Gregory K Schenter

List of Publications by Year in Descending Order

171 papers	8,386 citations	47 h-index	87 g-index
180 ext. papers	9,377 ext. citations	5.6 avg, IF	5.9 L-index

#	Paper	IF	Citations
171	Frustrated Coulombic and Cation Size Effects on Nanoscale Boehmite Aggregation: A Tumbler Small- and Ultra-Small-Angle Neutron Scattering Study. *Journal of Physical Chemistry C*, **2022**, 126, 4391-4414	3.8	2
170	Theory-Guided Inelastic Neutron Scattering of Crystalline Alkaline Aluminate Salts Bearing Principal Motifs of Solution-State Species. *Inorganic Chemistry*, **2021**, 60, 16223-16232	5.1	1
169	Moving beyond the Solvent-Tip Approximation to Determine Site-Specific Variations of Interfacial Water Structure through 3D Force Microscopy. *Journal of Physical Chemistry C*, **2021**, 125, 1282-1291	3.8	20
168	Toward a First-Principles Framework for Predicting Collective Properties of Electrolytes. *Accounts of Chemical Research*, **2021**, 54, 2833-2843	24.3	14
167	The Statistical Mechanics of Solution-Phase Nucleation: CaCO(_3) Revisited. *Molecular Modeling and Simulation*, **2021**, 101-122		1
166	Shear stress dependence of force networks in 3D dense suspensions. *Soft Matter*, **2021**, 17, 7476-7486	3.6	1
165	Resolving Heterogeneous Dynamics of Excess Protons in Aqueous Solution with Rate Theory. *Journal of Physical Chemistry B*, **2020**, 124, 5665-5675	3.4	10
164	Al27 NMR chemical shift of Al(OH) calculated from first principles: Assessment of error cancellation in chemically distinct reference and target systems. *Journal of Chemical Physics*, **2020**, 152, 134303	3.9	1
163	CP2K: An electronic structure and molecular dynamics software package - Quickstep: Efficient and accurate electronic structure calculations. *Journal of Chemical Physics*, **2020**, 152, 194103	3.9	421
162	Nanometer-Scale Correlations in Aqueous Salt Solutions. *Journal of Physical Chemistry Letters*, **2020**, 11, 2598-2604	6.4	7
161	Method for Accurately Predicting Solvation Structure. *Journal of Chemical Theory and Computation*, **2020**, 16, 5401-5409	6.4	8
160	Connecting energetics to dynamics in particle growth by oriented attachment using real-time observations. *Nature Communications*, **2020**, 11, 1045	17.4	45
159	Visualization of Aluminum Ions at the Mica Water Interface Links Hydrolysis State-to-Surface Potential and Particle Adhesion. *Journal of the American Chemical Society*, **2020**, 142, 6093-6102	16.4	11
158	Correlating inter-particle forces and particle shape to shear-induced aggregation/fragmentation and rheology for dilute anisotropic particle suspensions: A complementary study via capillary rheometry and in-situ small and ultra-small angle X-ray scattering. *Journal of Colloid and Interface Science*, **2020**, 576, 47-58	9.3	10
157	Quantifying the hydration structure of sodium and potassium ions: taking additional steps on Jacob's Ladder. *Physical Chemistry Chemical Physics*, **2020**, 22, 10641-10652	3.6	24
156	Heterolytic Scission of Hydrogen Within a Crystalline Frustrated Lewis Pair. *Inorganic Chemistry*, **2020**, 59, 15295-15301	5.1	5
155	Mechanisms of Al Dimerization in Alkaline Solutions. *Inorganic Chemistry*, **2020**, 59, 18181-18189	5.1	1

154	Solvent reaction coordinate for an S2 reaction. *Journal of Chemical Physics*, **2020**, 153, 024103	3.9	4
153	Correlation function approach for diffusion in confined geometries. *Physical Review E*, **2020**, 102, 022129	2.4	3
152	Inference of principal species in caustic aluminate solutions through solid-state spectroscopic characterization. *Dalton Transactions*, **2020**, 49, 5869-5880	4.3	6
151	Resolving local configurational contributions to X-ray and neutron radial distribution functions within solutions of concentrated electrolytes - a case study of concentrated NaOH. *Physical Chemistry Chemical Physics*, **2019**, 21, 6828-6838	3.6	10
