B J Berne

List of Publications by Year in descending order

Source: https://exaly.com/author-pdf/11323174/publications.pdf

Version: 2024-02-01

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	Reversible multiple time scale molecular dynamics. Journal of Chemical Physics, 1992, 97, 1990-2001.	3.0	3,008
2	Modification of the overlap potential to mimic a linear siteâ€“site potential. Journal of Chemical Physics, 1981, 74, 3316-3319.	3.0	1,180
3	Dynamical fluctuating charge force fields: Application to liquid water. Journal of Chemical Physics, 1994, 101, 6141-6156.	3.0	1,133
4	On the Simulation of Quantum Systems: Path Integral Methods. Annual Review of Physical Chemistry, 1986, 37, 401-424.	10.8	653
5	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
6	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
7	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
8	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
9	On the Calculation of Time Correlation Functions. Advances in Chemical Physics, 2007, , 63-227.	0.3	415
10	On path integral Monte Carlo simulations. Journal of Chemical Physics, 1982, 76, 5150-5155.	3.0	386
11	Observation of a dewetting transition in the collapse of the melittin tetramer. Nature, 2005, 437, 159-162.	27.8	362
12	Quantum and classical relaxation rates from classical simulations. Journal of Chemical Physics, 1994, 100, 8359-8366.	3.0	358
13	On the Calculation of Diffusion Coefficients in Confined Fluids and Interfaces with an Application to the Liquidâ^'Vapor Interface of Water. Journal of Physical Chemistry B, 2004, 108, 6595-6602.	2.6	337
14	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
15	A Monte Carlo simulation of the hydrophobic interaction. Journal of Chemical Physics, 1979, 71, 2975.	3.0	297
16	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
17	Ureaâ€™s Action on Hydrophobic Interactions. Journal of the American Chemical Society, 2009, 131, 1535-1541.	13.7	288
18	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
19	Computer Simulation of a â€œGreen Chemistryâ€•Room-Temperature Ionic Solvent. Journal of Physical Chemistry B, 2002, 106, 12017-12021.	2.6	268
20	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
21	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
22	Effects of Polarizability on the Hydration of the Chloride Ion. The Journal of Physical Chemistry, 1996, 100, 11934-11943.	2.9	258
23	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
24	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
25	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
26	Hydrogen-Bond Kinetics in the Solvation Shell of a Polypeptide. Journal of Physical Chemistry B, 2001, 105, 11929-11932.	2.6	225
27	Dynamical Fluctuating Charge Force Fields: The Aqueous Solvation of Amides. Journal of the American Chemical Society, 1996, 118, 672-679.	13.7	223
28	Effect of Ions on the Hydrophobic Interaction between Two Plates. Journal of the American Chemical Society, 2007, 129, 4678-4686.	13.7	223
29	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
30	Blue Gene: A vision for protein science using a petaflop supercomputer. IBM Systems Journal, 2001, 40, 310-327.	3.0	211
31	Advancing Drug Discovery through Enhanced Free Energy Calculations. Accounts of Chemical Research, 2017, 50, 1625-1632.	15.6	211
32	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
33	Role of Water in Mediating the Assembly of Alzheimer Amyloid-Î² AÎ²16â^22 Protofilaments. Journal of the American Chemical Society, 2008, 130, 11066-11072.	13.7	208
34	Novel methods of sampling phase space in the simulation of biological systems. Current Opinion in Structural Biology, 1997, 7, 181-189.	5.7	206
35	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
36	Can Water Polarizability Be Ignored in Hydrogen Bond Kinetics?. Journal of Physical Chemistry B, 2002, 106, 2054-2060.	2.6	195

#	Article	IF	Citations
37	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
38	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
39	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
40	Vibrational relaxation in simple fluids: Comparison of theory and simulation. Journal of Chemical Physics, 1993, 98, 7301-7318.	3.0	160
41	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
42	Hydrophobic hydration around a pair of apolar species in water. Journal of Chemical Physics, 1979, 71, 2982.	3.0	153
43	Effective potentials for liquid water using polarizable and nonpolarizable models. The Journal of Physical Chemistry, 1993, 97, 13841-13851.	2.9	140
44	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
45	Time-Correlation Functions, Memory Functions, and Molecular Dynamics. Physical Review A, 1970, 2, 975-996.	2.5	135
46	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
47	Constructing ab initio force fields for molecular dynamics simulations. Journal of Chemical Physics, 1998, 108, 4739-4755.	3.0	133
48	Intramolecular rate process: Isomerization dynamics and the transition to chaos. Journal of Chemical Physics, 1981, 75, 3495-3510.	3.0	126
49	Molecular dynamics with multiple time scales: The selection of efficient reference system propagators. Journal of Chemical Physics, 1996, 105, 1426-1436.	3.0	121
50	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
51	Hydrogen-Bond Dynamics in the Airâ"Water Interface. Journal of Physical Chemistry B, 2005, 109, 2949-2955.	2.6	121
52	Localization of an excess electron in water clusters. Journal of Chemical Physics, 1986, 85, 1583-1591.	3.0	120
53	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
54	Surface Curvature Effects in the Aqueous Ionic Solvation of the Chloride Ion. Journal of Physical Chemistry A, 1999, 103, 10300-10307.	2.5	117

