James T Hynes

List of Publications by Year in Descending Order

246 papers
19,950 citations
79 h-index
138 g-index
264 ext. papers
20,930 ext. citations
6.3 avg, IF
6.95 L-index

#	Paper	IF	Citations
246	Ultrafast Rotational and Translational Energy Relaxation in Neat Liquids. *Journal of Physical Chemistry B*, **2021**, 125, 12806-12819	3.4	
245	Electron Flow Characterization of Charge Transfer for Carbonic Acid to Strong Base Proton Transfer in Aqueous Solution. *Journal of Physical Chemistry B*, **2021**, 125, 11473-11490	3.4	0
244	Confined Water'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	6.4	12
243	A Model Electron Transfer Reaction in Confined Aqueous Solution. *ChemPhysChem*, **2021**, 22, 2247-2255	3.2	1
242	Water dynamics at electrified graphene interfaces: a jump model perspective. *Physical Chemistry Chemical Physics*, **2020**, 22, 10581-10591	3.6	9
241	Water Structure, Dynamics, and Sum-Frequency Generation Spectra at Electrified Graphene Interfaces. *Journal of Physical Chemistry Letters*, **2020**, 11, 624-631	6.4	28
240	Solvation Dynamics in Water. 4. On the Initial Regime of Solvation Relaxation. *Journal of Physical Chemistry B*, **2020**, 124, 7668-7681	3.4	4
239	Intact carbonic acid is a viable protonating agent for biological bases. *Proceedings of the National Academy of Sciences of the United States of America*, **2019**, 116, 20837-20843	11.5	5
238	Dynamical Recrossing in the Intercalation Process of the Anticancer Agent Proflavine into DNA. *Journal of Physical Chemistry B*, **2019**, 123, 10904-10914	3.4	2
237	Benzimidazoles as Metal-Free and Recyclable Hydrides for CO Reduction to Formate. *Journal of the American Chemical Society*, **2019**, 141, 272-280	16.4	40
236	Predicting Hydride Donor Strength via Quantum Chemical Calculations of Hydride Transfer Activation Free Energy. *Journal of Physical Chemistry B*, **2018**, 122, 1278-1288	3.4	11
235	Renewable Hydride Donors for the Catalytic Reduction of CO: A Thermodynamic and Kinetic Study. *Journal of Physical Chemistry B*, **2018**, 122, 10179-10189	3.4	9
234	Solvation Dynamics in Liquid Water. III. Energy Fluxes and Structural Changes. *Journal of Physical Chemistry B*, **2017**, 121, 1377-1385	3.4	9
233	Water Dynamics in the Hydration Shells of Biomolecules. *Chemical Reviews*, **2017**, 117, 10694-10725	68.1	410
232	Perspective: Structure and ultrafast dynamics of biomolecular hydration shells. *Structural Dynamics*, **2017**, 4, 044018	3.2	23
231	Nuclear Quantum Effects in Water Reorientation and Hydrogen-Bond Dynamics. *Journal of Physical Chemistry Letters*, **2017**, 8, 2602-2607	6.4	40
230	Translational versus rotational energy flow in water solvation dynamics. *Chemical Physics Letters*, **2017**, 683, 483-487	2.5	5

