James T Hynes

List of Publications by Year in descending order

247 papers	22,161 citations	5896 81 h-index	8866 145 g-index
264 all docs	264 docs citations	264 times ranked	9221 citing authors

#	Article	IF	Citations
1	The stable states picture of chemical reactions. II. Rate constants for condensed and gas phase reaction models. Journal of Chemical Physics, 1980, 73, 2715-2732.	3.0	1,242
2	A Molecular Jump Mechanism of Water Reorientation. Science, 2006, 311, 832-835.	12.6	988
3	Constrained reaction coordinate dynamics for the simulation of rare events. Chemical Physics Letters, 1989, 156, 472-477.	2.6	840
4	Water Dynamics in the Hydration Shells of Biomolecules. Chemical Reviews, 2017, 117, 10694-10725.	47.7	574
5	Time-dependent fluorescence solvent shifts, dielectric friction, and nonequilibrium solvation in polar solvents. The Journal of Physical Chemistry, 1985, 89, 4181-4188.	2.9	522
6	Outer-sphere electron-transfer reactions and frequency-dependent friction. The Journal of Physical Chemistry, 1986, 90, 3701-3706.	2.9	453
7	Solvation dynamics for an ion pair in a polar solvent: Timeâ€dependent fluorescence and photochemical charge transfer. Journal of Chemical Physics, 1991, 94, 5961-5979.	3.0	396
8	On the Molecular Mechanism of Water Reorientation. Journal of Physical Chemistry B, 2008, 112, 14230-14242.	2.6	380
9	A theoretical analysis of the sum frequency generation spectrum of the water surface. Chemical Physics, 2000, 258, 371-390.	1.9	340
10	Why Water Reorientation Slows without Iceberg Formation around Hydrophobic Solutes. Journal of Physical Chemistry B, 2009, 113, 2428-2435.	2.6	338
11	Intramolecular vibrational relaxation and spectra of CH and CD overtones in benzene and perdeuterobenzene. Journal of Chemical Physics, 1984, 81, 1115-1134.	3.0	330
12	Hydrogen Bond Dynamics in Water and Ultrafast Infrared Spectroscopy. Journal of Physical Chemistry A, 2002, 106, 11993-11996.	2.5	325
13	Molecularâ€dynamics simulation for a model nonadiabatic proton transfer reaction in solution. Journal of Chemical Physics, 1991, 94, 3619-3628.	3.0	323
14	Reorientation and Allied Dynamics in Water and Aqueous Solutions. Annual Review of Physical Chemistry, 2011, 62, 395-416.	10.8	310
15	Molecular Mechanism of HCl Acid Ionization in Water:â€‰ Ab Initio Potential Energy Surfaces and Monte Carlo Simulations. Journal of Physical Chemistry B, 1997, 101, 10464-10478.	2.6	299
16	Nonequilibrium solvation effects on reaction rates for model SN2 reactions in water. Journal of Chemical Physics, 1989, 90, 3537-3558.	3.0	289
17	Reorientional dynamics of water molecules in anionic hydration shells. Proceedings of the National Academy of Sciences of the United States of America, 2007, 104, 11167-11172.	7.1	279
18	Molecular dynamics of a modelSN2 reaction in water. Journal of Chemical Physics, 1987, 86, 1356-1376.	3.0	277

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19	Hydrogen Bond Dynamics in Water and Ultrafast Infrared Spectroscopy:â€‰ A Theoretical Study. Journal of Physical Chemistry A, 2004, 108, 1275-1289.	2.5	252
20	A Theoretical Analysis of the Sum Frequency Generation Spectrum of the Water Surface. II. Time-Dependent Approach. Journal of Physical Chemistry B, 2002, 106, 673-685.	2.6	251
21	Reactive modes in condensed phase reactions. Journal of Chemical Physics, 1981, 74, 4465-4475.	3.0	248
22	Vibrational energy relaxation of HOD in liquid D2O. Journal of Chemical Physics, 1996, 104, 2356-2368.	3.0	248
