B J Berne

List of Publications by Year in Descending Order

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	Efficient sampling of puckering states of monosaccharides through replica exchange with solute tempering and bond softening. *Journal of Chemical Physics*, **2018**, 149, 072306	3.9	9
205	Simulated Force Quench Dynamics Shows GB1 Protein Is Not a Two State Folder. *Journal of Physical Chemistry B*, **2017**, 121, 5162-5173	3.4	12
204	How and when does an anticancer drug leave its binding site?. *Science Advances*, **2017**, 3, e1700014	14.3	69
203	Predicting reaction coordinates in energy landscapes with diffusion anisotropy. *Journal of Chemical Physics*, **2017**, 147, 152701	3.9	26
202	Advancing Drug Discovery through Enhanced Free Energy Calculations. *Accounts of Chemical Research*, **2017**, 50, 1625-1632	24.3	126
201	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, 2839-44	11.5	135
200	How a Kinase Inhibitor Withstands Gatekeeper Residue Mutations. *Journal of the American Chemical Society*, **2016**, 138, 4608-15	16.4	26
199	How wet should be the reaction coordinate for ligand unbinding?. *Journal of Chemical Physics*, **2016**, 145, 054113	3.9	22
198	Kramers turnover: From energy diffusion to spatial diffusion using metadynamics. *Journal of Chemical Physics*, **2016**, 144, 134103	3.9	17
197	Prediction of Protein-Ligand Binding Poses via a Combination of Induced Fit Docking and Metadynamics Simulations. *Journal of Chemical Theory and Computation*, **2016**, 12, 2990-8	6.4	120
196	Role of water and steric constraints in the kinetics of cavity-ligand unbinding. *Proceedings of the National Academy of Sciences of the United States of America*, **2015**, 112, 12015-9	11.5	60
195	Role of Desolvation in Thermodynamics and Kinetics of Ligand Binding to a Kinase. *Journal of Chemical Theory and Computation*, **2014**, 10, 5696-5705	6.4	44
194	Elasticity, structure, and relaxation of extended proteins under force. *Proceedings of the National Academy of Sciences of the United States of America*, **2013**, 110, 3847-52	11.5	63
193	When does trimethylamine N-oxide fold a polymer chain and urea unfold it?. *Journal of Physical Chemistry B*, **2013**, 117, 8723-32	3.4	82
192	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, 13277-82	11.5	36
191	Are hydrodynamic interactions important in the kinetics of hydrophobic collapse?. *Journal of Physical Chemistry B*, **2012**, 116, 11537-44	3.4	27
190	Interplay between hydrodynamics and the free energy surface in the assembly of nanoscale hydrophobes. *Journal of Physical Chemistry B*, **2012**, 116, 378-89	3.4	46

189	Structure and Dynamics of Acetonitrile Confined in a Silica Nanopore. *Journal of Physical Chemistry C*, **2012**, 116, 9582-9593	3.8	33
188	Theory and simulations of quantum glass forming liquids. *Journal of Chemical Physics*, **2012**, 136, 074511	3.9	25
187	On achieving high accuracy and reliability in the calculation of relative protein-ligand binding affinities. *Proceedings of the National Academy of Sciences of the United States of America*, **2012**, 109, 1937-42	11.5	151
186	Unraveling quantum mechanical effects in water using isotopic fractionation. *Proceedings of the National Academy of Sciences of the United States of America*, **2012**, 109, 7988-91	11.5	88
185	Rate limit of protein elastic response is tether dependent. *Proceedings of the National Academy of Sciences of the United States of America*, **2012**, 109, 14416-21	11.5	48
184	Efficient multiple time scale molecular dynamics: Using colored noise thermostats to stabilize resonances. *Journal of Chemical Physics*, **2011**, 134, 014103	3.9	54
183	Replica exchange with solute scaling: a more efficient version of replica exchange with solute tempering (REST2). *Journal of Physical Chemistry B*, **2011**, 115, 9431-8	3.4	387
182	Comment on "urea-mediated protein denaturation: a consensus view". *Journal of Physical Chemistry B*, **2011**, 115, 1323-6; discussion 1327-8	3.4	33
181	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, 1326-30	11.5	156
180	Water's role in the force-induced unfolding of ubiquitin. *Proceedings of the National Academy of Sciences of the United States of America*, **2010**, 107, 19284-9	11.5	33
179	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, 11336-40	11.5	57
178	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	3.9	24
177	Thermal and structural stability of adsorbed proteins. *Biophysical Journal*, **2010**, 99, 1157-65	2.9	27
176	Competition of electrostatic and hydrophobic interactions between small hydrophobes and model enclosures. *Journal of Physical Chemistry B*, **2010**, 114, 7294-301	3.4	28
175	A displaced-solvent functional analysis of model hydrophobic enclosures. *Journal of Chemical Theory and Computation*, **2010**, 6, 2924-2934	6.4	27
174	Molecular Dynamics with Multiple Time Scales: How to Avoid Pitfalls. *Journal of Chemical Theory and Computation*, **2010**, 6, 1798-804	6.4	46
173	Hydrophobic interactions in model enclosures from small to large length scales: non-additivity in explicit and implicit solvent models. *Faraday Discussions*, **2010**, 146, 247-62; discussion 283-98, 395-401	3.6	27
172	Dewetting transitions in protein cavities. *Proteins: Structure, Function and Bioinformatics*, **2010**, 78, 1856-69	4.2	60