229	Dihydropteridine/Pteridine as a 2H/2e Redox Mediator for the Reduction of CO to Methanol: A Computational Study. *Journal of Physical Chemistry B*, **2017**, 121, 4158-4167	3.4	12
228	Solvation Dynamics in Water: 2. Energy Fluxes on Excited- and Ground-State Surfaces. *Journal of Physical Chemistry B*, **2016**, 120, 11287-11297	3.4	8
227	Dynamical Disorder in the DNA Hydration Shell. *Journal of the American Chemical Society*, **2016**, 138, 7610-20	16.4	80
226	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, 2281-90	3.4	9
225	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, 2271-80	3.4	22
224	Non-adiabatic transition probability dependence on conical intersection topography. *Journal of Chemical Physics*, **2016**, 145, 194104	3.9	16
223	How Acidic Is Carbonic Acid?. *Journal of Physical Chemistry B*, **2016**, 120, 2440-51	3.4	34
222	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, 9278-86	3.4	9
221	Are there dynamical effects in enzyme catalysis? Some thoughts concerning the enzymatic chemical step. *Archives of Biochemistry and Biophysics*, **2015**, 582, 42-55	4.1	30
220	Catalytic Reduction of CO2 by Renewable Organohydrides. *Journal of Physical Chemistry Letters*, **2015**, 6, 5078-92	6.4	51
219	Molecules in motion: chemical reaction and allied dynamics in solution and elsewhere. *Annual Review of Physical Chemistry*, **2015**, 66, 1-20	15.7	21
218	Solvation Dynamics in Liquid Water. 1. Ultrafast Energy Fluxes. *Journal of Physical Chemistry B*, **2015** , 119, 7558-70	3.4	20
217	Reduction of CO2 to methanol catalyzed by a biomimetic organo-hydride produced from pyridine. *Journal of the American Chemical Society*, **2014**, 136, 16081-95	16.4	113
216	Non-adiabatic dynamics close to conical intersections and the surface hopping perspective. *Frontiers in Chemistry*, **2014**, 2, 97	5	52
215	Conical intersection structure and dynamics for a model protonated schiff base photoisomerization in solution. *International Journal of Quantum Chemistry*, **2013**, 113, 296-305	2.1	7
214	Roles of the Lewis acid and base in the chemical reduction of CO2 catalyzed by frustrated Lewis pairs. *Inorganic Chemistry*, **2013**, 52, 10062-6	5.1	55
213	Biomolecular hydration dynamics: a jump model perspective. *Chemical Society Reviews*, **2013**, 42, 5672-83	38.5	81
212	Ultrafast librational relaxation of H2O in liquid water. *Journal of Physical Chemistry B*, **2013**, 117, 4541-52	3.4	30

211	Theoretical study of water oxidation by the ruthenium blue dimer. II. Proton relay chain mechanism for the step [bpy2(HOO)Ru(IV)ORu(IV)(OH)bpy2]4+ -[bpy2(O2(I))Ru(IV)ORu(III)(OH2)bpy2]4+. *Journal of Physical Chemistry B*, **2013**, 117, 15761-73	3.4	9
210	Water jump reorientation: from theoretical prediction to experimental observation. *Accounts of Chemical Research*, **2012**, 45, 53-62	24.3	82
209	Tracking energy transfer from excited to accepting modes: application to water bend vibrational relaxation. *Physical Chemistry Chemical Physics*, **2012**, 14, 6332-42	3.6	27
208	Photoisomerization for a model protonated Schiff base in solution: sloped/peaked conical intersection perspective. *Journal of Chemical Physics*, **2012**, 137, 22A543	3.9	21
207	Multistep drug intercalation: molecular dynamics and free energy studies of the binding of daunomycin to DNA. *Journal of the American Chemical Society*, **2012**, 134, 8588-96	16.4	69
206	Proton relay and electron flow in the OO single bond formation in water oxidation by the ruthenium blue dimer. *Energy and Environmental Science*, **2012**, 5, 7741	35.4	15
205	Water reorientation dynamics in the first hydration shells of F- and I-. *Physical Chemistry Chemical Physics*, **2011**, 13, 19895-901	3.6	49
204	Reorientation and allied dynamics in water and aqueous solutions. *Annual Review of Physical Chemistry*, **2011**, 62, 395-416	15.7	268
203	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, 19911-7	3.6	51
202	Dynamical friction effects on the photoisomerization of a model protonated Schiff base in solution. *Journal of Physical Chemistry A*, **2011**, 115, 3720-35	2.8	42
201	Theoretical study of O--O single bond formation in the oxidation of water by the ruthenium blue dimer. *Journal of Physical Chemistry A*, **2011**, 115, 8003-16	2.8	43
200	Vibrational symmetry breaking of NO3- in aqueous solution: NO asymmetric stretch frequency distribution and mean splitting. *Journal of Physical Chemistry A*, **2010**, 114, 1255-69	2.8	16
199	Water hydrogen-bond dynamics around amino acids: the key role of hydrophilic hydrogen-bond acceptor groups. *Journal of Physical Chemistry B*, **2010**, 114, 2083-9	3.4	100
198	Water reorientation, hydrogen-bond dynamics and 2D-IR spectroscopy next to an extended hydrophobic surface. *Faraday Discussions*, **2010**, 146, 263-81; discussion 283-98, 395-401	3.6	93
197	Water hydrogen bond dynamics in aqueous solutions of amphiphiles. *Journal of Physical Chemistry B*, **2010**, 114, 3052-9	3.4	97
196	Water reorientation in the hydration shells of hydrophilic and hydrophobic solutes. *Science China: Physics, Mechanics and Astronomy*, **2010**, 53, 1068-1072	3.6	10
195	Theoretical aspects of tunneling proton transfer reactions in a polar environment. *Journal of Physical Organic Chemistry*, **2010**, 23, 632-646	2.1	45
194	Local mode energy transfer: Ebb and flow. *International Journal of Quantum Chemistry*, **2009**, 22, 375-383	1.1	