23	Curve Crossing Formulation for Proton Transfer Reactions in Solution. The Journal of Physical Chemistry, 1996, 100, 1118-1128.	2.9	246
24	Nonequilibrium solvation dynamics in solution reactions. Journal of Chemical Physics, 1983, 78, 4174-4185.	3.0	241
25	Dynamical theory of proton tunneling transfer rates in solution: general formulation. Chemical Physics, 1993, 170, 315-346.	1.9	228
26	The stable states picture of chemical reactions. I. Formulation for rate constants and initial condition effects. Journal of Chemical Physics, 1980, 73, 2700-2714.	3.0	226
27	Dynamical polar solvent effects on solution reactions: A simple continuum model. Journal of Chemical Physics, 1982, 76, 2993-3001.	3.0	224
28	A dynamical theory of nonadiabatic proton and hydrogen atom transfer reaction rates in solution. Chemical Physics Letters, 1989, 162, 19-26.	2.6	223
29	Classical dynamics of energy transfer between bonds in ABA triatomics. Journal of Chemical Physics, 1982, 77, 3583-3594.	3.0	202
30	Vibrational relaxation of a dipolar molecule in water. Journal of Chemical Physics, 1992, 96, 5354-5369.	3.0	202
31	Proton transfer in hydrogenâ€bonded acidâ€“base complexes in polar solvents. Journal of Chemical Physics, 1995, 102, 2487-2505.	3.0	202
32	Solute-dependent solvent force constants for ion pairs and neutral pairs in a polar solvent. The Journal of Physical Chemistry, 1989, 93, 2184-2187.	2.9	188
33	Dynamics of ion pair interconversion in a polar solvent. Journal of Chemical Physics, 1990, 93, 7137-7147.	3.0	179
34	On the Molecular Mechanism of Drug Intercalation into DNA: A Simulation Study of the Intercalation Pathway, Free Energy, and DNA Structural Changes. Journal of the American Chemical Society, 2008, 130, 9747-9755.	13.7	176
35	Vibrational phase and energy relaxation of CNâ¯ in water. Journal of Chemical Physics, 1998, 108, 142-153.	3.0	173
36	Classical dynamics of highly excited CH and CD overtones in benzene and perdeuterobenzene. Journal of Chemical Physics, 1984, 81, 1135-1144.	3.0	170

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37	Nonadiabatic solvation model for SN2 reactions in polar solvents. Journal of Chemical Physics, 1987, 86, 1377-1386.	3.0	166
38	Equilibrium and nonequilibrium solvation and solute electronic structure. III. Quantum theory. Journal of Chemical Physics, 1992, 96, 5088-5110.	3.0	166
39	Ultrafast Vibrational Population Dynamics of Water and Related Systems:Â A Theoretical Perspective. Chemical Reviews, 2004, 104, 1915-1928.	47.7	163
40	Solution reaction path Hamiltonian for reactions in polar solvents. I. Formulation. Journal of Chemical Physics, 1988, 88, 6853-6862.	3.0	156
41	Slow vibrational relaxation in picosecond iodine recombination in liquids. Journal of Chemical Physics, 1982, 77, 2130-2143.	3.0	154
42	Equilibrium and nonequilibrium solvation and solute electronic structure. I. Formulation. Journal of Chemical Physics, 1990, 93, 5194-5210.	3.0	154
43	Short range caging effects for reactions in solution. I. Reaction rate constants and short range caging picture. Journal of Chemical Physics, 1979, 71, 871-883.	3.0	151
44	Frequency Shifts in the Hydrogen-Bonded OH Stretch in Halideâ^'Water Clusters. The Importance of Charge Transfer. Journal of the American Chemical Society, 2000, 122, 6278-6286.	13.7	150
45	Activation to the transition state: reactant and solvent energy flow for a model SN2 reaction in water. Journal of the American Chemical Society, 1991, 113, 74-87.	13.7	149