171	Single homopolypeptide chains collapse into mechanically rigid conformations. *Proceedings of the National Academy of Sciences of the United States of America*, **2009**, 106, 12605-10	11.5	78
170	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	3.8	22
169	Hydrophobic Interactions and Dewetting between Plates with Hydrophobic and Hydrophilic Domains. *Journal of Physical Chemistry C*, **2009**, 113, 5244-5253	3.8	93
168	Solvent Effects on the Self-Assembly of 1-Bromoeicosane on Graphite. Part II. Theory. *Journal of Physical Chemistry C*, **2009**, 113, 3641-3649	3.8	8
167	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	6.4	38
166	Urea's action on hydrophobic interactions. *Journal of the American Chemical Society*, **2009**, 131, 1535-41	16.4	261
165	Role of water in mediating the assembly of Alzheimer amyloid-beta Abeta16-22 protofilaments. *Journal of the American Chemical Society*, **2008**, 130, 11066-72	16.4	180
164	Massively parallel molecular dynamics simulations of lysozyme unfolding. *IBM Journal of Research and Development*, **2008**, 52, 19-30	2.5	10
163	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	3.8	34
162	Dissecting entropic coiling and poor solvent effects in protein collapse. *Journal of the American Chemical Society*, **2008**, 130, 11578-9	16.4	28
161	Scanning tunneling microscopy images of alkane derivatives on graphite: role of electronic effects. *Nano Letters*, **2008**, 8, 3160-5	11.5	77
160	Temperature dependence of dimerization and dewetting of large-scale hydrophobes: a molecular dynamics study. *Journal of Physical Chemistry B*, **2008**, 112, 8634-44	3.4	77
159	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, 16928-33	11.5	424
158	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, 7916-21	11.5	87
157	Serial replica exchange. *Journal of Physical Chemistry B*, **2007**, 111, 1416-23	3.4	31
156	Molecular Dynamics Simulation Studies of Self-Assembly of Racemic (R)/(S)-2-Bromohexadecanoic Acid on a Graphite Surface: Enantio-pure or Enantio-mixed Domains?. *Journal of Physical Chemistry C*, **2007**, 111, 18243-18250	3.8	9
155	Replica exchange with solute tempering: efficiency in large scale systems. *Journal of Physical Chemistry B*, **2007**, 111, 5405-10	3.4	95
154	Effect of ions on the hydrophobic interaction between two plates. *Journal of the American Chemical Society*, **2007**, 129, 4678-86	16.4	208

