Gregory K Schenter

List of Publications by Year
in descending order

175 papers	10,569 citations	38660 50 h-index	34900 98 g-index
180 all docs	180 docs citations	180 times ranked	10194 citing authors

#	Article	IF	Citations
1	²⁷Al NMR diffusometry of Al₁₃ Keggin nanoclusters. Magnetic Resonance in Chemistry, 2022, 60, 226-238.	1.1	3
2	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.	1.5	4
3	Toward a First-Principles Framework for Predicting Collective Properties of Electrolytes. Accounts of Chemical Research, 2021, 54, 2833-2843.	7.6	21
4	Visualizing Solution Structure at Solid-Liquid Interfaces using Three-Dimensional Fast Force Mapping. Journal of Visualized Experiments, 2021, , .	0.2	1
5	The Statistical Mechanics ofÂSolution-Phase Nucleation: CaCO$$_3$$ Revisited. Molecular Modeling and Simulation, 2021, , 101-122.	0.2	1
6	Shear stress dependence of force networks in 3D dense suspensions. Soft Matter, 2021, 17, 7476-7486.	1.2	9
7	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.	1.5	31
8	Theory-Guided Inelastic Neutron Scattering of Crystalline Alkaline Aluminate Salts Bearing Principal Motifs of Solution-State Species. Inorganic Chemistry, 2021, 60, 16223-16232.	1.9	4
9	Quantifying the hydration structure of sodium and potassium ions: taking additional steps on Jacob's Ladder. Physical Chemistry Chemical Physics, 2020, 22, 10641-10652.	1.3	38
10	Heterolytic Scission of Hydrogen Within a Crystalline Frustrated Lewis Pair. Inorganic Chemistry, 2020, 59, 15295-15301.	1.9	8
11	Mechanisms of Al³⁺ Dimerization in Alkaline Solutions. Inorganic Chemistry, 2020, 59, 18181-18189.	1.9	8
12	Solvent reaction coordinate for an SN2 reaction. Journal of Chemical Physics, 2020, 153, 024103.	1.2	11
13	Correlation function approach for diffusion in confined geometries. Physical Review E, 2020, 102, 022129.	0.8	6
14	Resolving Heterogeneous Dynamics of Excess Protons in Aqueous Solution with Rate Theory. Journal of Physical Chemistry B, 2020, 124, 5665-5675.	1.2	17
15	Al27 NMR chemical shift of Al(OH)4â˜ calculated from first principles: Assessment of error cancellation in chemically distinct reference and target systems. Journal of Chemical Physics, 2020, 152, 134303.	1.2	3
16	CP2K: An electronic structure and molecular dynamics software package - Quickstep: Efficient and accurate electronic structure calculations. Journal of Chemical Physics, 2020, 152, 194103.	1.2	1,371
17	Nanometer-Scale Correlations in Aqueous Salt Solutions. Journal of Physical Chemistry Letters, 2020, 11, 2598-2604.	2.1	10
18	Method for Accurately Predicting Solvation Structure. Journal of Chemical Theory and Computation, 2020, 16, 5401-5409.	2.3	12

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19	Connecting energetics to dynamics in particle growth by oriented attachment using real-time observations. Nature Communications, 2020, 11, 1045.	5.8	74
20	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.	6.6	24
21	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.	5.0	18
22	Inference of principal species in caustic aluminate solutions through solid-state spectroscopic characterization. Dalton Transactions, 2020, 49, 5869-5880.	1.6	10
23	Resolving local configurational contributions to X-ray and neutron radial distribution functions within solutions of concentrated electrolytes â€“ a case study of concentrated NaOH. Physical Chemistry Chemical Physics, 2019, 21, 6828-6838.	1.3	14
24	Effect of fine-tuning pore structures on the dynamics of confined water. Journal of Chemical Physics, 2019, 150, 204706.	1.2	10