46	Fast vibrational relaxation for a dipolar molecule in a polar solvent. The Journal of Physical Chemistry, 1990, 94, 8625-8628.	2.9	147
47	A Theoretical Investigation of Excited-State Acidity of Phenol and Cyanophenols. Journal of the American Chemical Society, 2000, 122, 12243-12253.	13.7	145
48	Quantum mechanics of local mode ABA triatomic molecules. Journal of Chemical Physics, 1982, 77, 3595-3604.	3.0	143
49	On the Residence Time for Water in a Solute Hydration Shell: Application to Aqueous Halide Solutions. Journal of Physical Chemistry B, 2008, 112, 7697-7701.	2.6	143
50	HCl acid ionization in water: A theoretical molecular modeling. Journal of Molecular Liquids, 1995, 64, 25-37.	4.9	142
51	Energy diffusionâ€controlled reactions in solution. Journal of Chemical Physics, 1982, 77, 3736-3743.	3.0	140
52	Molecular dynamics simulation of electron-transfer reactions in solution. The Journal of Physical Chemistry, 1989, 93, 6261-6265.	2.9	138
53	Molecular dynamics of the A+BC reaction in rare gas solution. Journal of Chemical Physics, 1986, 85, 5625-5643.	3.0	134
54	Reduction of CO₂ to Methanol Catalyzed by a Biomimetic Organo-Hydride Produced from Pyridine. Journal of the American Chemical Society, 2014, 136, 16081-16095.	13.7	131

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55	Nonlinear resonances and vibrational energy flow in model hydrocarbon chains. Journal of Chemical Physics, 1983, 79, 4247-4260.	3.0	122
56	A theoretical model for SN1 ionic dissociation in solution. 1. Activation free energetics and transition-state structure. Journal of the American Chemical Society, 1992, 114, 10508-10528.	13.7	117
57	Kinetic Isotope Effects for Nonadiabatic Proton Transfer Reactions in a Polar Environment. 1. Interpretation of Tunneling Kinetic Isotopic Effects. Journal of Physical Chemistry A, 2004, 108, 11793-11808.	2.5	115
58	Do more strongly hydrogen-bonded water molecules reorient more slowly ?. Chemical Physics Letters, 2006, 433, 80-85.	2.6	115
59	Intermolecular photochemical proton transfer in solution: new insights and perspectives. Journal of Photochemistry and Photobiology A: Chemistry, 2002, 154, 3-11.	3.9	113
60	Water Hydrogen-Bond Dynamics around Amino Acids: The Key Role of Hydrophilic Hydrogen-Bond Acceptor Groups. Journal of Physical Chemistry B, 2010, 114, 2083-2089.	2.6	113
61	Molecular Mechanism of HF Acid Ionization in Water:Â An Electronic Structureâ^'Monte Carlo Study. Journal of Physical Chemistry A, 1999, 103, 10398-10408.	2.5	111
62	Nonlinear Free Energy Relations for Adiabatic Proton Transfer Reactions in a Polar Environment. I. Fixed Proton Donorâ^'Acceptor Separation. Journal of Physical Chemistry A, 2002, 106, 1834-1849.	2.5	106
63	Water Hydrogen Bond Dynamics in Aqueous Solutions of Amphiphiles. Journal of Physical Chemistry B, 2010, 114, 3052-3059.	2.6	106
64	Nonequilibrium free energy surfaces for hydrogen-bonded proton-transfer complexes in solution. The Journal of Physical Chemistry, 1991, 95, 10431-10442.	2.9	105
65	Vibrational predissociation in hydrogen-bonded OHâ€¦O complexes via OH stretch-OO stretch energy transfer. Chemical Physics Letters, 1993, 204, 197-205.	2.6	104
66	Molecular dynamics of a modelSN1 reaction in water. Journal of Chemical Physics, 1991, 95, 5256-5267.	3.0	103
67	Dynamical Disorder in the DNA Hydration Shell. Journal of the American Chemical Society, 2016, 138, 7610-7620.	13.7	103
68	Model molecular dynamics simulation of hydrochloric acid ionization at the surface of stratospheric ice. Faraday Discussions, 1998, 110, 301-322.	3.2	102