193	Ultrafast energy transfer from the intramolecular bending vibration to librations in liquid water. *Journal of Physical Chemistry A*, **2009**, 113, 6657-65	2.8	50
192	Pathways for H2O bend vibrational relaxation in liquid water. *Journal of Physical Chemistry A*, **2009**, 113, 8949-62	2.8	67
191	Why water reorientation slows without iceberg formation around hydrophobic solutes. *Journal of Physical Chemistry B*, **2009**, 113, 2428-35	3.4	310
190	Nitric Acid Dissociation at an Aqueous Surface: Occurrence and Mechanism. *Israel Journal of Chemistry*, **2009**, 49, 251-259	3.4	4
189	Depth-dependent dissociation of nitric acid at an aqueous surface: Car-Parrinello molecular dynamics. *Journal of Physical Chemistry A*, **2009**, 113, 1295-307	2.8	51
188	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, 7477-88	16.4	57
187	On the residence time for water in a solute hydration shell: application to aqueous halide solutions. *Journal of Physical Chemistry B*, **2008**, 112, 7697-701	3.4	131
186	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, 9747-55	16.4	151
185	On the molecular mechanism of water reorientation. *Journal of Physical Chemistry B*, **2008**, 112, 14230-42	3.4	335
184	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	3.8	57
183	Theoretical study of the dissociation of nitric acid at a model aqueous surface. *Journal of Physical Chemistry A*, **2007**, 111, 11033-42	2.8	42
182	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	3.8	43
181	Reorientional dynamics of water molecules in anionic hydration shells. *Proceedings of the National Academy of Sciences of the United States of America*, **2007**, 104, 11167-72	11.5	255
180	Acid-Base Proton Transfer and Ion Pair Formation in Solution. *Advances in Chemical Physics*, **2007**, 381-430		21
179	Conical intersections in solution: non-equilibrium versus equilibrium solvation. *Molecular Physics*, **2006**, 104, 903-914	1.7	40
178	A molecular jump mechanism of water reorientation. *Science*, **2006**, 311, 832-5	33.3	866
177	Multiple time scales in solvation dynamics of DNA in aqueous solution: the role of water, counterions, and cross-correlations. *Journal of Physical Chemistry B*, **2006**, 110, 26396-402	3.4	82
176	Coupling between protein and reaction dynamics in enzymatic processes: application of Grote-Hynes Theory to catechol O-methyltransferase. *Journal of the American Chemical Society*, **2006**, 128, 6186-93	16.4	53

175	Excited-state charge transfer at a conical intersection: effects of an environment. *Journal of Physical Chemistry A*, **2006**, 110, 11411-23	2.8	77
174	On the ultrafast infrared spectroscopy of anion hydration shell hydrogen bond dynamics. *Journal of Physical Chemistry A*, **2006**, 110, 11237-43	2.8	60
173	Entropy of water in the hydration layer of major and minor grooves of DNA. *Journal of Physical Chemistry B*, **2006**, 110, 19611-8	3.4	71
172	Do more strongly hydrogen-bonded water molecules reorient more slowly ?. *Chemical Physics Letters*, **2006**, 433, 80-85	2.5	106
171	A theoretical study of the H2SO4+H2O -HSO4 H3O+ reaction at the surface of aqueous aerosols. *Theoretical Chemistry Accounts*, **2004**, 111, 182-187	1.9	25
170	Environmental effects on a conical intersection: a model study. *Faraday Discussions*, **2004**, 127, 395-411	3.6	80
169	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	2.8	47
168	Ultrafast vibrational population dynamics of water and related systems: a theoretical perspective. *Chemical Reviews*, **2004**, 104, 1915-28	68.1	152
167	Temperature-Dependent Solvent Polarity Effects on Adiabatic Proton Transfer Rate Constants and Kinetic Isotope Effects. *Israel Journal of Chemistry*, **2004**, 44, 171-184	3.4	13
166	Hydrogen Bond Dynamics in Water and Ultrafast Infrared Spectroscopy: A Theoretical Study. *Journal of Physical Chemistry A*, **2004**, 108, 1275-1289	2.8	236
165	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	2.8	100
164	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	2.8	35
163	Rate and Mechanisms for Water Exchange around Li+(aq) from MD Simulations. *Journal of Physical Chemistry B*, **2003**, 107, 4470-4477	3.4	69
162	Charged Push Pull Polyenes in Solution: Anomalous Solvatochromism and Nonlinear Optical Properties. *Journal of Physical Chemistry A*, **2003**, 107, 6032-6046	2.8	52
161	Kinetic Isotope Effects for Adiabatic Proton Transfer Reactions in a Polar Environment. *Journal of Physical Chemistry A*, **2003**, 107, 9022-9039	2.8	60
160	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	2.8	38
159	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	3.9	21
158	Intermolecular photochemical proton transfer in solution: new insights and perspectives. *Journal of Photochemistry and Photobiology A: Chemistry*, **2002**, 154, 3-11	4.7	102