150	Effect of fine-tuning pore structures on the dynamics of confined water. *Journal of Chemical Physics* , **2019**, 150, 204706	3.9	5
149	PageRank as a collective variable to study complex chemical transformations and their energy landscapes. *Journal of Chemical Physics*, **2019**, 150, 134102	3.9	7
148	Global topology of contact force networks: Insight into shear thickening suspensions. *Physical Review E*, **2019**, 99, 012607	2.4	7
147	Many-Body Effects Determine the Local Hydration Structure of Cs in Solution. *Journal of Physical Chemistry Letters*, **2019**, 10, 406-412	6.4	28
146	Water Lone Pair Delocalization in Classical and Quantum Descriptions of the Hydration of Model Ions. *Journal of Physical Chemistry B*, **2018**, 122, 3519-3527	3.4	17
145	Supersaturated calcium carbonate solutions are classical. *Science Advances*, **2018**, 4, eaao6283	14.3	75
144	On the relation between Marcus theory and ultrafast spectroscopy of solvation kinetics. *Chemical Physics Letters*, **2018**, 692, 407-415	2.5	9
143	Silver Nanocube and Nanobar Growth via Anisotropic Monomer Addition and Particle Attachment Processes. *Langmuir*, **2018**, 34, 1466-1472	4	8
142	In Situ Al NMR Spectroscopy of Aluminate in Sodium Hydroxide Solutions above and below Saturation with Respect to Gibbsite. *Inorganic Chemistry*, **2018**, 57, 11864-11873	5.1	23
141	Rate theory of ion pairing at the water liquid-vapor interface: A case of sodium iodide. *Journal of Chemical Physics*, **2018**, 148, 222820	3.9	4
140	Al Pulsed Field Gradient, Diffusion-NMR Spectroscopy of Solvation Dynamics and Ion Pairing in Alkaline Aluminate Solutions. *Journal of Physical Chemistry B*, **2018**, 122, 10907-10912	3.4	11
139	Unraveling the spectral signatures of solvent ordering in K-edge XANES of aqueous Na. *Journal of Chemical Physics*, **2018**, 149, 124503	3.9	7
138	Effects of Ionic Strength, Salt, and pH on Aggregation of Boehmite Nanocrystals: Tumbler Small-Angle Neutron and X-ray Scattering and Imaging Analysis. *Langmuir*, **2018**, 34, 15839-15853	4	20
137	Impact of Solution Chemistry and Particle Anisotropy on the Collective Dynamics of Oriented Aggregation. *ACS Nano*, **2018**, 12, 10114-10122	16.7	28

136	Ab Initio Molecular Dynamics Reveal Spectroscopic Siblings and Ion Pairing as New Challenges for Elucidating Prenucleation Aluminum Speciation. *Journal of Physical Chemistry B*, **2018**, 122, 7394-7402	3.4	25
135	Revisiting the hydration structure of aqueous Na. *Journal of Chemical Physics*, **2017**, 146, 084504	3.9	66
134	Probing equilibrium of molecular and deprotonated water on TiO(110). *Proceedings of the National Academy of Sciences of the United States of America*, **2017**, 114, 1801-1805	11.5	71
133	Rate Theory of Ion Pairing at the Water Liquid⁄Vapor Interface. *Journal of Physical Chemistry C*, **2017**, 121, 10018-10026	3.8	13
132	Electrostatic solvation free energies of charged hard spheres using molecular dynamics with density functional theory interactions. *Journal of Chemical Physics*, **2017**, 147, 161716	3.9	38
131	Marcus Theory of Ion-Pairing. *Journal of Chemical Theory and Computation*, **2017**, 13, 3470-3477	6.4	40
130	Real single ion solvation free energies with quantum mechanical simulation. *Chemical Science*, **2017** , 8, 6131-6140	9.4	49
129	Trends in mica-mica adhesion reflect the influence of molecular details on long-range dispersion forces underlying aggregation and coalignment. *Proceedings of the National Academy of Sciences of the United States of America*, **2017**, 114, 7537-7542	11.5	39
128	Mass density fluctuations in quantum and classical descriptions of liquid water. *Journal of Chemical Physics*, **2017**, 146, 244501	3.9	37
127	Molecular Dynamics Simulations and XAFS (MD-XAFS) **2017**, 251-270		6
126	Applying the scientific method to cybersecurity research **2016**,		3