#	Article	IF	Citations
55	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
56	Path integral Monte Carlo study of the hydrated electron. Journal of Chemical Physics, 1987, 86, 6404-6418.	3.0	116
57	Dynamic friction on rigid and flexible bonds. Journal of Chemical Physics, 1990, 93, 5084-5095.	3.0	115
58	How and when does an anticancer drug leave its binding site?. Science Advances, 2017, 3, e1700014.	10.3	111
59	Behavior of the hydrated electron at different temperatures: structure and absorption spectrum. The Journal of Physical Chemistry, 1988, 92, 1721-1730.	2.9	110
60	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
61	Nonergodicity in path integral molecular dynamics. Journal of Chemical Physics, 1984, 81, 3641-3643.	3.0	105
62	Hydrophobic Interactions and Dewetting between Plates with Hydrophobic and Hydrophilic Domains. Journal of Physical Chemistry C, 2009, 113, 5244-5253.	3.1	104
63	Replica Exchange with Solute Tempering:Â Efficiency in Large Scale Systems. Journal of Physical Chemistry B, 2007, 111, 5405-5410.	2.6	103
64	Computer simulation of the nucleation and thermodynamics of microclusters. Journal of Chemical Physics, 1978, 68, 1325-1336.	3.0	100
65	Can imaginary instantaneous normal mode frequencies predict barriers to self-diffusion?. Journal of Chemical Physics, 1997, 107, 4618-4627.	3.0	99
66	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
67	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
68	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
69	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
70	Effect of pressure on hydrogen bonding in glycerol: A molecular dynamics investigation. Journal of Chemical Physics, 1997, 107, 4350-4357.	3.0	94
71	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
72	Dynamics of Water Confined in the Interdomain Region of a Multidomain Proteinâ€. Journal of Physical Chemistry B, 2006, 110, 3704-3711.	2.6	93

#	Article	IF	Citations
73	Aggregation and Dispersion of Small Hydrophobic Particles in Aqueous Electrolyte Solutions. Journal of Physical Chemistry B, 2006, 110, 22736-22741.	2.6	92
74	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
75	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
76	Smart walking: A new method for Boltzmann sampling of protein conformations. Journal of Chemical Physics, 1997, 107, 9185-9196.	3.0	87
77	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
78	Scanning Tunneling Microscopy Images of Alkane Derivatives on Graphite: Role of Electronic Effects. Nano Letters, 2008, 8, 3160-3165.	9.1	86
79	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
80	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
81	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
82	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
83	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
84	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
85	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
86	Molecular Reorientation in Liquids and Gases. Journal of Chemical Physics, 1968, 49, 3125-3129.	3.0	75
87	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
88	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
89	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
90	Topics in Time-Dependent Statistical Mechanics. Annual Review of Physical Chemistry, 1971, 22, 563-596.	10.8	72

#	Article	IF	Citations
91	On the Adequacy of Mixed Quantum-Classical Dynamics in Condensed Phase Systems. Journal of Physical Chemistry B, 1999, 103, 10978-10991.	2.6	72
92	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
93	On the force bias Monte Carlo simulation of simple liquids. Journal of Chemical Physics, 1979, 71, 129-132.	3.0	71
94	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
95	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
96	Solvation and reorganization energies in polarizable molecular and continuum solvents. Journal of Chemical Physics, 1997, 106, 2372-2387.	3.0	70
97	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
98	Theory of correlated hops in surface diffusion. Physical Review Letters, 1993, 70, 3299-3302.	7.8	68
99	Global Optimization:Â Quantum Thermal Annealing with Path Integral Monte Carlo. Journal of Physical Chemistry A, 2000, 104, 86-95.	2.5	68
100	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
101	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
102	Density dependence of excess electronic groundâ€state energies in simple atomic fluids. Journal of Chemical Physics, 1992, 97, 2002-2021.	3.0	65
103	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
104	Nonradiative relaxation processes in condensed phases: Quantum versus classical baths. Journal of Chemical Physics, 1999, 110, 5238-5248.	3.0	64
105	Dewetting transitions in protein cavities. Proteins: Structure, Function and Bioinformatics, 2010, 78, 1856-1869.	2.6	64
106	Time correlation functions in quantum systems. Journal of Chemical Physics, 1984, 81, 2512-2513.	3.0	61
107	Efficient multiple time scale molecular dynamics: Using colored noise thermostats to stabilize resonances. Journal of Chemical Physics, 2011, 134, 014103.	3.0	61
108	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