157	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	2.8	69
156	Nonlinear Free Energy Relations for Adiabatic Proton Transfer Reactions in a Polar Environment. I. Fixed Proton Donor□Acceptor Separation. *Journal of Physical Chemistry A*, **2002**, 106, 1834-1849	2.8	95
155	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	3.4	223
154	Hydrogen Bond Dynamics in Water and Ultrafast Infrared Spectroscopy. *Journal of Physical Chemistry A*, **2002**, 106, 11993-11996	2.8	309
153	Crossing the Transition State in Solution **2002**, 231-258		6
152	A theoretical analysis of the sum frequency generation spectrum of the water surface. *Chemical Physics*, **2000**, 258, 371-390	2.3	310
151	A Theoretical Investigation of Excited-State Acidity of Phenol and Cyanophenols. *Journal of the American Chemical Society*, **2000**, 122, 12243-12253	16.4	122
150	Frequency Shifts in the Hydrogen-Bonded OH Stretch in Halide□Water Clusters. The Importance of Charge Transfer. *Journal of the American Chemical Society*, **2000**, 122, 6278-6286	16.4	144
149	Molecular Mechanism of HF Acid Ionization in Water:□An Electronic Structure□Monte Carlo Study. *Journal of Physical Chemistry A*, **1999**, 103, 10398-10408	2.8	100
148	Theoretical studies of heterogeneous reaction mechanisms relevant for stratospheric ozone depletion. *International Journal of Quantum Chemistry*, **1999**, 75, 683-692	2.1	18
147	A Theoretical Study of the Reaction of ClONO2 with HCl on Ice. *Journal of Physical Chemistry A*, **1999**, 103, 3797-3801	2.8	55
146	Acid Ionization of HBr in a Small Water Cluster. *Israel Journal of Chemistry*, **1999**, 39, 273-281	3.4	32
145	Ab Initio Model Study of the Mechanism of Chlorine Nitrate Hydrolysis on Ice. *Journal of Physical Chemistry A*, **1998**, 102, 309-314	2.8	65
144	Ab Initio Study of Nitromethane Deprotonation by (OH)-□hH2O Clusters. *Journal of Physical Chemistry A*, **1998**, 102, 3977-3984	2.8	13
143	Two Valence Bond State Model for Molecular Nonlinear Optical Properties. Nonequilibrium Solvation Formulation. *Journal of Physical Chemistry A*, **1998**, 102, 7712-7722	2.8	52
142	Model molecular dynamics simulation of hydrochloric acid ionization at the surface of stratospheric ice. *Faraday Discussions*, **1998**, 110, 301-322	3.6	96
141	Vibrational phase and energy relaxation of CN□in water. *Journal of Chemical Physics*, **1998**, 108, 142-153	3.9	171
140	On the photodissociation of alkali-metal halides insolution. *Journal of the Chemical Society, Faraday Transactions*, **1997**, 93, 977-988		47