125	Dependence of the Rate of LiF Ion-Pairing on the Description of Molecular Interaction. *Journal of Physical Chemistry B*, **2016**, 120, 1749-58	3.4	12
124	Solvent exchange in liquid methanol and rate theory. *Chemical Physics Letters*, **2016**, 643, 142-148	2.5	5
123	The structure of liquid water up to 360 MPa from x-ray diffraction measurements using a high Q-range and from molecular simulation. *Journal of Chemical Physics*, **2016**, 144, 134504	3.9	32
122	Reaction Rate Theory in Coordination Number Space: An Application to Ion Solvation. *Journal of Physical Chemistry C*, **2016**, 120, 7597-7605	3.8	31
121	Smoothed dissipative particle dynamics model for mesoscopic multiphase flows in the presence of thermal fluctuations. *Physical Review E*, **2016**, 94, 023304	2.4	7
120	The role of solvent heterogeneity in determining the dispersion interaction between nanoassemblies. *Journal of Physical Chemistry B*, **2015**, 119, 5873-81	3.4	20
119	Modeling nanoscale hydrodynamics by smoothed dissipative particle dynamics. *Journal of Chemical Physics*, **2015**, 142, 194504	3.9	15

118	Experimental and theoretical study of molecular response of amine bases in organic solvents. *Journal of Physical Chemistry B*, **2014**, 118, 4883-8	3.4	9
117	The Role of Broken Symmetry in Solvation of a Spherical Cavity in Classical and Quantum Water Models. *Journal of Physical Chemistry Letters*, **2014**, 5, 2767-74	6.4	64
116	Quantitatively probing the Al distribution in zeolites. *Journal of the American Chemical Society*, **2014**, 136, 8296-306	16.4	146
115	Persistent ion pairing in aqueous hydrochloric acid. *Journal of Physical Chemistry B*, **2014**, 118, 7211-20	3.4	49
114	The aqueous Ca2+ system, in comparison with Zn2+, Fe3+, and Al3+: an ab initio molecular dynamics study. *Chemistry - A European Journal*, **2013**, 19, 3047-60	4.8	36
113	Near-Quantitative Agreement of Model-Free DFT-MD Predictions with XAFS Observations of the Hydration Structure of Highly Charged Transition-Metal Ions. *Journal of Physical Chemistry Letters*, **2012**, 3, 2588-93	6.4	33
112	Understanding Vibrational Anharmonicity and Phonon Dispersion in Solid Ammonia Borane. *Journal of Physical Chemistry C*, **2012**, 116, 5926-5931	3.8	10
111	Role of Solvents on the Thermodynamics and Kinetics of Forming Frustrated Lewis Pairs. *Journal of Physical Chemistry Letters*, **2012**, 3, 3312-3319	6.4	19
110	Structure and hydrolysis of the U(IV), U(V), and U(VI) aqua ions from ab initio molecular simulations. *Inorganic Chemistry*, **2012**, 51, 3016-24	5.1	50
109	Analysis of the activation and heterolytic dissociation of H2 by frustrated Lewis pairs: NH3/BX3 (X = H, F, and Cl). *Journal of Physical Chemistry A*, **2012**, 116, 7228-37	2.8	47
108	Understanding the surface potential of water. *Journal of Physical Chemistry B*, **2011**, 115, 4369-77	3.4	136
107	Is Iodate a Strongly Hydrated Cation?. *Journal of Physical Chemistry Letters*, **2011**, 2, 2650-2654	6.4	60
106	Semiempirical self-consistent polarization description of bulk water, the liquid-vapor interface, and cubic ice. *Journal of Physical Chemistry A*, **2011**, 115, 6046-53	2.8	21
105	Hydration shell structure and dynamics of curium(III) in aqueous solution: first principles and empirical studies. *Journal of Physical Chemistry A*, **2011**, 115, 4665-77	2.8	49
104	Improving the density functional theory description of water with self-consistent polarization. *Journal of Chemical Physics*, **2010**, 132, 164102	3.9	30
103	Theoretical investigations on the formation and dehydrogenation reaction pathways of H(NH2BH2)(n)H (n = 1-4) oligomers: importance of dihydrogen interactions. *Inorganic Chemistry*, **2010**, 49, 7710-20	5.1	36
102	Probing the hydration structure of polarizable halides: a multiedge XAFS and molecular dynamics study of the iodide anion. *Journal of Physical Chemistry B*, **2010**, 114, 12926-37	3.4	68