69	Biomolecular hydration dynamics: a jump model perspective. Chemical Society Reviews, 2013, 42, 5672.	38.1	100
70	Classical dynamics of intramolecular energy flow and overtoneâ€induced dissociation in HO2H and HO2D. Journal of Chemical Physics, 1986, 85, 5791-5804.	3.0	99
71	Water reorientation, hydrogen-bond dynamics and 2D-IR spectroscopy next to an extended hydrophobic surface. Faraday Discussions, 2010, 146, 263.	3.2	98
72	The protean proton in water. Nature, 1999, 397, 565-567.	27.8	94

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73	Multiple Time Scales in Solvation Dynamics of DNA in Aqueous Solution:Â The Role of Water, Counterions, and Cross-Correlations. Journal of Physical Chemistry B, 2006, 110, 26396-26402.	2.6	92
74	A simple dipole isomerization model for non-equilibrium solvation dynamics in reactions in polar solvents. Chemical Physics, 1984, 90, 21-35.	1.9	91
75	Chemical reaction rates and solvent friction. Journal of Statistical Physics, 1986, 42, 149-168.	1.2	91
76	Stochastic trajectory simulation of iodine recombination in liquids. Journal of Chemical Physics, 1980, 72, 177-188.	3.0	90
77	Nonequilibrium Free Energy Functions, Recombination Dynamics, and Vibrational Relaxation of I2- in Acetonitrile: Molecular Dynamics of Charge Flow in the Electronically Adiabatic Limit. The Journal of Physical Chemistry, 1995, 99, 7557-7567.	2.9	90
78	Water Jump Reorientation: From Theoretical Prediction to Experimental Observation. Accounts of Chemical Research, 2012, 45, 53-62.	15.6	90
79	Vibrational energy transfer from highly excited anharmonic oscillators. Dependence on quantum state and interaction potential. Journal of Chemical Physics, 1982, 76, 6002-6014.	3.0	85
80	Environmental effects on a conical intersection: A model study. Faraday Discussions, 2004, 127, 395.	3.2	85
81	Entropy of Water in the Hydration Layer of Major and Minor Grooves of DNA. Journal of Physical Chemistry B, 2006, 110, 19611-19618.	2.6	85
82	Saddle point model for atom transfer reactions in solution. Journal of Chemical Physics, 1981, 75, 2191-2198.	3.0	84
83	Excited-State Charge Transfer at a Conical Intersection:â€‰ Effects of an Environment. Journal of Physical Chemistry A, 2006, 110, 11411-11423.	2.5	82
84	Electronic friction and electron transfer rates at metallic electrodes. Journal of Chemical Physics, 1993, 99, 6517-6530.	3.0	80
85	Equilibrium and nonequilibrium solvation and solute electronic structure. II. Strong coupling limit. Journal of Chemical Physics, 1990, 93, 5211-5223.	3.0	79
86	Nonlinear Free Energy Relations for Adiabatic Proton Transfer Reactions in a Polar Environment. II. Inclusion of the Hydrogen Bond Vibration. Journal of Physical Chemistry A, 2002, 106, 1850-1861.	2.5	78
87	Multistep Drug Intercalation: Molecular Dynamics and Free Energy Studies of the Binding of Daunomycin to DNA. Journal of the American Chemical Society, 2012, 134, 8588-8596.	13.7	78
88	Chemical reaction rates and solvation dynamics in electrolyte solutions: ion atmosphere friction. Chemical Physics, 1991, 152, 169-183.	1.9	76
89	Reactive dynamics for diffusive barrier crossing. Journal of Chemical Physics, 1978, 69, 5246-5260.	3.0	73
90	Ab Initio Model Study of the Mechanism of Chlorine Nitrate Hydrolysis on Ice. Journal of Physical Chemistry A, 1998, 102, 309-314.	2.5	73

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91	Pathways for H₂O Bend Vibrational Relaxation in Liquid Water. Journal of Physical Chemistry A, 2009, 113, 8949-8962.	2.5	73
