Carlo simulation of the hydrophobic interaction. Journal of Chemical Physics, 1979, 71, 2975.	3.0	297
190	Hydrophobic hydration around a pair of apolar species in water. Journal of Chemical Physics, 1979, 71, 2982.	3.0	153
191	Radial correlations in associated liquids. Journal of Chemical Physics, 1979, 71, 3889-3891.	3.0	9
192	Nucleation in finite systems: Theory and computer simulation. Astrophysics and Space Science, 1979, 65, 39-46.	1.4	13
193	On the force bias Monte Carlo simulation of simple liquids. Journal of Chemical Physics, 1979, 71, 129-132.	3.0	71
194	Computer simulation of the nucleation and thermodynamics of microclusters. Journal of Chemical Physics, 1978, 68, 1325-1336.	3.0	100
195	Monte Carlo Simulation of Water. ACS Symposium Series, 1978, , 29-31.	0.5	6
196	Determination of the Mean Force of Two Noble Gas Atoms Dissolved in Water. ACS Symposium Series, 1978, , 32-34.	0.5	5
197	On the effects of translationâ€“rotation coupling on hydrodynamic diffusion tensors. Journal of Chemical Physics, 1977, 67, 5971-5972.	3.0	7
198	Characterization of heterogeneous solutions using laser light scattering: study of the tubulin system. Biochemistry, 1977, 16, 5776-5781.	2.5	15

#	Article	IF	Citations
199	Laser Light Scattering from Liquids. Annual Review of Physical Chemistry, 1974, 25, 233-253.	10.8	54
200	Topics in Time-Dependent Statistical Mechanics. Annual Review of Physical Chemistry, 1971, 22, 563-596.	10.8	72
201	Comments on the Coupling between Linear and Angular Momentum of Structured Molecules. Journal of Chemical Physics, 1970, 52, 5193-5194.	3.0	5
202	Time-Correlation Functions, Memory Functions, and Molecular Dynamics. Physical Review A, 1970, 2, 975-996.	2.5	135
203	Dispersion of the Electrically Induced Refractiveâ€Index Anisotropy in Nonpolar Liquids as a Probe of Reaction Kinetics. Journal of Chemical Physics, 1970, 52, 1259-1261.	3.0	4
204	Molecular Reorientation in Liquids and Gases. Journal of Chemical Physics, 1968, 49, 3125-3129.	3.0	75
205	Light Scattering as a Probe of Fast Reaction Kinetics. Journal of Chemical Physics, 1967, 47, 3675-3676.	3.0	53