101	The diammoniate of diborane: crystal structure and hydrogen release. *Chemical Communications*, **2010**, 46, 8564-6	5.8	44

100	Structure and dynamics of the hydration shells of the Zn(2+) ion from ab initio molecular dynamics and combined ab initio and classical molecular dynamics simulations. *Journal of Chemical Physics*, **2010**, 132, 194502	3.9	78
99	Experimental and computational studies on collective hydrogen dynamics in ammonia borane: incoherent inelastic neutron scattering. *Journal of Chemical Physics*, **2009**, 130, 024507	3.9	25
98	Self-consistent polarization density functional theory: application to argon. *Journal of Physical Chemistry A*, **2009**, 113, 2075-85	2.8	19
97	Interaction of ClO radical with liquid water. *Journal of the American Chemical Society*, **2009**, 131, 14778-85	16.4	16
96	The oil-water interface: mapping the solvation potential. *Journal of the American Chemical Society*, **2009**, 131, 1037-42	16.4	3
95	Hydrated structure of Ag(I) ion from symmetry-dependent, K- and L-edge XAFS multiple scattering and molecular dynamics simulations. *Journal of Physical Chemistry A*, **2009**, 113, 13976-84	2.8	46
94	Thermodynamic and Structural Investigations of Ammonium Borohydride, a Solid with a Highest Content of Thermodynamically and Kinetically Accessible Hydrogen. *Chemistry of Materials*, **2009**, 21, 4356-4358	9.6	48
93	Neutron powder diffraction and molecular simulation study of the structural evolution of ammonia borane from 15 to 340 K. *Journal of Physical Chemistry A*, **2009**, 113, 5723-35	2.8	53
92	Defining active catalyst structure and reaction pathways from ab initio molecular dynamics and operando XAFS: dehydrogenation of dimethylaminoborane by rhodium clusters. *Journal of the American Chemical Society*, **2009**, 131, 10516-24	16.4	63
91	Thermodynamics and Kinetics of Nanoclusters Controlling Gas-to-Particle Nucleation. *Journal of Physical Chemistry C*, **2009**, 113, 10354-10370	3.8	51
90	Spectroscopic studies of the phase transition in ammonia borane: Raman spectroscopy of single crystal NH3BH3 as a function of temperature from 88 to 330 K. *Journal of Chemical Physics*, **2008**, 128, 034508	3.9	80
89	Pyroelectricity of water ice. *Journal of Physical Chemistry B*, **2008**, 112, 6379-89	3.4	18
88	Materials for hydrogen storage: structure and dynamics of borane ammonia complex. *Dalton Transactions*, **2008**, 4514-22	4.3	41
87	On the determination of monomer dissociation energies of small water clusters from photoionization experiments. *Journal of Physical Chemistry A*, **2008**, 112, 1851-3	2.8	5
86	Molecular structure and dynamics in the low temperature (orthorhombic) phase of NH3BH3. *Journal of Physical Chemistry A*, **2008**, 112, 4277-83	2.8	30
85	Equatorial and apical solvent shells of the UO2 2+ ion. *Journal of Chemical Physics*, **2008**, 128, 124507	3.9	74
84	Self-consistent polarization neglect of diatomic differential overlap: application to water clusters. *Journal of Chemical Physics*, **2008**, 128, 164111	3.9	24
83	Activation energies and potentials of mean force for water cluster evaporation. *Journal of Chemical Physics*, **2008**, 128, 064306	3.9	10

82	Electron-driven acid-base chemistry: proton transfer from hydrogen chloride to ammonia. *Science*, **2008**, 319, 936-9	33.3	67
81	The Impact of Molecular Interactions on Atmospheric Aerosol Radiative Forcing. *Advances in Quantum Chemistry*, **2008**, 55, 429-447	1.4	5
80	Many-body decomposition of the binding energies for OH.(H2O)2 and OH.(H2O)3 complexes. *Journal of Chemical Physics*, **2008**, 128, 084307	3.9	13
79	A molecular approach to understanding complex systems: computational statistical mechanics using state-of-the-art algorithms on terascale computational platforms. *Journal of Physics: Conference Series*, **2008**, 125, 012014	0.3	0