92	Rate and Mechanisms for Water Exchange around Li+(aq) from MD Simulations. Journal of Physical Chemistry B, 2003, 107, 4470-4477.	2.6	70
93	Benzimidazoles as Metal-Free and Recyclable Hydrides for CO₂ Reduction to Formate. Journal of the American Chemical Society, 2019, 141, 272-280.	13.7	67
94	Solution reaction path Hamiltonian for reactions in polar solvents. II. Applications. Journal of Chemical Physics, 1988, 88, 6863-6869.	3.0	66
95	Hydration Shell Exchange Kinetics:Â An MD Study for Na+(aq). The Journal of Physical Chemistry, 1996, 100, 5611-5615.	2.9	66
96	Well and barrier dynamics and electron transfer rates. A molecular dynamics study. Chemical Physics, 1993, 176, 521-537.	1.9	65
97	A Theoretical Study of the Formation of the Aminoacetonitrile Precursor of Glycine on Icy Grain Mantles in the Interstellar Medium. Journal of Physical Chemistry C, 2008, 112, 2972-2980.	3.1	64
98	Non-adiabatic dynamics close to conical intersections and the surface hopping perspective. Frontiers in Chemistry, 2014, 2, 97.	3.6	64
99	Microscopic boundary layer effects and rough sphere rotation. Journal of Chemical Physics, 1977, 67, 3256-3267.	3.0	63
100	Quantum dynamics of energy transfer between bonds in coupled Morse oscillator systems. Journal of Chemical Physics, 1984, 81, 1314-1326.	3.0	63
101	A Theoretical Study of the Reaction of ClONO2 with HCl on Ice. Journal of Physical Chemistry A, 1999, 103, 3797-3801.	2.5	63
102	Charged Pushâ^'Pull Polyenes in Solution:â€‰ Anomalous Solvatochromism and Nonlinear Optical Properties. Journal of Physical Chemistry A, 2003, 107, 6032-6046.	2.5	63
103	Kinetic Isotope Effects for Adiabatic Proton Transfer Reactions in a Polar Environment. Journal of Physical Chemistry A, 2003, 107, 9022-9039.	2.5	63
104	On the Ultrafast Infrared Spectroscopy of Anion Hydration Shell Hydrogen Bond Dynamics. Journal of Physical Chemistry A, 2006, 110, 11237-11243.	2.5	63
105	How Acidic Is Carbonic Acid?. Journal of Physical Chemistry B, 2016, 120, 2440-2451.	2.6	63
106	Dynamic Effects on Reaction Rates in a Michael Addition Catalyzed by Chalcone Isomerase. Beyond the Frozen Environment Approach. Journal of the American Chemical Society, 2008, 130, 7477-7488.	13.7	61
107	Non-monotonic dependence of water reorientation dynamics on surface hydrophilicity: competing effects of the hydration structure and hydrogen-bond strength. Physical Chemistry Chemical Physics, 2011, 13, 19911.	2.8	60
108	Catalytic Reduction of CO₂ by Renewable Organohydrides. Journal of Physical Chemistry Letters, 2015, 6, 5078-5092.	4.6	59

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109	Reactive paths in the diffusion limit. Journal of Chemical Physics, 1982, 77, 1295-1301.	3.0	58
110	Vibrational relaxation times for a model hydrogen-bonded complex in a polar solvent. Chemical Physics, 1993, 175, 205-221.	1.9	58
111	Two Valence Bond State Model for Molecular Nonlinear Optical Properties. Nonequilibrium Solvation Formulation. Journal of Physical Chemistry A, 1998, 102, 7712-7722.	2.5	58
112	Roles of the Lewis Acid and Base in the Chemical Reduction of CO₂ Catalyzed by Frustrated Lewis Pairs. Inorganic Chemistry, 2013, 52, 10062-10066.	4.0	58
113	Coupling between Protein and Reaction Dynamics in Enzymatic Processes:Â Application of Groteâ^'Hynes Theory to CatecholO-Methyltransferase. Journal of the American Chemical Society, 2006, 128, 6186-6193.	13.7	57
