

Gregory K Schenter

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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	Reversible work transition state theory: application to dissociative adsorption of hydrogen. <i>Surface Science</i> , 1995 , 324, 305-337	1.8	1699
170	Role of water in electron-initiated processes and radical chemistry: issues and scientific advances. <i>Chemical Reviews</i> , 2005 , 105, 355-90	68.1	469
169	CP2K: An electronic structure and molecular dynamics software package - Quickstep: Efficient and accurate electronic structure calculations. <i>Journal of Chemical Physics</i> , 2020 , 152, 194103	3.9	421
168	Excited States of the Bacteriochlorophyll b Dimer of Rhodospseudomonas viridis: A QM/MM Study of the Photosynthetic Reaction Center That Includes MM Polarization. <i>The Journal of Physical Chemistry</i> , 1995 , 99, 6374-6386		252
167	Reactor antineutrino spectra and their application to antineutrino-induced reactions. II. <i>Physical Review C</i> , 1981 , 24, 1543-1553	2.7	173
166	Quantitatively probing the Al distribution in zeolites. <i>Journal of the American Chemical Society</i> , 2014 , 136, 8296-306	16.4	146
165	Understanding the surface potential of water. <i>Journal of Physical Chemistry B</i> , 2011 , 115, 4369-77	3.4	136
164	Statistical Analyses and Theoretical Models of Single-Molecule Enzymatic Dynamics. <i>Journal of Physical Chemistry A</i> , 1999 , 103, 10477-10488	2.8	124
163	Molecular simulations of the transport of molecules across the liquid/vapor interface of water. <i>Chemical Reviews</i> , 2006 , 106, 1355-74	68.1	120
162	Natural Energy Decomposition Analysis: The Linear Response Electrical Self Energy. <i>The Journal of Physical Chemistry</i> , 1996 , 100, 17152-17156		116
161	Dynamical Nucleation Theory: A New Molecular Approach to Vapor-Liquid Nucleation. <i>Physical Review Letters</i> , 1999 , 82, 3484-3487	7.4	111
160	Molecular simulation analysis and X-ray absorption measurement of Ca ²⁺ , K ⁺ and Cl ⁻ ions in solution. <i>Journal of Physical Chemistry B</i> , 2006 , 110, 23644-54	3.4	107
159	Structure and Dynamics of the Water/MgO Interface. <i>The Journal of Physical Chemistry</i> , 1996 , 100, 16989-16995		102
158	Generalized transition state theory in terms of the potential of mean force. <i>Journal of Chemical Physics</i> , 2003 , 119, 5828-5833	3.9	100
157	Generalized path integral based quantum transition state theory. <i>Chemical Physics Letters</i> , 1997 , 278, 91-96	2.5	98
156	Spectroscopic studies of the phase transition in ammonia borane: Raman spectroscopy of single crystal NH ₃ BH ₃ as a function of temperature from 88 to 330 K. <i>Journal of Chemical Physics</i> , 2008 , 128, 034508	3.9	80
155	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. <i>Journal of Chemical Physics</i> , 2010 , 132, 194502	3.9	78

154	Supersaturated calcium carbonate solutions are classical. <i>Science Advances</i> , 2018 , 4, eaao6283	14.3	75
153	Equatorial and apical solvent shells of the UO ₂ ²⁺ ion. <i>Journal of Chemical Physics</i> , 2008 , 128, 124507	3.9	74
152	A quantitative account of quantum effects in liquid water. <i>Journal of Chemical Physics</i> , 2006 , 125, 141102	3.9	74
151	Intermolecular potential and second virial coefficient of the water-hydrogen complex. <i>Journal of Chemical Physics</i> , 2004 , 120, 710-20	3.9	73
150	Probing equilibrium of molecular and deprotonated water on TiO(110). <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2017 , 114, 1801-1805	11.5	71