78	Isomers and Conformers of H(NH2BH2)nH Oligomers: Understanding the Geometries and Electronic Structure of Boron□Nitrogen□Hydrogen Compounds as Potential Hydrogen Storage Materials. *Journal of Physical Chemistry C*, **2007**, 111, 3294-3299	3.8	38
77	The Critical Role of Anharmonicity in Aqueous Ionic Clusters Relevant to Nucleation. *Journal of Physical Chemistry C*, **2007**, 111, 4977-4983	3.8	35
76	Ab initio and analytical intermolecular potential for ClO-H2O. *Journal of Chemical Physics*, **2007**, 126, 114304	3.9	10
75	Comment on "Quantum nature of the sign preference in ion-induced nucleation". *Physical Review Letters*, **2007**, 98, 109603; discussion 109604	7.4	11
74	Hybrid approach for free energy calculations with high-level methods: application to the SN2 reaction of CHCl3 and OH- in water. *Journal of Chemical Physics*, **2007**, 127, 051102	3.9	69
73	Electronic structure, statistical mechanical simulations, and EXAFS spectroscopy of aqueous potassium. *Theoretical Chemistry Accounts*, **2006**, 115, 86-99	1.9	54
72	A quantitative account of quantum effects in liquid water. *Journal of Chemical Physics*, **2006**, 125, 141102	3.9	74
71	Critical comparison of classical and quantum mechanical treatments of the phase equilibria of water. *Journal of Chemical Physics*, **2006**, 124, 114505	3.9	8
70	The OH radical-H2O molecular interaction potential. *Journal of Chemical Physics*, **2006**, 124, 224318	3.9	66
69	Molecular simulations of the transport of molecules across the liquid/vapor interface of water. *Chemical Reviews*, **2006**, 106, 1355-74	68.1	120
68	Molecular simulation analysis and X-ray absorption measurement of Ca2+, K+ and Cl- ions in solution. *Journal of Physical Chemistry B*, **2006**, 110, 23644-54	3.4	107
67	Sensitivity analysis of thermodynamic properties of liquid water: a general approach to improve empirical potentials. *Journal of Physical Chemistry A*, **2006**, 110, 762-71	2.8	18
66	Role of water in electron-initiated processes and radical chemistry: issues and scientific advances. *Chemical Reviews*, **2005**, 105, 355-90	68.1	469
65	Ion-induced nucleation: the importance of chemistry. *Physical Review Letters*, **2005**, 94, 116104	7.4	52

64	Helium diffusion through H2O and D2O amorphous ice: observation of a lattice inverse isotope effect. *Physical Review Letters*, **2004**, 92, 198306	7.4	11
63	Multicomponent dynamical nucleation theory and sensitivity analysis. *Journal of Chemical Physics*, **2004**, 120, 9133-41	3.9	25
62	Intermolecular potential and second virial coefficient of the water-hydrogen complex. *Journal of Chemical Physics*, **2004**, 120, 710-20	3.9	73
61	Nanosurface enhanced Raman scattering fluctuation dynamics **2003**, 4962, 70		5
60	Potentials of mean force with ab initio mixed Hamiltonian models of solvation. *Computational and Theoretical Chemistry*, **2003**, 632, 173-183		10
59	Probing nanoscale surface enhanced Raman-scattering fluctuation dynamics using correlated AFM and confocal ultramicroscopy. *Ultramicroscopy*, **2003**, 97, 89-102	3.1	46
58	EXAFS Spectra of the Dilute Solutions of Ca2+ and Sr2+ in Water and Methanol. *Journal of Physical Chemistry B*, **2003**, 107, 14119-14123	3.4	40
57	Thermochemistry and Kinetics of Evaporation and Condensation for Small Water Clusters. *Springer Series in Cluster Physics*, **2003**, 25-51		
56	Generalized transition state theory in terms of the potential of mean force. *Journal of Chemical Physics*, **2003**, 119, 5828-5833	3.9	100
55	The development of effective classical potentials and the quantum statistical mechanical second virial coefficient of water. *Journal of Chemical Physics*, **2002**, 117, 6573-6581	3.9	40
54	Understanding the sensitivity of nucleation kinetics: A case study on water. *Journal of Chemical Physics*, **2002**, 116, 5046	3.9	56
53	Equilibrium Constant for Water Dimerization: Analysis of the Partition Function for a Weakly Bound System. *Journal of Physical Chemistry A*, **2002**, 106, 1557-1566	2.8	41