25	PageRank as a collective variable to study complex chemical transformations and their energy landscapes. Journal of Chemical Physics, 2019, 150, 134102.	1.2	10
26	Global topology of contact force networks: Insight into shear thickening suspensions. Physical Review E, 2019, 99, 012607.	0.8	8
27	Many-Body Effects Determine the Local Hydration Structure of Cs⁺ in Solution. Journal of Physical Chemistry Letters, 2019, 10, 406-412.	2.1	45
28	Water Lone Pair Delocalization in Classical and Quantum Descriptions of the Hydration of Model Ions. Journal of Physical Chemistry B, 2018, 122, 3519-3527.	1.2	27
29	Supersaturated calcium carbonate solutions are classical. Science Advances, 2018, 4, eaao6283.	4.7	116
30	On the relation between Marcus theory and ultrafast spectroscopy of solvation kinetics. Chemical Physics Letters, 2018, 692, 407-415.	1.2	10
31	Silver Nanocube and Nanobar Growth via Anisotropic Monomer Addition and Particle Attachment Processes. Langmuir, 2018, 34, 1466-1472.	1.6	13
32	²⁷Al Pulsed Field Gradient, Diffusionâ€“NMR Spectroscopy of Solvation Dynamics and Ion Pairing in Alkaline Aluminate Solutions. Journal of Physical Chemistry B, 2018, 122, 10907-10912.	1.2	15
33	Unraveling the spectral signatures of solvent ordering in K-edge XANES of aqueous Na+. Journal of Chemical Physics, 2018, 149, 124503.	1.2	12
34	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.	1.6	25
35	Impact of Solution Chemistry and Particle Anisotropy on the Collective Dynamics of Oriented Aggregation. ACS Nano, 2018, 12, 10114-10122.	7.3	40
36	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.	1.2	34

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37	In Situ ²⁷Al NMR Spectroscopy of Aluminate in Sodium Hydroxide Solutions above and below Saturation with Respect to Gibbsite. Inorganic Chemistry, 2018, 57, 11864-11873.	1.9	33
38	Rate theory of ion pairing at the water liquidâ€“vapor interface: A case of sodium iodide. Journal of Chemical Physics, 2018, 148, 222820.	1.2	5
39	Revisiting the hydration structure of aqueous Na+. Journal of Chemical Physics, 2017, 146, 084504.	1.2	90
40	Probing equilibrium of molecular and deprotonated water on TiO ₂ (110). Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, 1801-1805.	3.3	90
41	Rate Theory of Ion Pairing at the Water Liquidâ€“Vapor Interface. Journal of Physical Chemistry C, 2017, 121, 10018-10026.	1.5	15
42	Electrostatic solvation free energies of charged hard spheres using molecular dynamics with density functional theory interactions. Journal of Chemical Physics, 2017, 147, 161716.	1.2	42
43	Marcus Theory of Ion-Pairing. Journal of Chemical Theory and Computation, 2017, 13, 3470-3477.	2.3	53
44	Real single ion solvation free energies with quantum mechanical simulation. Chemical Science, 2017, 8, 6131-6140.	3.7	63
45	Trends in micaâ€“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.	3.3	56
46	Mass density fluctuations in quantum and classical descriptions of liquid water. Journal of Chemical Physics, 2017, 146, 244501.	1.2	44
47	Molecular Dynamics Simulations and XAFS (MD-XAFS). , 2017, , 251-270.		6
48	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.	1.2	38
49	Reaction Rate Theory in Coordination Number Space: An Application to Ion Solvation. Journal of Physical Chemistry C, 2016, 120, 7597-7605.	1.5	36
50	Smoothed dissipative particle dynamics model for mesoscopic multiphase flows in the presence of thermal fluctuations. Physical Review E, 2016, 94, 023304.	0.8	11
51	Applying the scientific method to cybersecurity research. , 2016, , .		4