149	Hybrid approach for free energy calculations with high-level methods: application to the SN ₂ reaction of CHCl ₃ and OH ⁻ in water. <i>Journal of Chemical Physics</i> , 2007 , 127, 051102	3.9	69
148	Probing the hydration structure of polarizable halides: a multiedge XAFS and molecular dynamics study of the iodide anion. <i>Journal of Physical Chemistry B</i> , 2010 , 114, 12926-37	3.4	68
147	Tunneling in the Presence of a Bath: A Generalized Transition State Theory Approach. <i>The Journal of Physical Chemistry</i> , 1994 , 98, 8396-8405		68
146	Electron-driven acid-base chemistry: proton transfer from hydrogen chloride to ammonia. <i>Science</i> , 2008 , 319, 936-9	33.3	67
145	Revisiting the hydration structure of aqueous Na. <i>Journal of Chemical Physics</i> , 2017 , 146, 084504	3.9	66
144	The OH radical-H ₂ O molecular interaction potential. <i>Journal of Chemical Physics</i> , 2006 , 124, 224318	3.9	66
143	The Role of Broken Symmetry in Solvation of a Spherical Cavity in Classical and Quantum Water Models. <i>Journal of Physical Chemistry Letters</i> , 2014 , 5, 2767-74	6.4	64
142	Reversible work based quantum transition state theory. <i>Journal of Chemical Physics</i> , 1994 , 101, 8964-8973	3.9	64
141	Defining active catalyst structure and reaction pathways from ab initio molecular dynamics and operando XAFS: dehydrogenation of dimethylaminoborane by rhodium clusters. <i>Journal of the American Chemical Society</i> , 2009 , 131, 10516-24	16.4	63
140	Is Iodate a Strongly Hydrated Cation?. <i>Journal of Physical Chemistry Letters</i> , 2011 , 2, 2650-2654	6.4	60
139	Inclusion of nonequilibrium continuum solvation effects in variational transition state theory. <i>Journal of Chemical Physics</i> , 1993 , 98, 5756-5770	3.9	57
138	Understanding the sensitivity of nucleation kinetics: A case study on water. <i>Journal of Chemical Physics</i> , 2002 , 116, 5046	3.9	56
137	Electronic structure, statistical mechanical simulations, and EXAFS spectroscopy of aqueous potassium. <i>Theoretical Chemistry Accounts</i> , 2006 , 115, 86-99	1.9	54

136	Neutron powder diffraction and molecular simulation study of the structural evolution of ammonia borane from 15 to 340 K. <i>Journal of Physical Chemistry A</i> , 2009 , 113, 5723-35	2.8	53
135	Ion-induced nucleation: the importance of chemistry. <i>Physical Review Letters</i> , 2005 , 94, 116104	7.4	52
134	The Role of Collective Solvent Coordinates and Nonequilibrium Solvation in Charge-Transfer Reactions. <i>Journal of Physical Chemistry B</i> , 2001 , 105, 9672-9685	3.4	52
133	Thermodynamics and Kinetics of Nanoclusters Controlling Gas-to-Particle Nucleation. <i>Journal of Physical Chemistry C</i> , 2009 , 113, 10354-10370	3.8	51
132	Variational transition state theory evaluation of the rate constant for proton transfer in a polar solvent. <i>Journal of Chemical Physics</i> , 2001 , 115, 8460-8480	3.9	51
131	Structure and hydrolysis of the U(IV), U(V), and U(VI) aqua ions from ab initio molecular simulations. <i>Inorganic Chemistry</i> , 2012 , 51, 3016-24	5.1	50
130	Persistent ion pairing in aqueous hydrochloric acid. <i>Journal of Physical Chemistry B</i> , 2014 , 118, 7211-20	3.4	49
129	Real single ion solvation free energies with quantum mechanical simulation. <i>Chemical Science</i> , 2017 , 8, 6131-6140	9.4	49