#	Article	IF	Citations
109	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
110	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
111	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
112	A new quantum propagator for hard sphere and cavity systems. Journal of Chemical Physics, 1992, 97, 2382-2385.	3.0	58
113	Molecular Dynamics with Multiple Time Scales: How to Avoid Pitfalls. Journal of Chemical Theory and Computation, 2010, 6, 1798-1804.	5.3	57
114	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
115	Laser Light Scattering from Liquids. Annual Review of Physical Chemistry, 1974, 25, 233-253.	10.8	54
116	Light Scattering as a Probe of Fast Reaction Kinetics. Journal of Chemical Physics, 1967, 47, 3675-3676.	3.0	53
117	Method for accelerating chain folding and mixing. Journal of Chemical Physics, 1993, 99, 6071-6077.	3.0	52
118	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
119	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
120	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
121	Quantum Rate Constants from Short-Time Dynamics:Â An Analytic Continuation Approachâ€. Journal of Physical Chemistry A, 2001, 105, 2824-2833.	2.5	50
122	The energy relaxation of a nonlinear oscillator coupled to a linear bath. Journal of Chemical Physics, 1996, 104, 1111-1119.	3.0	49
123	Manyâ€body dispersion forces of polarizable clusters and liquids. Journal of Chemical Physics, 1992, 97, 8628-8636.	3.0	48
124	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
125	Computer simulation of solid C60 using multiple timeâ€step algorithms. Journal of Chemical Physics, 1994, 101, 2421-2431.	3.0	47
126	Multiple â€œtime stepâ€•Monte Carlo. Journal of Chemical Physics, 2002, 117, 8203-8207.	3.0	47

#	Article	IF	Citations
127	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
128	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
129	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
130	Impulsive stochastic models of molecular relaxation and isomerization reactions. Journal of Chemical Physics, 1980, 73, 4314-4320.	3.0	44
131	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
132	How a Kinase Inhibitor Withstands Gatekeeper Residue Mutations. Journal of the American Chemical Society, 2016, 138, 4608-4615.	13.7	44
133	Theory and simulation of polar and nonpolar polarizable fluids. Journal of Chemical Physics, 1993, 99, 6998-7011.	3.0	40
134	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
135	Multicanonical jump walking: A method for efficiently sampling rough energy landscapes. Journal of Chemical Physics, 1999, 110, 10299-10306.	3.0	40
136	Classical Approximation to Nonradiative Electronic Relaxation in Condensed Phase Systems. Journal of Physical Chemistry A, 1999, 103, 9539-9544.	2.5	39
137	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
138	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
139	Structure and Dynamics of Acetonitrile Confined in a Silica Nanopore. Journal of Physical Chemistry C, 2012, 116, 9582-9593.	3.1	38
140	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
141	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
142	Predicting reaction coordinates in energy landscapes with diffusion anisotropy. Journal of Chemical Physics, 2017, 147, 152701.	3.0	37
143	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
144	Serial Replica Exchange. Journal of Physical Chemistry B, 2007, 111, 1416-1423.	2.6	35