114	Short range caging effects for reactions in solution. II. Escape probability and time dependent reactivity. Journal of Chemical Physics, 1979, 71, 884-893.	3.0	56
115	Depth-Dependent Dissociation of Nitric Acid at an Aqueous Surface: Carâ^'Parrinello Molecular Dynamics. Journal of Physical Chemistry A, 2009, 113, 1295-1307.	2.5	54
116	Charge Transfer Reactions and Solvation Dynamics. , 1994, , 345-381.		54
117	Confined Waterâ€™s Dielectric Constant Reduction Is Due to the Surrounding Low Dielectric Media and Not to Interfacial Molecular Ordering. Journal of Physical Chemistry Letters, 2021, 12, 4319-4326.	4.6	53
118	Coupling of translational and reactive dynamics for a Fokkerâ€“Planck model. Journal of Chemical Physics, 1978, 68, 3203-3216.	3.0	52
119	On the photodissociation of alkali-metal halides in solution. Journal of the Chemical Society, Faraday Transactions, 1997, 93, 977-988.	1.7	52
120	Ultrafast Energy Transfer from the Intramolecular Bending Vibration to Librations in Liquid Water. Journal of Physical Chemistry A, 2009, 113, 6657-6665.	2.5	52
121	Water reorientation dynamics in the first hydration shells of Fâ^' and Iâ^'. Physical Chemistry Chemical Physics, 2011, 13, 19895.	2.8	52
122	Excited state intramolecular charge transfer rates of p-dirnethylaminobenzonitrile (DMABN) in solution: a two-dimensional dynamics perspective. Journal of Photochemistry and Photobiology A: Chemistry, 1997, 105, 337-343.	3.9	51
123	Kinetic Isotope Effects for Nonadiabatic Proton Transfer Reactions in a Polar Environment. 2. Comparison with an Electronically Diabatic Description. Journal of Physical Chemistry A, 2004, 108, 11809-11818.	2.5	51
124	Nuclear Quantum Effects in Water Reorientation and Hydrogen-Bond Dynamics. Journal of Physical Chemistry Letters, 2017, 8, 2602-2607.	4.6	51
125	A dynamical theory of unimolecular ionic dissociation reactions in polar solvents. Journal of Chemical Physics, 1988, 88, 2513-2525.	3.0	49
126	Theoretical aspects of tunneling proton transfer reactions in a polar environment. Journal of Physical Organic Chemistry, 2010, 23, 632-646.	1.9	49

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127	Dielectric friction and solvation dynamics: a molecular dynamics study. The Journal of Physical Chemistry, 1992, 96, 4068-4074.	2.9	48
128	Theoretical Study of Oâ€“O Single Bond Formation in the Oxidation of Water by the Ruthenium Blue Dimer. Journal of Physical Chemistry A, 2011, 115, 8003-8016.	2.5	46
129	Theoretical Study of the Dissociation of Nitric Acid at a Model Aqueous Surface. Journal of Physical Chemistry A, 2007, 111, 11033-11042.	2.5	45
130	Water Structure, Dynamics, and Sum-Frequency Generation Spectra at Electrified Graphene Interfaces. Journal of Physical Chemistry Letters, 2020, 11, 624-631.	4.6	45
131	Dynamical Friction Effects on the Photoisomerization of a Model Protonated Schiff Base in Solution. Journal of Physical Chemistry A, 2011, 115, 3720-3735.	2.5	43
132	VB resonance theory in solution. I. Multistate formulation. Journal of Chemical Physics, 1995, 102, 7864-7884.	3.0	40
133	On the Dissociation of Aromatic Radical Anions in Solution. 1. Formulation and Application top-Cyanochlorobenzene Radical Anion. Journal of Physical Chemistry A, 2003, 107, 11271-11291.	2.5	40
134	On the Dissociation of Aromatic Radical Anions in Solution. 2. Reaction Path and Rate Constant Analysis. Journal of Physical Chemistry A, 2003, 107, 11292-11306.	2.5	40
135	Conical intersections in solution: non-equilibrium versus equilibrium solvation. Molecular Physics, 2006, 104, 903-914.	1.7	40