52	Dependence of the Rate of LiF Ion-Pairing on the Description of Molecular Interaction. Journal of Physical Chemistry B, 2016, 120, 1749-1758.	1.2	13
53	Solvent exchange in liquid methanol and rate theory. Chemical Physics Letters, 2016, 643, 142-148.	1.2	5
54	The Role of Solvent Heterogeneity in Determining the Dispersion Interaction between Nanoassemblies. Journal of Physical Chemistry B, 2015, 119, 5873-5881.	1.2	26

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55	Modeling nanoscale hydrodynamics by smoothed dissipative particle dynamics. Journal of Chemical Physics, 2015, 142, 194504.	1.2	17
56	Experimental and Theoretical Study of Molecular Response of Amine Bases in Organic Solvents. Journal of Physical Chemistry B, 2014, 118, 4883-4888.	1.2	9
57	The Role of Broken Symmetry in Solvation of a Spherical Cavity in Classical and Quantum Water Models. Journal of Physical Chemistry Letters, 2014, 5, 2767-2774.	2.1	71
58	Quantitatively Probing the Al Distribution in Zeolites. Journal of the American Chemical Society, 2014, 136, 8296-8306.	6.6	199
59	Persistent Ion Pairing in Aqueous Hydrochloric Acid. Journal of Physical Chemistry B, 2014, 118, 7211-7220.	1.2	53
60	The Aqueous Ca²⁺ System, in Comparison with Zn²⁺, Fe^{3 +}, and Al^{3 +}: An Abâ€...Initio Molecular Dynamics Study. Chemistry - A European Journal, 2013, 19, 3047-3060.	1.7	45
61	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, 2588-2593.	2.1	40
62	Understanding Vibrational Anharmonicity and Phonon Dispersion in Solid Ammonia Borane. Journal of Physical Chemistry C, 2012, 116, 5926-5931.	1.5	10
63	Role of Solvents on the Thermodynamics and Kinetics of Forming Frustrated Lewis Pairs. Journal of Physical Chemistry Letters, 2012, 3, 3312-3319.	2.1	20
64	Structure and Hydrolysis of the U(IV), U(V), and U(VI) Aqua Ions from Ab Initio Molecular Simulations. Inorganic Chemistry, 2012, 51, 3016-3024.	1.9	58
65	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, 7228-7237.	1.1	51
66	Hydration Shell Structure and Dynamics of Curium(III) in Aqueous Solution: First Principles and Empirical Studies. Journal of Physical Chemistry A, 2011, 115, 4665-4677.	1.1	52
67	Understanding the Surface Potential of Water. Journal of Physical Chemistry B, 2011, 115, 4369-4377.	1.2	157
68	Is Iodate a Strongly Hydrated Cation?. Journal of Physical Chemistry Letters, 2011, 2, 2650-2654.	2.1	68
69	Semiempirical Self-Consistent Polarization Description of Bulk Water, the Liquidâ^'Vapor Interface, and Cubic Ice. Journal of Physical Chemistry A, 2011, 115, 6046-6053.	1.1	22
70	Improving the density functional theory description of water with self-consistent polarization. Journal of Chemical Physics, 2010, 132, 164102.	1.2	30
71	Theoretical Investigations on the Formation and Dehydrogenation Reaction Pathways of H(NH₂BH₂)_nH (n = 1â^'4) Oligomers: Importance of Dihydrogen Interactions. Inorganic Chemistry, 2010, 49, 7710-7720.	1.9	38
72	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, 12926-12937.	1.2	78

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73	The diammoniate of diborane: crystal structure and hydrogen release. Chemical Communications, 2010, 46, 8564.	2.2	47
74	Structure and dynamics of the hydration shells of the Zn2+ ion from ab initio molecular dynamics and combined ab initio and classical molecular dynamics simulations. Journal of Chemical Physics, 2010, 132, 194502.	1.2	95
75	Experimental and computational studies on collective hydrogen dynamics in ammonia borane: Incoherent inelastic neutron scattering. Journal of Chemical Physics, 2009, 130, 024507.	1.2	25