139	Molecular Mechanism of HCl Acid Ionization in Water: Ab Initio Potential Energy Surfaces and Monte Carlo Simulations. *Journal of Physical Chemistry B*, **1997**, 101, 10464-10478	3.4	283
138	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	4.7	46
137	Curve Crossing Formulation for Proton Transfer Reactions in Solution. *The Journal of Physical Chemistry*, **1996**, 100, 1118-1128		232
136	Hydration Shell Exchange Kinetics: An MD Study for Na+(aq). *The Journal of Physical Chemistry*, **1996**, 100, 5611-5615		63
135	Hydration shell exchange dynamics for in water. *Journal of Physics Condensed Matter*, **1996**, 8, 9411-9416	1.8	15
134	Adiabatic acid-base proton transfer in solution. *AIP Conference Proceedings*, **1996**,	0	2
133	Vibrational energy relaxation of HOD in liquid D2O. *Journal of Chemical Physics*, **1996**, 104, 2356-2368	3.9	233
132	HCl acid ionization in water: A theoretical molecular modeling. *Journal of Molecular Liquids*, **1995**, 64, 25-37	6	127
131	VB resonance theory in solution. I. Multistate formulation. *Journal of Chemical Physics*, **1995**, 102, 7864-7884	3.9	35
130	VB resonance theory in solution. II. I2□+I□ in acetonitrile. *Journal of Chemical Physics*, **1995**, 102, 7885-7904	3.9	25
129	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		85
128	Proton transfer in hydrogen-bonded acid□base complexes in polar solvents. *Journal of Chemical Physics*, **1995**, 102, 2487-2505	3.9	188
127	Ionization of Acids in Water. *ACS Symposium Series*, **1994**, 143-153	0.4	10
126	Twisted intramolecular charge transfer dynamics in polar solvents. *Journal of Photochemistry and Photobiology A: Chemistry*, **1994**, 82, 67-79	4.7	37
125	Bihalide ion combination reactions in solution: electronic structure and solvation aspects. *Chemical Physics*, **1994**, 183, 309-323	2.3	32
124	Charge Transfer Reactions and Solvation Dynamics **1994**, 345-381		46
123	Electronic friction and electron transfer rates at metallic electrodes. *Journal of Chemical Physics*, **1993**, 99, 6517-6530	3.9	71
122	Vibrational predissociation in hydrogen-bonded OH□O complexes via OH stretch-OO stretch energy transfer. *Chemical Physics Letters*, **1993**, 204, 197-205	2.5	99

121	Vibrational relaxation times for a model hydrogen-bonded complex in a polar solvent. *Chemical Physics*, **1993**, 175, 205-221	2.3	56
120	Well and barrier dynamics and electron transfer rates. A molecular dynamics study. *Chemical Physics*, **1993**, 176, 521-537	2.3	62
119	Dynamical theory of proton tunneling transfer rates in solution: general formulation. *Chemical Physics*, **1993**, 170, 315-346	2.3	211
118	Dielectric friction and solvation dynamics: a molecular dynamics study. *The Journal of Physical Chemistry*, **1992**, 96, 4068-4074		45
117	Vibrational relaxation of a dipolar molecule in water. *Journal of Chemical Physics*, **1992**, 96, 5354-5369	3.9	191
116	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	16.4	108
115	Equilibrium and nonequilibrium solvation and solute electronic structure. III. Quantum theory. *Journal of Chemical Physics*, **1992**, 96, 5088-5110	3.9	162
114	Direct and indirect solvent coupling vibrational dephasing mechanisms in hydrogen-bonded molecules. *The Journal of Physical Chemistry*, **1991**, 95, 4651-4659		17
113	Nonequilibrium free energy surfaces for hydrogen-bonded proton-transfer complexes in solution. *The Journal of Physical Chemistry*, **1991**, 95, 10431-10442		94
112	Chemical reaction rates and solvation dynamics in electrolyte solutions: ion atmosphere friction. *Chemical Physics*, **1991**, 152, 169-183	2.3	70
111	Solvation dynamics for an ion pair in a polar solvent: Time-dependent fluorescence and photochemical charge transfer. *Journal of Chemical Physics*, **1991**, 94, 5961-5979	3.9	379
110	Molecular dynamics of a model SN1 reaction in water. *Journal of Chemical Physics*, **1991**, 95, 5256-5267	3.9	95
109	Molecular-dynamics simulation for a model nonadiabatic proton transfer reaction in solution. *Journal of Chemical Physics*, **1991**, 94, 3619-3628	3.9	299
108	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	16.4	137
107	Fast vibrational relaxation for a dipolar molecule in a polar solvent. *The Journal of Physical Chemistry*, **1990**, 94, 8625-8628		137
106	Equilibrium and nonequilibrium solvation and solute electronic structure. I. Formulation. *Journal of Chemical Physics*, **1990**, 93, 5194-5210	3.9	145
105	Equilibrium and nonequilibrium solvation and solute electronic structure. II. Strong coupling limit. *Journal of Chemical Physics*, **1990**, 93, 5211-5223	3.9	66
104	Equilibrium and nonequilibrium solvation and solute electronic structure. *International Journal of Quantum Chemistry*, **1990**, 38, 821-833	2.1	19