#	Article	IF	Citations
145	Comment on â€œUrea-Mediated Protein Denaturation: A Consensus Viewâ€• Journal of Physical Chemistry B, 2011, 115, 1323-1326.	2.6	35
146	Excess electronic states in fluid helium. Journal of Chemical Physics, 1988, 89, 2128-2137.	3.0	34
147	A scaling and mapping theory for excess electrons in simple fluids. Journal of Chemical Physics, 1995, 102, 432-436.	3.0	34
148	Comment on â€œCan a Continuum Solvent Model Reproduce the Free Energy Landscape of a Î²-Hairpin Folding in Water?â€•The Poissonâ^'Boltzmann Equation. Journal of Physical Chemistry B, 2004, 108, 7528-7530.	2.6	34
149	Theory and simulations of quantum glass forming liquids. Journal of Chemical Physics, 2012, 136, 074511.	3.0	34
150	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
151	Thermal and Structural Stability of Adsorbed Proteins. Biophysical Journal, 2010, 99, 1157-1165.	0.5	32
152	Competition of Electrostatic and Hydrophobic Interactions between Small Hydrophobes and Model Enclosures. Journal of Physical Chemistry B, 2010, 114, 7294-7301.	2.6	32
153	Real time quantum correlation functions. I. Centroid molecular dynamics of anharmonic systems. Journal of Chemical Physics, 1999, 111, 9140-9146.	3.0	31
154	Dissecting Entropic Coiling and Poor Solvent Effects in Protein Collapse. Journal of the American Chemical Society, 2008, 130, 11578-11579.	13.7	31
155	A Displaced-Solvent Functional Analysis of Model Hydrophobic Enclosures. Journal of Chemical Theory and Computation, 2010, 6, 2924-2934.	5.3	31
156	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
157	How wet should be the reaction coordinate for ligand unbinding?. Journal of Chemical Physics, 2016, 145, 054113.	3.0	31
158	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
159	Reply to Comment on: Reversible multiple time scale molecular dynamics. Journal of Chemical Physics, 1993, 99, 2278-2279.	3.0	29
160	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
161	Multicanonical jump walk annealing: An efficient method for geometric optimization. Journal of Chemical Physics, 2000, 112, 2701-2708.	3.0	29
162	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
163	Quantum path minimization: An efficient method for global optimization. Journal of Chemical Physics, 2003, 118, 2999-3005.	3.0	28
164	Activated rate processes: The reactive flux method for oneâ€dimensional surface diffusion. Journal of Chemical Physics, 1995, 102, 4037-4055.	3.0	27
165	Calculating the hopping rate for diffusion in molecular liquids: CS2. Journal of Chemical Physics, 1999, 110, 3444-3452.	3.0	26
166	Evaluation of microcanonical rate constants for bimolecular reactions by path integral techniques. Journal of Chemical Physics, 1985, 83, 2972-2975.	3.0	25
167	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
168	Quantum Thermal Annealing with Renormalization:Â Application to a Frustrated Model Protein. Journal of Physical Chemistry A, 2001, 105, 459-464.	2.5	23
169	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
170	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
171	Massively parallel molecular dynamics simulations of lysozyme unfolding. IBM Journal of Research and Development, 2008, 52, 19-30.	3.1	22
172	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
173	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
174	Transport properties of normal liquid helium: Comparison of various methodologies. Journal of Chemical Physics, 2005, 123, 184506.	3.0	18
175	Kramers turnover: From energy diffusion to spatial diffusion using metadynamics. Journal of Chemical Physics, 2016, 144, 134103.	3.0	18
176	Characterization of heterogeneous solutions using laser light scattering: study of the tubulin system. Biochemistry, 1977, 16, 5776-5781.	2.5	15
177	Multiple â€œtime stepâ€•Monte Carlo simulations: Application to charged systems with Ewald summation. Journal of Chemical Physics, 2004, 121, 44.	3.0	15
178	Second-Order Reentrant Phase Transition in the Quantum Anisotropic Planar Rotor Model. Physical Review Letters, 1999, 83, 4606-4609.	7.8	14
179	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
180	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

#	Article	IF	Citations
181	Nucleation in finite systems: Theory and computer simulation. Astrophysics and Space Science, 1979, 65, 39-46.	1.4	13
182	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
183	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
184	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
185	Path-integral Monte Carlo simulations of electron localization in water clusters. Journal of Statistical Physics, 1986, 43, 973-984.	1.2	11
186	Theory of polarizable liquid crystals: Optical birefringence. Journal of Chemical Physics, 1993, 99, 2213-2220.	3.0	11
187	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
188	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
189	Radial correlations in associated liquids. Journal of Chemical Physics, 1979, 71, 3889-3891.	3.0	9
190	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
191	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
192	On the effects of translationâ€“rotation coupling on hydrodynamic diffusion tensors. Journal of Chemical Physics, 1977, 67, 5971-5972.	3.0	7
193	Rabani, Gezelter, and Berne Reply:. Physical Review Letters, 2000, 85, 467-467.	7.8	7
194	Monte Carlo Simulation of Water. ACS Symposium Series, 1978, , 29-31.	0.5	6
195	Comments on the Coupling between Linear and Angular Momentum of Structured Molecules. Journal of Chemical Physics, 1970, 52, 5193-5194.	3.0	5
196	Determination of the Mean Force of Two Noble Gas Atoms Dissolved in Water. ACS Symposium Series, 1978, , 32-34.	0.5	5
197	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
198	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

#	Article	IF	Citations
199	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
200	Fluctuations in lattice Monte Carlo simulations. Physical Review D, 1984, 30, 1791-1794.	4.7	1
201	Perspective on "Statistical mechanics of isomerization dynamics in liquids and the transition state approximation". Theoretical Chemistry Accounts, 2000, 103, 335-336.	1.4	1
202	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
203	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
204	Computer Experiments on Heterogeneous Systems. Topics in Current Physics, 1982, , 99-127.	0.5	0
205	Multiple Time Scales in Molecular Dynamics: Applications to Vibrational Relaxation. Jerusalem Symposia on Quantum Chemistry and Biochemistry, 1994, , 471-494.	0.2	0