76	Self-Consistent Polarization Density Functional Theory: Application to Argon. Journal of Physical Chemistry A, 2009, 113, 2075-2085.	1.1	19
77	Interaction of ClO Radical with Liquid Water. Journal of the American Chemical Society, 2009, 131, 14778-14785.	6.6	20
78	The Oilâˆ'Water Interface: Mapping the Solvation Potential. Journal of the American Chemical Society, 2009, 131, 1037-1042.	6.6	3
79	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, 13976-13984.	1.1	51
80	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.	3.2	55
81	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, 5723-5735.	1.1	56
82	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, 10516-10524.	6.6	67
83	Thermodynamics and Kinetics of Nanoclusters Controlling Gas-to-Particle Nucleation. Journal of Physical Chemistry C, 2009, 113, 10354-10370.	1.5	59
84	Spectroscopic studies of the phase transition in ammonia borane: Raman spectroscopy of single crystal NH3BH3 as a function of temperature from 88to330K. Journal of Chemical Physics, 2008, 128, 034508.	1.2	90
85	Pyroelectricity of Water Ice. Journal of Physical Chemistry B, 2008, 112, 6379-6389.	1.2	22
86	Materials for hydrogen storage: structure and dynamics of borane ammonia complex. Dalton Transactions, 2008, , 4514.	1.6	43
87	On the Determination of Monomer Dissociation Energies of Small Water Clusters from Photoionization Experiments. Journal of Physical Chemistry A, 2008, 112, 1851-1853.	1.1	5
88	Molecular Structure and Dynamics in the Low Temperature (Orthorhombic) Phase of NH3BH3. Journal of Physical Chemistry A, 2008, 112, 4277-4283.	1.1	32
89	Equatorial and apical solvent shells of the UO22+ ion. Journal of Chemical Physics, 2008, 128, 124507.	1.2	79
90	Self-consistent polarization neglect of diatomic differential overlap: Application to water clusters. Journal of Chemical Physics, 2008, 128, 164111.	1.2	24

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91	Activation energies and potentials of mean force for water cluster evaporation. Journal of Chemical Physics, 2008, 128, 064306.	1.2	12
92	Electron-Driven Acid-Base Chemistry: Proton Transfer from Hydrogen Chloride to Ammonia. Science, 2008, 319, 936-939.	6.0	73
93	The Impact of Molecular Interactions on Atmospheric Aerosol Radiative Forcing. Advances in Quantum Chemistry, 2008, 55, 429-447.	0.4	5
94	Many-body decomposition of the binding energies for OHâ‹…(H2O)2 and OHâ‹…(H2O)3 complexes. Journal of Chemical Physics, 2008, 128, 084307.	1.2	13
95	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	1
96	Ab initio and analytical intermolecular potential for ClOâ€“H2O. Journal of Chemical Physics, 2007, 126, 114304.	1.2	11
97	Comment on â€œQuantum Nature of the Sign Preference in Ion-Induced Nucleationâ€. Physical Review Letters, 2007, 98, 109603; discussion 109604.	2.9	11
98	Hybrid approach for free energy calculations with high-level methods: Application to the SN2 reaction of CHCl3 and OHâ^' in water. Journal of Chemical Physics, 2007, 127, 051102.	1.2	70
99	Isomers and Conformers of H(NH2BH2)nH Oligomers:â€‰ Understanding the Geometries and Electronic Structure of Boronâ^'Nitrogenâ^'Hydrogen Compounds as Potential Hydrogen Storage Materials. Journal of Physical Chemistry C, 2007, 111, 3294-3299.	1.5	38
100	The Critical Role of Anharmonicity in Aqueous Ionic Clusters Relevant to Nucleation. Journal of Physical Chemistry C, 2007, 111, 4977-4983.	1.5	35
101	Molecular Simulations of the Transport of Molecules across the Liquid/Vapor Interface of Water. Chemical Reviews, 2006, 106, 1355-1374.	23.0	134