153	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, 5824-9	11.5	66
152	On the Calculation of Time Correlation Functions. *Advances in Chemical Physics*, **2007**, 63-227		346
151	Hydrophobic aided replica exchange: an efficient algorithm for protein folding in explicit solvent. *Journal of Physical Chemistry B*, **2006**, 110, 19018-22	3.4	71
150	Aggregation and dispersion of small hydrophobic particles in aqueous electrolyte solutions. *Journal of Physical Chemistry B*, **2006**, 110, 22736-41	3.4	84
149	Dynamics of water confined in the interdomain region of a multidomain protein. *Journal of Physical Chemistry B*, **2006**, 110, 3704-11	3.4	88
148	Elastic bag model for molecular dynamics simulations of solvated systems: application to liquid water and solvated peptides. *Journal of Physical Chemistry B*, **2006**, 110, 13256-63	3.4	9
147	Elastic bag model for molecular dynamics simulations of solvated systems: application to liquid argon. *Journal of Physical Chemistry B*, **2005**, 109, 463-70	3.4	13
146	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. *Journal of Physical Chemistry B*, **2005**, 109, 16529-38	3.4	51
145	Efficient Simulation Method for Polarizable Protein Force Fields: Application to the Simulation of BPTI in Liquid Water. *Journal of Chemical Theory and Computation*, **2005**, 1, 169-80	6.4	65
144	Hydrogen-bond dynamics in the air-water interface. *Journal of Physical Chemistry B*, **2005**, 109, 2949-55	3.4	110
143	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, 13749-54	11.5	530
142	Observation of a dewetting transition in the collapse of the melittin tetramer. *Nature*, **2005**, 437, 159-62	50.4	333
141	Transport properties of normal liquid helium: comparison of various methodologies. *Journal of Chemical Physics*, **2005**, 123, 184506	3.9	18
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, 5315-22	11.5	36
139	Polarizable molecules in the vibrational spectroscopy of water. *Proceedings of the National Academy of Sciences of the United States of America*, **2005**, 102, 11611-6	11.5	74
138	Multiple "time step" Monte Carlo simulations: application to charged systems with Ewald summation. *Journal of Chemical Physics*, **2004**, 121, 44-50	3.9	14
137	Reply to the Comment on Do 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	3.4	
136	Comment on Can a Continuum Solvent Model Reproduce the Free Energy Landscape of a Hairpin Folding in Water? The PoissonBoltzmann Equation. *Journal of Physical Chemistry B*, **2004**, 108, 7528-7530	3.4	31

135	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	2.8	209
134	On the Calculation of Diffusion Coefficients in Confined Fluids and Interfaces with an Application to the Liquid Vapor Interface of Water. *Journal of Physical Chemistry B*, **2004**, 108, 6595-6602	3.4	281
133	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	3.4	62
132	Quantum path minimization: An efficient method for global optimization. *Journal of Chemical Physics*, **2003**, 118, 2999-3005	3.9	27
131	Dewetting-induced collapse of hydrophobic particles. *Proceedings of the National Academy of Sciences of the United States of America*, **2003**, 100, 11953-8	11.5	245
130	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, 1515-31	3.5	276
129	Can a continuum solvent model reproduce the free energy landscape of a beta -hairpin folding in water?. *Proceedings of the National Academy of Sciences of the United States of America*, **2002**, 99, 12777-82	11.5	308
128	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, 1129-33	11.5	88
127	Computer Simulation of a Green Chemistry Room-Temperature Ionic Solvent. *Journal of Physical Chemistry B*, **2002**, 106, 12017-12021	3.4	253
126	Helix Unfolding and Intramolecular Hydrogen Bond Dynamics in Small Helices in Explicit Solvent. *Journal of Physical Chemistry B*, **2002**, 106, 10748-10752	3.4	32
125	Multiple time step Monte Carlo. *Journal of Chemical Physics*, **2002**, 117, 8203-8207	3.9	41
124	Can Water Polarizability Be Ignored in Hydrogen Bond Kinetics?. *Journal of Physical Chemistry B*, **2002**, 106, 2054-2060	3.4	183
123	The free energy landscape for beta hairpin folding in explicit water. *Proceedings of the National Academy of Sciences of the United States of America*, **2001**, 98, 14931-6	11.5	458
122	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	3.9	104
121	Quantum effects in liquid water: Path-integral simulations of a flexible and polarizable ab initio model. *Journal of Chemical Physics*, **2001**, 115, 7622-7628	3.9	147
120	Combined fluctuating charge and polarizable dipole models: Application to a five-site water potential function. *Journal of Chemical Physics*, **2001**, 115, 2237-2251	3.9	256
119	Quantum time correlation functions from complex time Monte Carlo simulations: A maximum entropy approach. *Journal of Chemical Physics*, **2001**, 114, 1075-1088	3.9	45
118	Blue Gene: A vision for protein science using a petaflop supercomputer. *IBM Systems Journal*, **2001**, 40, 310-327		175