103	Dynamics of ion pair interconversion in a polar solvent. *Journal of Chemical Physics*, **1990**, 93, 7137-7147	3.9	166
102	Environmental Dynamics and Electron Transfer Reactions. *Jerusalem Symposia on Quantum Chemistry and Biochemistry*, **1990**, 133-148		3
101	Radical recombination rate constants from gas to liquid phase. *The Journal of Physical Chemistry*, **1989**, 93, 7031-7036		11
100	Nonequilibrium solvation effects on reaction rates for model SN2 reactions in water. *Journal of Chemical Physics*, **1989**, 90, 3537-3558	3.9	268
99	A dynamical theory of nonadiabatic proton and hydrogen atom transfer reaction rates in solution. *Chemical Physics Letters*, **1989**, 162, 19-26	2.5	207
98	Constrained reaction coordinate dynamics for the simulation of rare events. *Chemical Physics Letters*, **1989**, 156, 472-477	2.5	726
97	A stochastic theory of chemical reaction rates. I. Formalism. *Journal of Statistical Physics*, **1989**, 56, 879-893	1.5	13
96	A stochastic theory of chemical reaction rates. II. Applications. *Journal of Statistical Physics*, **1989**, 56, 895-910	1.5	10
95	Molecular dynamics simulation of electron-transfer reactions in solution. *The Journal of Physical Chemistry*, **1989**, 93, 6261-6265		125
94	Solute-dependent solvent force constants for ion pairs and neutral pairs in a polar solvent. *The Journal of Physical Chemistry*, **1989**, 93, 2184-2187		177
93	Solution reaction path Hamiltonian for reactions in polar solvents. I. Formulation. *Journal of Chemical Physics*, **1988**, 88, 6853-6862	3.9	146
92	A dynamical theory of unimolecular ionic dissociation reactions in polar solvents. *Journal of Chemical Physics*, **1988**, 88, 2513-2525	3.9	47
91	Solution reaction path Hamiltonian for reactions in polar solvents. II. Applications. *Journal of Chemical Physics*, **1988**, 88, 6863-6869	3.9	54
90	Nonadiabatic solvation model for SN2 reactions in polar solvents. *Journal of Chemical Physics*, **1987**, 86, 1377-1386	3.9	158
89	Molecular dynamics of a model SN2 reaction in water. *Journal of Chemical Physics*, **1987**, 86, 1356-1376	3.9	258
88	Chemical reaction rates and solvent friction. *Journal of Statistical Physics*, **1986**, 42, 149-168	1.5	82
87	Probability oscillations in single pass curve crossings: Semiclassical predictions of nonmonotonic dependence on crossing velocity. *Journal of Chemical Physics*, **1986**, 84, 1554-1564	3.9	5
86	Classical dynamics of intramolecular energy flow and overtone-induced dissociation in HO2H and HO2D. *Journal of Chemical Physics*, **1986**, 85, 5791-5804	3.9	93