102	Molecular Simulation Analysis and X-ray Absorption Measurement of Ca2+, K+and Cl-Ions in Solution. Journal of Physical Chemistry B, 2006, 110, 23644-23654.	1.2	115
103	Sensitivity Analysis of Thermodynamic Properties of Liquid Water:Â A General Approach to Improve Empirical Potentialsâ€. Journal of Physical Chemistry A, 2006, 110, 762-771.	1.1	18
104	Electronic structure, statistical mechanical simulations, and EXAFS spectroscopy of aqueous potassium. Theoretical Chemistry Accounts, 2006, 115, 86-99.	0.5	63
105	A quantitative account of quantum effects in liquid water. Journal of Chemical Physics, 2006, 125, 141102.	1.2	77
106	Critical comparison of classical and quantum mechanical treatments of the phase equilibria of water. Journal of Chemical Physics, 2006, 124, 114505.	1.2	8
107	The OH radical-H2O molecular interaction potential. Journal of Chemical Physics, 2006, 124, 224318.	1.2	67
108	Ion-Induced Nucleation: The Importance of Chemistry. Physical Review Letters, 2005, 94, 116104.	2.9	56

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109	Role of Water in Electron-Initiated Processes and Radical Chemistry:â€‰ Issues and Scientific Advances. Chemical Reviews, 2005, 105, 355-390.	23.0	560
110	Helium Diffusion throughH2OandD2OAmorphous Ice: Observation of a Lattice Inverse Isotope Effect. Physical Review Letters, 2004, 92, 198306.	2.9	12
111	Multicomponent dynamical nucleation theory and sensitivity analysis. Journal of Chemical Physics, 2004, 120, 9133-9141.	1.2	26
112	Intermolecular potential and second virial coefficient of the waterâ€“hydrogen complex. Journal of Chemical Physics, 2004, 120, 710-720.	1.2	82
113	Potentials of mean force with ab initio mixed Hamiltonian models of solvation. Computational and Theoretical Chemistry, 2003, 632, 173-183.	1.5	10
114	Probing nanoscale surface enhanced Raman-scattering fluctuation dynamics using correlated AFM and confocal ultramicroscopy. Ultramicroscopy, 2003, 97, 89-102.	0.8	47
115	EXAFS Spectra of the Dilute Solutions of Ca2+ and Sr2+ in Water and Methanol. Journal of Physical Chemistry B, 2003, 107, 14119-14123.	1.2	41
116	Thermochemistry and Kinetics of Evaporation and Condensation for Small Water Clusters. Springer Series in Cluster Physics, 2003, , 25-51.	0.3	1
117	Generalized transition state theory in terms of the potential of mean force. Journal of Chemical Physics, 2003, 119, 5828-5833.	1.2	110
118	Nanosurface enhanced Raman scattering fluctuation dynamics. , 2003, 4962, 70.		6
119	The development of effective classical potentials and the quantum statistical mechanical second virial coefficient of water. Journal of Chemical Physics, 2002, 117, 6573-6581.	1.2	46
120	Understanding the sensitivity of nucleation kinetics: A case study on water. Journal of Chemical Physics, 2002, 116, 5046.	1.2	61
121	Equilibrium Constant for Water Dimerization:â€‰ Analysis of the Partition Function for a Weakly Bound System. Journal of Physical Chemistry A, 2002, 106, 1557-1566.	1.1	46
122	Dynamical benchmarks of the nucleation kinetics of water. Journal of Chemical Physics, 2002, 116, 4275-4280.	1.2	46
123	Sculpting the Oilâˆ'Water Interface to Probe Ion Solvation. Journal of Physical Chemistry B, 2001, 105, 2483-2498.	1.2	7
124	The Role of Collective Solvent Coordinates and Nonequilibrium Solvation in Charge-Transfer Reactions. Journal of Physical Chemistry B, 2001, 105, 9672-9685.	1.2	55
125	Variational transition state theory evaluation of the rate constant for proton transfer in a polar solvent. Journal of Chemical Physics, 2001, 115, 8460-8480.	1.2	54