117	Hydrogen-Bond Kinetics in the Solvation Shell of a Polypeptide. *Journal of Physical Chemistry B*, **2001**, 105, 11929-11932	3.4	206
116	Quantum Rate Constants from Short-Time Dynamics: An Analytic Continuation Approach *Journal of Physical Chemistry A*, **2001**, 105, 2824-2833	2.8	48
115	Quantum Thermal Annealing with Renormalization: Application to a Frustrated Model Protein. *Journal of Physical Chemistry A*, **2001**, 105, 459-464	2.8	21
114	Perspective on Statistical mechanics of isomerization dynamics in liquids and the transition state approximation *Theoretical Chemistry Accounts*, **2000**, 103, 335-336	1.9	1
113	Multicanonical jump walk annealing: An efficient method for geometric optimization. *Journal of Chemical Physics*, **2000**, 112, 2701-2708	3.9	27
112	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	3.9	69
111	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, 11164-9	11.5	21
110	Rabani, gezelter, and berne reply:. *Physical Review Letters*, **2000**, 85, 467	7.4	7
109	Global Optimization: Quantum Thermal Annealing with Path Integral Monte Carlo. *Journal of Physical Chemistry A*, **2000**, 104, 86-95	2.8	65
108	Multicanonical jump walking: A method for efficiently sampling rough energy landscapes. *Journal of Chemical Physics*, **1999**, 110, 10299-10306	3.9	37
107	Real time quantum correlation functions. I. Centroid molecular dynamics of anharmonic systems. *Journal of Chemical Physics*, **1999**, 111, 9140-9146	3.9	30
106	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	3.9	8
105	Path-integral diffusion Monte Carlo: Calculation of observables of many-body systems in the ground state. *Journal of Chemical Physics*, **1999**, 110, 6143-6153	3.9	18
104	Calculating the hopping rate for diffusion in molecular liquids: CS2. *Journal of Chemical Physics*, **1999**, 110, 3444-3452	3.9	23
103	Direct Observation of Stretched-Exponential Relaxation in Low-Temperature Lennard-Jones Systems Using the Cage Correlation Function. *Physical Review Letters*, **1999**, 82, 3649-3652	7.4	69
102	Second-Order Reentrant Phase Transition in the Quantum Anisotropic Planar Rotor Model. *Physical Review Letters*, **1999**, 83, 4606-4609	7.4	11
101	Electronic properties of CdSe nanocrystals in the absence and presence of a dielectric medium. *Journal of Chemical Physics*, **1999**, 110, 5355-5369	3.9	209
100	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	3.9	45

99	Nonradiative relaxation processes in condensed phases: Quantum versus classical baths. *Journal of Chemical Physics*, **1999**, 110, 5238-5248	3.9	60
98	Parametrizing a polarizable force field from ab initio data. I. The fluctuating point charge model. *Journal of Chemical Physics*, **1999**, 110, 741-754	3.9	225
97	Classical Approximation to Nonradiative Electronic Relaxation in Condensed Phase Systems. *Journal of Physical Chemistry A*, **1999**, 103, 9539-9544	2.8	36
96	Fluctuating Charge, Polarizable Dipole, and Combined Models: Parameterization from ab Initio Quantum Chemistry. *Journal of Physical Chemistry B*, **1999**, 103, 4730-4737	3.4	239
95	On the Adequacy of Mixed Quantum-Classical Dynamics in Condensed Phase Systems. *Journal of Physical Chemistry B*, **1999**, 103, 10978-10991	3.4	68
94	Surface Curvature Effects in the Aqueous Ionic Solvation of the Chloride Ion. *Journal of Physical Chemistry A*, **1999**, 103, 10300-10307	2.8	112
93	Energy Dissipation in Nonlinear Systems Coupled to a Bath:□On the Use of Perturbative Maps. *Journal of Physical Chemistry A*, **1998**, 102, 9380-9389	2.8	1
92	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	3.9	37
91	Constructing ab initio force fields for molecular dynamics simulations. *Journal of Chemical Physics*, **1998**, 108, 4739-4755	3.9	126
90	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	3.9	81
89	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	3.9	43
88	Response to □Comment on a critique of the instantaneous normal mode (INM) approach to diffusion□[J. Chem. Phys. 109, 4693 (1998)]. *Journal of Chemical Physics*, **1998**, 109, 4695-4696	3.9	17
87	Can imaginary instantaneous normal mode frequencies predict barriers to self-diffusion?. *Journal of Chemical Physics*, **1997**, 107, 4618-4627	3.9	91
86	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	3.9	98
85	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	3.9	39
84	Effect of pressure on hydrogen bonding in glycerol: A molecular dynamics investigation. *Journal of Chemical Physics*, **1997**, 107, 4350-4357	3.9	83
83	Circumventing the pathological behavior of path-integral Monte Carlo for systems with Coulomb potentials. *Journal of Chemical Physics*, **1997**, 107, 571-575	3.9	21
82	Calculating the hopping rate for self-diffusion on rough potential energy surfaces: Cage correlations. *Journal of Chemical Physics*, **1997**, 107, 6867-6876	3.9	110