52	Dynamical benchmarks of the nucleation kinetics of water. *Journal of Chemical Physics*, **2002**, 116, 4275-4280	3.9	36
51	Variational transition state theory evaluation of the rate constant for proton transfer in a polar solvent. *Journal of Chemical Physics*, **2001**, 115, 8460-8480	3.9	51
50	Sculpting the Oil/Water Interface to Probe Ion Solvation. *Journal of Physical Chemistry B*, **2001**, 105, 2483-2498	3.4	7
49	The Role of Collective Solvent Coordinates and Nonequilibrium Solvation in Charge-Transfer Reactions. *Journal of Physical Chemistry B*, **2001**, 105, 9672-9685	3.4	52
48	The quantum vibrational dynamics of Cl(H2O)n clusters. *Journal of Chemical Physics*, **2000**, 113, 5171	3.9	33
47	Statistical Analyses and Theoretical Models of Single-Molecule Enzymatic Dynamics. *Journal of Physical Chemistry A*, **1999**, 103, 10477-10488	2.8	124

46	Stimulated Desorption by Surface Electron Standing Waves. *Physical Review Letters*, **1999**, 82, 3348-3351	7.4	9
45	XAFS Debye-Waller factors in aqueous Cr+3 from molecular dynamics. *Journal of Synchrotron Radiation*, **1999**, 6, 310-2	2.4	47
44	Dynamical Nucleation Theory: A New Molecular Approach to Vapor-Liquid Nucleation. *Physical Review Letters*, **1999**, 82, 3484-3487	7.4	111
43	Variational transition state theory of vapor phase nucleation. *Journal of Chemical Physics*, **1999**, 110, 7951-7959	3.9	45
42	Dynamical nucleation theory: Calculation of condensation rate constants for small water clusters. *Journal of Chemical Physics*, **1999**, 111, 4688-4697	3.9	42
41	A quantum statistical mechanical study of the enthalpy of formation of the water dimer. *Journal of Chemical Physics*, **1998**, 108, 6222-6232	3.9	27
40	Prediction of extended x-ray-absorption fine-structure spectra from molecular interaction models: Na+(H2O)n/MgO(100) interface. *Physical Review B*, **1997**, 56, 9925-9936	3.3	29
39	Dynamic solvent effects on activated chemical reactions PartII. Quantum mechanicaleffects. *Journal of the Chemical Society, Faraday Transactions*, **1997**, 93, 997-1009		8
38	Generalized path integral based quantum transition state theory. *Chemical Physics Letters*, **1997**, 278, 91-96	2.5	98
37	Structure and Dynamics of the Water/MgO Interface. *The Journal of Physical Chemistry*, **1996**, 100, 16989-16995		102
36	Natural Energy Decomposition Analysis: The Linear Response Electrical Self Energy. *The Journal of Physical Chemistry*, **1996**, 100, 17152-17156		116
35	Quantum statistical mechanical simulation of the ion/water cluster I(H2O)n: The importance of nuclear quantum effects and anharmonicity. *Journal of Chemical Physics*, **1996**, 105, 8835-8841	3.9	44
34	Quantum simulation of high-density amorphous ice. *Physical Review B*, **1996**, 54, 14873-14876	3.3	10
33	Classical and quantum mechanical studies of ice Ih near the melting temperature. *Journal of Chemical Physics*, **1996**, 104, 680-685	3.9	22
32	Electron-phonon scattering contributions to metallic resistivity at 0 K. *Physical Review B*, **1996**, 54, 16591-16601	3.3	4
31	A variational centroid density procedure for the calculation of transmission coefficients for asymmetric barriers at low temperature. *Journal of Chemical Physics*, **1995**, 103, 3430-3435	3.9	39
30	The reactive flux method in the energy diffusion regime. II. Importance of the solvent's spectral profile. *Journal of Chemical Physics*, **1995**, 102, 104-118	3.9	28
29	Quantum Simulation of Aqueous Ionic Clusters. *The Journal of Physical Chemistry*, **1995**, 99, 13303-13306		25

28	Reversible work transition state theory: application to dissociative adsorption of hydrogen. *Surface Science*, **1995**, 324, 305-337	1.8	1699
27	Excited States of the Bacteriochlorophyll b Dimer of Rhodopseudomonas viridis: A QM/MM Study of the Photosynthetic Reaction Center That Includes MM Polarization. *The Journal of Physical Chemistry*, **1995**, 99, 6374-6386		252