128	Hydration shell structure and dynamics of curium(III) in aqueous solution: first principles and empirical studies. <i>Journal of Physical Chemistry A</i> , 2011 , 115, 4665-77	2.8	49
127	Thermodynamic and Structural Investigations of Ammonium Borohydride, a Solid with a Highest Content of Thermodynamically and Kinetically Accessible Hydrogen. <i>Chemistry of Materials</i> , 2009 , 21, 4356-4358	9.6	48
126	Analysis of the activation and heterolytic dissociation of H ₂ by frustrated Lewis pairs: NH ₃ /BX ₃ (X = H, F, and Cl). <i>Journal of Physical Chemistry A</i> , 2012 , 116, 7228-37	2.8	47
125	XAFS Debye-Waller factors in aqueous Cr ³⁺ from molecular dynamics. <i>Journal of Synchrotron Radiation</i> , 1999 , 6, 310-2	2.4	47
124	Hydrated structure of Ag(I) ion from symmetry-dependent, K- and L-edge XAFS multiple scattering and molecular dynamics simulations. <i>Journal of Physical Chemistry A</i> , 2009 , 113, 13976-84	2.8	46
123	Probing nanoscale surface enhanced Raman-scattering fluctuation dynamics using correlated AFM and confocal ultramicroscopy. <i>Ultramicroscopy</i> , 2003 , 97, 89-102	3.1	46
122	Connecting energetics to dynamics in particle growth by oriented attachment using real-time observations. <i>Nature Communications</i> , 2020 , 11, 1045	17.4	45
121	Variational transition state theory of vapor phase nucleation. <i>Journal of Chemical Physics</i> , 1999 , 110, 7951-7959	3.9	45
120	The diammoniate of diborane: crystal structure and hydrogen release. <i>Chemical Communications</i> , 2010 , 46, 8564-6	5.8	44
119	Quantum statistical mechanical simulation of the ion-water cluster I ⁻ (H ₂ O) _n : The importance of nuclear quantum effects and anharmonicity. <i>Journal of Chemical Physics</i> , 1996 , 105, 8835-8841	3.9	44

118	Dynamical nucleation theory: Calculation of condensation rate constants for small water clusters. <i>Journal of Chemical Physics</i> , 1999 , 111, 4688-4697	3.9	42
117	Critical comparison of approximate and accurate quantum-mechanical calculations of rate constants for a model activated reaction in solution. <i>Journal of Chemical Physics</i> , 1992 , 97, 7392-7404	3.9	42
116	Materials for hydrogen storage: structure and dynamics of borane ammonia complex. <i>Dalton Transactions</i> , 2008 , 4514-22	4.3	41
115	Equilibrium Constant for Water Dimerization: Analysis of the Partition Function for a Weakly Bound System. <i>Journal of Physical Chemistry A</i> , 2002 , 106, 1557-1566	2.8	41
114	Marcus Theory of Ion-Pairing. <i>Journal of Chemical Theory and Computation</i> , 2017 , 13, 3470-3477	6.4	40
113	EXAFS Spectra of the Dilute Solutions of Ca ²⁺ and Sr ²⁺ in Water and Methanol. <i>Journal of Physical Chemistry B</i> , 2003 , 107, 14119-14123	3.4	40
112	The development of effective classical potentials and the quantum statistical mechanical second virial coefficient of water. <i>Journal of Chemical Physics</i> , 2002 , 117, 6573-6581	3.9	40
111	Trends in mica-mica adhesion reflect the influence of molecular details on long-range dispersion forces underlying aggregation and coalignment. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2017 , 114, 7537-7542	11.5	39
110	A variational centroid density procedure for the calculation of transmission coefficients for asymmetric barriers at low temperature. <i>Journal of Chemical Physics</i> , 1995 , 103, 3430-3435	3.9	39
109	Centroid-density quantum rate theory: Variational optimization of the dividing surface. <i>Journal of Chemical Physics</i> , 1993 , 98, 8525-8536	3.9	39