136	Twisted intramolecular charge transfer dynamics in polar solvents. Journal of Photochemistry and Photobiology A: Chemistry, 1994, 82, 67-79.	3.9	39
137	Bihalide ion combination reactions in solution: electronic structure and solvation aspects. Chemical Physics, 1994, 183, 309-323.	1.9	38
138	Acid Ionization of HBr in a Small Water Cluster. Israel Journal of Chemistry, 1999, 39, 273-281.	2.3	37
139	Are there dynamical effects in enzyme catalysis? Some thoughts concerning the enzymatic chemical step. Archives of Biochemistry and Biophysics, 2015, 582, 42-55.	3.0	36
140	Ultrafast Librational Relaxation of H₂O in Liquid Water. Journal of Physical Chemistry B, 2013, 117, 4541-4552.	2.6	35
141	Perspective: Structure and ultrafast dynamics of biomolecular hydration shells. Structural Dynamics, 2017, 4, 044018.	2.3	34
142	On Hydrodynamic Models for Brownian Motion. Journal of Chemical Physics, 1972, 57, 5612-5613.	3.0	33
143	Acid-Base Proton Transfer and Ion Pair Formation in Solution. Advances in Chemical Physics, 2007, , 381-430.	0.3	33
144	Transient initial condition effects for Brownian particle motion. Journal of Chemical Physics, 1973, 59, 3459-3467.	3.0	32

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145	Tracking energy transfer from excited to accepting modes: application to water bend vibrational relaxation. Physical Chemistry Chemical Physics, 2012, 14, 6332.	2.8	29
146	VB resonance theory in solution. II. I2â^'â–I+Iâ^' in acetonitrile. Journal of Chemical Physics, 1995, 102, 7885-7901.	3.0	28
147	A theoretical study of the H2SO4+H2O â†' HSO4 â^'+H3O+ reaction at the surface of aqueous aerosols. Theoretical Chemistry Accounts, 2004, 111, 182-187.	1.4	28
148	Vibrational-translational energy transfer from highly excited anharmonic oscillators. Chemical Physics Letters, 1981, 82, 252-254.	2.6	26
149	Photoisomerization for a model protonated Schiff base in solution: Sloped/peaked conical intersection perspective. Journal of Chemical Physics, 2012, 137, 22A543.	3.0	26
150	Solvation Dynamics in Liquid Water. 1. Ultrafast Energy Fluxes. Journal of Physical Chemistry B, 2015, 119, 7558-7570.	2.6	26
151	Initial condition effects for diffusive barrier crossing. Journal of Chemical Physics, 1978, 69, 5261-5266.	3.0	25
152	Molecules in Motion: Chemical Reaction and Allied Dynamics in Solution and Elsewhere. Annual Review of Physical Chemistry, 2015, 66, 1-20.	10.8	25
153	On the Fokker-Planck equation for the linear chain. Molecular Physics, 1974, 28, 997-1004.	1.7	24
154	Adsorption of HF and HCl molecules on ice at 190 and 235 K from molecular dynamics simulations: Free energy profiles and residence times. Journal of Chemical Physics, 2003, 118, 9814-9823.	3.0	24
155	Non-adiabatic transition probability dependence on conical intersection topography. Journal of Chemical Physics, 2016, 145, 194104.	3.0	24
156	Reaction Mechanism for Direct Proton Transfer from Carbonic Acid to a Strong Base in Aqueous Solution I: Acid and Base Coordinate and Charge Dynamics. Journal of Physical Chemistry B, 2016, 120, 2271-2280.	2.6	24
157	Equilibrium and nonequilibrium solvation and solute electronic structure. International Journal of Quantum Chemistry, 1990, 38, 821-833.	2.0	20
158	Theoretical studies of heterogeneous reaction mechanisms relevant for stratospheric ozone depletion. International Journal of Quantum Chemistry, 1999, 75, 683-692.	2.0	20