126	Dynamical nucleation theory. AIP Conference Proceedings, 2000, , .	0.3	1

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127	Kinetics of cluster evaporation and condensation important in homogeneous vapor phase nucleation. AIP Conference Proceedings, 2000, , .	0.3	0
128	The quantum vibrational dynamics of Cl[sup â^'](H[sub 2]O)[sub n] clusters. Journal of Chemical Physics, 2000, 113, 5171.	1.2	33
129	Statistical Analyses and Theoretical Models of Single-Molecule Enzymatic Dynamics. Journal of Physical Chemistry A, 1999, 103, 10477-10488.	1.1	130
130	Stimulated Desorption by Surface Electron Standing Waves. Physical Review Letters, 1999, 82, 3348-3351.	2.9	11
131	XAFS Debyeâ€“Waller factors in aqueous Cr+3 from molecular dynamics. Journal of Synchrotron Radiation, 1999, 6, 310-312.	1.0	52
132	Dynamical Nucleation Theory: A New Molecular Approach to Vapor-Liquid Nucleation. Physical Review Letters, 1999, 82, 3484-3487.	2.9	123
133	Variational transition state theory of vapor phase nucleation. Journal of Chemical Physics, 1999, 110, 7951-7959.	1.2	47
134	Dynamical nucleation theory: Calculation of condensation rate constants for small water clusters. Journal of Chemical Physics, 1999, 111, 4688-4697.	1.2	46
135	A quantum statistical mechanical study of the enthalpy of formation of the water dimer. Journal of Chemical Physics, 1998, 108, 6222-6232.	1.2	29
136	Prediction of extended x-ray-absorption fine-structure spectra from molecular interaction models:Na+(H2O)nâ^'MgO(100) interface. Physical Review B, 1997, 56, 9925-9936.	1.1	34
137	Dynamic solvent effects on activated chemical reactions Part II.â€”Quantum mechanical effects. Journal of the Chemical Society, Faraday Transactions, 1997, 93, 997-1009.	1.7	9
138	Generalized path integral based quantum transition state theory. Chemical Physics Letters, 1997, 278, 91-96.	1.2	105
139	Natural Energy Decomposition Analysis:Â The Linear Response Electrical Self Energy. The Journal of Physical Chemistry, 1996, 100, 17152-17156.	2.9	131
140	Quantum statistical mechanical simulation of the ionâ€“water cluster Iâ^'(H2O)n: The importance of nuclear quantum effects and anharmonicity. Journal of Chemical Physics, 1996, 105, 8835-8841.	1.2	45
141	Quantum simulation of high-density amorphous ice. Physical Review B, 1996, 54, 14873-14876.	1.1	10
142	Classical and quantum mechanical studies of ice Ih near the melting temperature. Journal of Chemical Physics, 1996, 104, 680-685.	1.2	22
143	Electron-phonon scattering contributions to metallic resistivity at 0 K. Physical Review B, 1996, 54, 16591-16601.	1.1	7
144	Structure and Dynamics of the Water/MgO Interface. The Journal of Physical Chemistry, 1996, 100, 16989-16995.	2.9	110

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145	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.	1.2	39
146	The reactive flux method in the energy diffusion regime. II. Importance of the solventâ€™s spectral profile. Journal of Chemical Physics, 1995, 102, 104-118.	1.2	30
147	Quantum Simulation of Aqueous Ionic Clusters. The Journal of Physical Chemistry, 1995, 99, 13303-13306.	2.9	25
148	Reversible work transition state theory: application to dissociative adsorption of hydrogen. Surface Science, 1995, 324, 305-337.	0.8	1,953
149	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.	2.9	278
150	Tunneling in the Presence of a Bath: A Generalized Transition State Theory Approach. The Journal of Physical Chemistry, 1994, 98, 8396-8405.	2.9	73
151	Variational solutions for the thermal and real time propagator using the McLachlan variational principle. Journal of Chemical Physics, 1994, 100, 6570-6577.	1.2	12