81	Solvation and reorganization energies in polarizable molecular and continuum solvents. *Journal of Chemical Physics*, **1997**, 106, 2372-2387	3.9	63
80	Vibrational energy relaxation in the condensed phases: Quantum vs classical bath for multiphonon processes. *Journal of Chemical Physics*, **1997**, 107, 6050-6061	3.9	89
79	Smart walking: A new method for Boltzmann sampling of protein conformations. *Journal of Chemical Physics*, **1997**, 107, 9185-9196	3.9	83
78	Free Energy of the Hydrophobic Interaction from Molecular Dynamics Simulations: The Effects of Solute and Solvent Polarizability. *Journal of Physical Chemistry B*, **1997**, 101, 10488-10493	3.4	86
77	Novel methods of sampling phase space in the simulation of biological systems. *Current Opinion in Structural Biology*, **1997**, 7, 181-9	8.1	196
76	Effects of Polarizability on the Hydration of the Chloride Ion. *The Journal of Physical Chemistry*, **1996**, 100, 11934-11943		242
75	Dynamical Fluctuating Charge Force Fields: The Aqueous Solvation of Amides. *Journal of the American Chemical Society*, **1996**, 118, 672-679	16.4	199
74	Molecular dynamics with multiple time scales: The selection of efficient reference system propagators. *Journal of Chemical Physics*, **1996**, 105, 1426-1436	3.9	88
73	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, 8800-3	11.5	48
72	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	7.4	27
71	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	3.9	2
70	Solvation energies and electronic spectra in polar, polarizable media: Simulation tests of dielectric continuum theory. *Journal of Chemical Physics*, **1996**, 104, 1293-1308	3.9	90
69	The energy relaxation of a nonlinear oscillator coupled to a linear bath. *Journal of Chemical Physics*, **1996**, 104, 1111-1119	3.9	44
68	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	3.9	82
67	A scaling and mapping theory for excess electrons in simple fluids. *Journal of Chemical Physics*, **1995**, 102, 432-436	3.9	3
66	Activated rate processes: The reactive flux method for one-dimensional surface diffusion. *Journal of Chemical Physics*, **1995**, 102, 4037-4055	3.9	27
65	The energy-dependent transmission coefficient and the energy distribution of classical particles escaping from a metastable well. *Journal of Chemical Physics*, **1995**, 102, 7953-7965	3.9	13
64	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		129