26	Tunneling in the Presence of a Bath: A Generalized Transition State Theory Approach. *The Journal of Physical Chemistry*, **1994**, 98, 8396-8405		68
25	Variational solutions for the thermal and real time propagator using the McLachlan variational principle. *Journal of Chemical Physics*, **1994**, 100, 6570-6577	3.9	12
24	Reversible work based quantum transition state theory. *Journal of Chemical Physics*, **1994**, 101, 8964-8973	3.9	64
23	Variational transition state theory for activated chemical reactions in solution. *International Reviews in Physical Chemistry*, **1994**, 13, 263-289	7	29
22	Nonequilibrium Solvation for an Aqueous-Phase Reaction. *ACS Symposium Series*, **1994**, 122-142	0.4	11
21	Inclusion of nonequilibrium continuum solvation effects in variational transition state theory. *Journal of Chemical Physics*, **1993**, 98, 5756-5770	3.9	57
20	Quantum activated rate theory: Variational optimization of planar dividing surfaces. *Journal of Chemical Physics*, **1993**, 99, 8644-8653	3.9	22
19	Approximate path integral methods for partition functions. *Journal of Chemical Physics*, **1993**, 98, 4120-4127	3.9	22
18	Centroid-density quantum rate theory: Dynamical treatment of classical recrossing. *Journal of Chemical Physics*, **1993**, 99, 1674-1684	3.9	28
17	Centroid-density quantum rate theory: Variational optimization of the dividing surface. *Journal of Chemical Physics*, **1993**, 98, 8525-8536	3.9	39
16	Critical comparison of approximate and accurate quantum-mechanical calculations of rate constants for a model activated reaction in solution. *Journal of Chemical Physics*, **1992**, 97, 7392-7404	3.9	42
15	Dynamic solvent effects on activated chemical reactions. I. Classical effects of reaction path curvature. *Journal of Chemical Physics*, **1992**, 97, 9116-9137	3.9	33
14	Semiconductor surface and interface dynamics from tight-binding molecular dynamics simulations. *Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films*, **1992**, 10, 2429-2435	2.9	12
13	The electronic structure and conformation of dimethylaminobenzonitrile. *Structural Chemistry*, **1992**, 3, 9-14	1.8	1
12	Theory of photoinduced twisting dynamics in polar solvents: application to dimethylaminobenzonitrile in propanol at low temperatures. *Chemical Physics Letters*, **1991**, 176, 563-570	2.5	22
11	Twisted intramolecular charge transfer and the torsional potential function of dimethylaminobenzonitrile. *Journal of Chemical Physics*, **1991**, 94, 7558-7559	3.9	7

10	Analytic distribution for charge carriers in a semiconductor dominated by equivalent intervalley scattering. *Physical Review B*, **1989**, 40, 5624-5631	3.3	2
9	Distribution functions and fluid variables in a semiconductor. *Journal of Applied Physics*, **1988**, 63, 5363-5368	2.5	8
8	Nonlinear electrical conductivity for a strongly coupled plasma. *Physics of Fluids*, **1987**, 30, 1789		2
7	Quasiclassical kinetic equation for charge-carrier transport in a semiconductor. *Journal of Applied Physics*, **1987**, 62, 177-184	2.5	7
6	Solution of a new nonlinear equation for the distribution of charge carriers in a semiconductor. *Physical Review B*, **1986**, 34, 7063-7068	3.3	11
5	Unified equation of state for weakly and strongly coupled laboratory plasmas. *Physical Review A*, **1986**, 34, 3217-3220	2.6	4
4	Fundamental relativistic solution for the rail gun. *Journal of Applied Physics*, **1986**, 59, 1749-1751	2.5	1
3	Criterion for phase change in terms of oscillation of the pair distribution function. *Journal of Chemical Physics*, **1986**, 84, 7005-7008	3.9	2
2	A Simple Approximation of the Fermi Function in Nuclear Beta Decay. *Nuclear Science and Engineering*, **1983**, 83, 393-396	1.2	34
1	Reactor antineutrino spectra and their application to antineutrino-induced reactions. II. *Physical Review C*, **1981**, 24, 1543-1553	2.7	173