159	Concerted Proton-Transfer Mechanism and Solvation Effects in the HNC/HCN Isomerization on the Surface of Icy Grain Mantles in the Interstellar Medium. Journal of Physical Chemistry C, 2007, 111, 15026-15033.	3.1	20
160	Water dynamics at electrified graphene interfaces: a jump model perspective. Physical Chemistry Chemical Physics, 2020, 22, 10581-10591.	2.8	19
161	Direct and indirect solvent coupling vibrational dephasing mechanisms in hydrogen-bonded molecules. The Journal of Physical Chemistry, 1991, 95, 4651-4659.	2.9	18
162	Vibrational Symmetry Breaking of NO₃^{â^'} in Aqueous Solution: NO Asymmetric Stretch Frequency Distribution and Mean Splitting. Journal of Physical Chemistry A, 2010, 114, 1255-1269.	2.5	18

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163	Nonlinear fluctuations in master equation systems. I. Velocity correlation function for the Rayleigh model. Journal of Chemical Physics, 1975, 62, 2972-2981.	3.0	17
164	Hydration shell exchange dynamics for in water. Journal of Physics Condensed Matter, 1996, 8, 9411-9416.	1.8	17
165	Proton relay and electron flow in the Oâ€“O single bond formation in water oxidation by the ruthenium blue dimer. Energy and Environmental Science, 2012, 5, 7741.	30.8	16
166	Temperature-Dependent Solvent Polarity Effects on Adiabatic Proton Transfer Rate Constants and Kinetic Isotope Effects. Israel Journal of Chemistry, 2004, 44, 171-184.	2.3	15
167	Predicting Hydride Donor Strength via Quantum Chemical Calculations of Hydride Transfer Activation Free Energy. Journal of Physical Chemistry B, 2018, 122, 1278-1288.	2.6	15
168	A stochastic theory of chemical reaction rates. I. Formalism. Journal of Statistical Physics, 1989, 56, 879-893.	1.2	14
169	Wet chemistry. Nature, 1994, 369, 439-440.	27.8	14
170	Ab Initio Study of Nitromethane Deprotonation by (OH)-Â·nH2O Clusters. Journal of Physical Chemistry A, 1998, 102, 3977-3984.	2.5	14
171	Solvation Dynamics in Liquid Water. III. Energy Fluxes and Structural Changes. Journal of Physical Chemistry B, 2017, 121, 1377-1385.	2.6	14
172	Radical recombination rate constants from gas to liquid phase. The Journal of Physical Chemistry, 1989, 93, 7031-7036.	2.9	13
173	Dihydropteridine/Pteridine as a 2H⁺/2e^{â€“} Redox Mediator for the Reduction of CO₂ to Methanol: A Computational Study. Journal of Physical Chemistry B, 2017, 121, 4158-4167.	2.6	13
174	Renewable Hydride Donors for the Catalytic Reduction of CO₂: A Thermodynamic and Kinetic Study. Journal of Physical Chemistry B, 2018, 122, 10179-10189.	2.6	13
175	Solvation Dynamics in Water: 2. Energy Fluxes on Excited- and Ground-State Surfaces. Journal of Physical Chemistry B, 2016, 120, 11287-11297.	2.6	12
176	Reaction Mechanism for Direct Proton Transfer from Carbonic Acid to a Strong Base in Aqueous Solution II: Solvent Coordinate-Dependent Reaction Path. Journal of Physical Chemistry B, 2016, 120, 2281-2290.	2.6	12
177	A stochastic theory of chemical reaction rates. II. Applications. Journal of Statistical Physics, 1989, 56, 895-910.	1.2	11
178	Ionization of Acids in Water. ACS Symposium Series, 1994, , 143-153.	0.5	11
179	Water reorientation in the hydration shells of hydrophilic and hydrophobic solutes. Science China: Physics, Mechanics and Astronomy, 2010, 53, 1068-1072.	5.1	11
180	Effect of Solvent Dielectric Constant and Acidity on the OH Vibration Frequency in Hydrogen-Bonded Complexes of Fluorinated Ethanols. Journal of Physical Chemistry B, 2015, 119, 9278-9286.	2.6	11

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