85	Outer-sphere electron-transfer reactions and frequency-dependent friction. *The Journal of Physical Chemistry*, **1986**, 90, 3701-3706		432
84	Molecular dynamics of the A+BC reaction in rare gas solution. *Journal of Chemical Physics*, **1986**, 85, 5625-5643	3.9	126
83	Time-dependent fluorescence solvent shifts, dielectric friction, and nonequilibrium solvation in polar solvents. *The Journal of Physical Chemistry*, **1985**, 89, 4181-4188		496
82	Intramolecular vibrational relaxation and spectra of CH and CD overtones in benzene and perdeuterobenzene. *Journal of Chemical Physics*, **1984**, 81, 1115-1134	3.9	315
81	Classical dynamics of highly excited CH and CD overtones in benzene and perdeuterobenzene. *Journal of Chemical Physics*, **1984**, 81, 1135-1144	3.9	160
80	A simple dipole isomerization model for non-equilibrium solvation dynamics in reactions in polar solvents. *Chemical Physics*, **1984**, 90, 21-35	2.3	88
79	Quantum dynamics of energy transfer between bonds in coupled Morse oscillator systems. *Journal of Chemical Physics*, **1984**, 81, 1314-1326	3.9	61
78	Nonequilibrium solvation dynamics in solution reactions. *Journal of Chemical Physics*, **1983**, 78, 4174-4185	3.9	233
77	Nonlinear resonances and vibrational energy flow in model hydrocarbon chains. *Journal of Chemical Physics*, **1983**, 79, 4247-4260	3.9	119
76	Slow vibrational relaxation in picosecond iodine recombination in liquids. *Journal of Chemical Physics*, **1982**, 77, 2130-2143	3.9	143
75	Hydrodynamic interaction effects on isomerization rates in chain molecules. *Journal of Chemical Physics*, **1982**, 77, 4739-4746	3.9	5
74	Energy diffusion-controlled reactions in solution. *Journal of Chemical Physics*, **1982**, 77, 3736-3743	3.9	123
73	Reactive paths in the diffusion limit. *Journal of Chemical Physics*, **1982**, 77, 1295-1301	3.9	52
72	Dynamical polar solvent effects on solution reactions: A simple continuum model. *Journal of Chemical Physics*, **1982**, 76, 2993-3001	3.9	213
71	Classical dynamics of energy transfer between bonds in ABA triatomics. *Journal of Chemical Physics*, **1982**, 77, 3583-3594	3.9	195
70	Quantum mechanics of local mode ABA triatomic molecules. *Journal of Chemical Physics*, **1982**, 77, 3595-3604	3.9	128
69	Vibrational energy transfer from highly excited anharmonic oscillators. Dependence on quantum state and interaction potential. *Journal of Chemical Physics*, **1982**, 76, 6002-6014	3.9	78
68	Vibrational-translational energy transfer from highly excited anharmonic oscillators. *Chemical Physics Letters*, **1981**, 82, 252-254	2.5	18

67	Saddle point model for atom transfer reactions in solution. *Journal of Chemical Physics*, **1981**, 75, 2191-2198	3.9	75
66	Reactive modes in condensed phase reactions. *Journal of Chemical Physics*, **1981**, 74, 4465-4475	3.9	233
65	The stable states picture of chemical reactions. I. Formulation for rate constants and initial condition effects. *Journal of Chemical Physics*, **1980**, 73, 2700-2714	3.9	213
64	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	3.9	1122
63	Stochastic trajectory simulation of iodine recombination in liquids. *Journal of Chemical Physics*, **1980**, 72, 177-188	3.9	82
62	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	3.9	143
61	Short range caging effects for reactions in solution. II. Escape probability and time dependent reactivity. *Journal of Chemical Physics*, **1979**, 71, 884-893	3.9	31
60	Kinetic energy relaxation of a test particle in a dense fluid. *Journal of Chemical Physics*, **1979**, 71, 4492-4501	3.9	7
59	Coupling of translational and reactive dynamics for a Fokker-Planck model. *Journal of Chemical Physics*, **1978**, 68, 3203-3216	3.9	47
58	Reactive dynamics for diffusive barrier crossing. *Journal of Chemical Physics*, **1978**, 69, 5246-5260	3.9	64
57	Initial condition effects for diffusive barrier crossing. *Journal of Chemical Physics*, **1978**, 69, 5261-5266	3.9	20
56	Microscopic boundary layer effects and rough sphere rotation. *Journal of Chemical Physics*, **1977**, 67, 3256-3267	3.9	58
55	Nonlinear fluctuations in master equation systems. I. Velocity correlation function for the Rayleigh model. *Journal of Chemical Physics*, **1975**, 62, 2972-2981	3.9	14
54	On the Fokker-Planck equation for the linear chain. *Molecular Physics*, **1974**, 28, 997-1004	1.7	19
53	Transient initial condition effects for Brownian particle motion. *Journal of Chemical Physics*, **1973**, 59, 3459-3467	3.9	28
52	On Hydrodynamic Models for Brownian Motion. *Journal of Chemical Physics*, **1972**, 57, 5612-5613	3.9	31
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