152	Reversible work based quantum transition state theory. Journal of Chemical Physics, 1994, 101, 8964-8971.	1.2	72
153	Variational transition state theory for activated chemical reactions in solution. International Reviews in Physical Chemistry, 1994, 13, 263-289.	0.9	33
154	Nonequilibrium Solvation for an Aqueous-Phase Reaction. ACS Symposium Series, 1994, , 122-142.	0.5	12
155	Inclusion of nonequilibrium continuum solvation effects in variational transition state theory. Journal of Chemical Physics, 1993, 98, 5756-5770.	1.2	60
156	Quantum activated rate theory: Variational optimization of planar dividing surfaces. Journal of Chemical Physics, 1993, 99, 8644-8653.	1.2	22
157	Approximate path integral methods for partition functions. Journal of Chemical Physics, 1993, 98, 4120-4127.	1.2	24
158	Centroidâ€density quantum rate theory: Dynamical treatment of classical recrossing. Journal of Chemical Physics, 1993, 99, 1674-1684.	1.2	31
159	Centroidâ€density quantum rate theory: Variational optimization of the dividing surface. Journal of Chemical Physics, 1993, 98, 8525-8536.	1.2	39
160	Critical comparison of approximate and accurate quantumâ€mechanical calculations of rate constants for a model activated reaction in solution. Journal of Chemical Physics, 1992, 97, 7392-7404.	1.2	47
161	Dynamic solvent effects on activated chemical reactions. I. Classical effects of reaction path curvature. Journal of Chemical Physics, 1992, 97, 9116-9137.	1.2	35
162	Semiconductor surface and interface dynamics from tightâ€binding molecular dynamics simulations. Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films, 1992, 10, 2429-2435.	0.9	13

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163	The electronic structure and conformation of dimethylaminobenzonitrile. Structural Chemistry, 1992, 3, 9-14.	1.0	1
164	Twisted intramolecular charge transfer and the torsional potential function of dimethylaminobenzonitrile. Journal of Chemical Physics, 1991, 94, 7558-7559.	1.2	8
165	Theory of photoinduced twisting dynamics in polar solvents: application to dimethylaminobenzonitrile in propanol at low temperatures. Chemical Physics Letters, 1991, 176, 563-570.	1.2	23
166	Analytic distribution for charge carriers in a semiconductor dominated by equivalent intervalley scattering. Physical Review B, 1989, 40, 5624-5631.	1.1	2
167	Distribution functions and fluid variables in a semiconductor. Journal of Applied Physics, 1988, 63, 5363-5368.	1.1	0
168	Nonlinear electrical conductivity for a strongly coupled plasma. Physics of Fluids, 1987, 30, 1789.	1.4	2
169	Quasiclassical kinetic equation for chargeâ€carrier transport in a semiconductor. Journal of Applied Physics, 1987, 62, 177-184.	1.1	8
170	Criterion for phase change in terms of oscillation of the pair distribution function. Journal of Chemical Physics, 1986, 84, 7005-7008.	1.2	2
171	Solution of a new nonlinear equation for the distribution of charge carriers in a semiconductor. Physical Review B, 1986, 34, 7063-7068.	1.1	12
172	Unified equation of state for weakly and strongly coupled laboratory plasmas. Physical Review A, 1986, 34, 3217-3220.	1.0	4
173	Fundamental relativistic solution for the rail gun. Journal of Applied Physics, 1986, 59, 1749-1751.	1.1	1
174	A Simple Approximation of the Fermi Function in Nuclear Beta Decay. Nuclear Science and Engineering, 1983, 83, 393-396.	0.5	40
175	Reactor antineutrino spectra and their application to antineutrino-induced reactions. II. Physical Review C, 1981, 24, 1543-1553.	1.1	194