63	Computer Simulation of Hydrophobic Hydration Forces on Stacked Plates at Short Range. *The Journal of Physical Chemistry*, **1995**, 99, 2893-2899		256
62	Molecular Dynamics Calculation of the Effect of Solvent Polarizability on the Hydrophobic Interaction. *Journal of the American Chemical Society*, **1995**, 117, 7172-7179	16.4	69
61	Hydrodynamic calculation of the frequency dependent friction on the bond of a diatomic molecule. *Journal of Chemical Physics*, **1995**, 103, 1160-1174	3.9	9
60	The Theory of Multi-Barrier Crossing **1995**, 67-92		3
59	Computer simulation of solid C60 using multiple time-step algorithms. *Journal of Chemical Physics*, **1994**, 101, 2421-2431	3.9	43
58	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	3.9	72
57	Dynamical fluctuating charge force fields: Application to liquid water. *Journal of Chemical Physics*, **1994**, 101, 6141-6156	3.9	1048
56	Quantum and classical relaxation rates from classical simulations. *Journal of Chemical Physics*, **1994**, 100, 8359-8366	3.9	328
55	The Aqueous Solvation of Water: A Comparison of Continuum Methods with Molecular Dynamics. *Journal of the American Chemical Society*, **1994**, 116, 3949-3954	16.4	118
54	Multiple Time Scales in Molecular Dynamics: Applications to Vibrational Relaxation. *Jerusalem Symposia on Quantum Chemistry and Biochemistry*, **1994**, 471-494		
53	Theory and simulation of polar and nonpolar polarizable fluids. *Journal of Chemical Physics*, **1993**, 99, 6998-7011	3.9	36
52	Effective potentials for liquid water using polarizable and nonpolarizable models. *The Journal of Physical Chemistry*, **1993**, 97, 13841-13851		134
51	Reply to Comment on: Reversible multiple time scale molecular dynamics. *Journal of Chemical Physics*, **1993**, 99, 2278-2279	3.9	27
50	Vibrational relaxation in simple fluids: Comparison of theory and simulation. *Journal of Chemical Physics*, **1993**, 98, 7301-7318	3.9	148
49	Theory of polarizable liquid crystals: Optical birefringence. *Journal of Chemical Physics*, **1993**, 99, 2213-2220	3.9	9
48	Method for accelerating chain folding and mixing. *Journal of Chemical Physics*, **1993**, 99, 6071-6077	3.9	45
47	Theory of correlated hops in surface diffusion. *Physical Review Letters*, **1993**, 70, 3299-3302	7.4	68
46	A Born□Oppenheimer approximation for path integrals with an application to electron solvation in polarizable fluids. *Journal of Chemical Physics*, **1993**, 99, 2902-2916	3.9	65

45	Many-body dispersion forces of polarizable clusters and liquids. *Journal of Chemical Physics*, **1992**, 97, 8628-8636	3.9	44
44	A new quantum propagator for hard sphere and cavity systems. *Journal of Chemical Physics*, **1992**, 97, 2382-2385	3.9	54
43	Density dependence of excess electronic ground-state energies in simple atomic fluids. *Journal of Chemical Physics*, **1992**, 97, 2002-2021	3.9	61
42	Reversible multiple time scale molecular dynamics. *Journal of Chemical Physics*, **1992**, 97, 1990-2001	3.9	2628
41	Monte Carlo methods for accelerating barrier crossing: Anti-force-bias and variable step algorithms. *Journal of Chemical Physics*, **1990**, 92, 1980-1985	3.9	38
40	Dynamic friction on rigid and flexible bonds. *Journal of Chemical Physics*, **1990**, 93, 5084-5095	3.9	108
39	Low-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	3.9	56
38	Excess electronic states in fluid helium. *Journal of Chemical Physics*, **1988**, 89, 2128-2137	3.9	33
37	Behavior of the hydrated electron at different temperatures: structure and absorption spectrum. *The Journal of Physical Chemistry*, **1988**, 92, 1721-1730		106
36	Path integral Monte Carlo studies of the behavior of excess electrons in simple fluids. *Journal of Chemical Physics*, **1987**, 86, 5689-5702	3.9	138
35	Path integral Monte Carlo study of the hydrated electron. *Journal of Chemical Physics*, **1987**, 86, 6404-6418	3.9	107
34	Path-integral Monte Carlo simulations of electron localization in water clusters. *Journal of Statistical Physics*, **1986**, 43, 973-984	1.5	10
33	Localization of an excess electron in water clusters. *Journal of Chemical Physics*, **1986**, 85, 1583-1591	3.9	111
32	On the Simulation of Quantum Systems: Path Integral Methods. *Annual Review of Physical Chemistry*, **1986**, 37, 401-424	15.7	619
31	Evaluation of microcanonical rate constants for bimolecular reactions by path integral techniques. *Journal of Chemical Physics*, **1985**, 83, 2972-2975	3.9	24
30	On the use of semiclassical dynamics in determining electronic spectra of Br2 in an Ar matrix. *Journal of Chemical Physics*, **1985**, 83, 230-238	3.9	67
29	Nonergodicity in path integral molecular dynamics. *Journal of Chemical Physics*, **1984**, 81, 3641-3643	3.9	100
28	Fluctuations in lattice Monte Carlo simulations. *Physical Review D*, **1984**, 30, 1791-1794	4.9	1

27	A path integral Monte Carlo study of liquid neon and the quantum effective pair potential. *Journal of Chemical Physics*, **1984**, 81, 2523-2527	3.9	107
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