108	Electrostatic solvation free energies of charged hard spheres using molecular dynamics with density functional theory interactions. <i>Journal of Chemical Physics</i> , 2017 , 147, 161716	3.9	38
107	Isomers and Conformers of H(NH ₂ BH ₂) _n H Oligomers: Understanding the Geometries and Electronic Structure of Boron-Nitrogen-Hydrogen Compounds as Potential Hydrogen Storage Materials. <i>Journal of Physical Chemistry C</i> , 2007 , 111, 3294-3299	3.8	38
106	Mass density fluctuations in quantum and classical descriptions of liquid water. <i>Journal of Chemical Physics</i> , 2017 , 146, 244501	3.9	37
105	The aqueous Ca ²⁺ system, in comparison with Zn ²⁺ , Fe ³⁺ , and Al ³⁺ : an ab initio molecular dynamics study. <i>Chemistry - A European Journal</i> , 2013 , 19, 3047-60	4.8	36
104	Theoretical investigations on the formation and dehydrogenation reaction pathways of H(NH ₂ BH ₂) _(n) H (n = 1-4) oligomers: importance of dihydrogen interactions. <i>Inorganic Chemistry</i> , 2010 , 49, 7710-20	5.1	36
103	Dynamical benchmarks of the nucleation kinetics of water. <i>Journal of Chemical Physics</i> , 2002 , 116, 4275-4280	3.9	36
102	The Critical Role of Anharmonicity in Aqueous Ionic Clusters Relevant to Nucleation. <i>Journal of Physical Chemistry C</i> , 2007 , 111, 4977-4983	3.8	35
101	A Simple Approximation of the Fermi Function in Nuclear Beta Decay. <i>Nuclear Science and Engineering</i> , 1983 , 83, 393-396	1.2	34

100	Near-Quantitative Agreement of Model-Free DFT-MD Predictions with XAFS Observations of the Hydration Structure of Highly Charged Transition-Metal Ions. <i>Journal of Physical Chemistry Letters</i> , 2012 , 3, 2588-93	6.4	33
99	The quantum vibrational dynamics of Cl(H ₂ O) _n clusters. <i>Journal of Chemical Physics</i> , 2000 , 113, 5171	3.9	33
98	Dynamic solvent effects on activated chemical reactions. I. Classical effects of reaction path curvature. <i>Journal of Chemical Physics</i> , 1992 , 97, 9116-9137	3.9	33
97	The structure of liquid water up to 360 MPa from x-ray diffraction measurements using a high Q-range and from molecular simulation. <i>Journal of Chemical Physics</i> , 2016 , 144, 134504	3.9	32
96	Reaction Rate Theory in Coordination Number Space: An Application to Ion Solvation. <i>Journal of Physical Chemistry C</i> , 2016 , 120, 7597-7605	3.8	31
95	Improving the density functional theory description of water with self-consistent polarization. <i>Journal of Chemical Physics</i> , 2010 , 132, 164102	3.9	30
94	Molecular structure and dynamics in the low temperature (orthorhombic) phase of NH ₃ BH ₃ . <i>Journal of Physical Chemistry A</i> , 2008 , 112, 4277-83	2.8	30
93	Prediction of extended x-ray-absorption fine-structure spectra from molecular interaction models: Na+(H ₂ O) _n MgO(100) interface. <i>Physical Review B</i> , 1997 , 56, 9925-9936	3.3	29
92	Variational transition state theory for activated chemical reactions in solution. <i>International Reviews in Physical Chemistry</i> , 1994 , 13, 263-289	7	29
91	The reactive flux method in the energy diffusion regime. II. Importance of the solvent's spectral profile. <i>Journal of Chemical Physics</i> , 1995 , 102, 104-118	3.9	28
90	Centroid-density quantum rate theory: Dynamical treatment of classical recrossing. <i>Journal of Chemical Physics</i> , 1993 , 99, 1674-1684	3.9	28
89	Many-Body Effects Determine the Local Hydration Structure of Cs in Solution. <i>Journal of Physical Chemistry Letters</i> , 2019 , 10, 406-412	6.4	28
88	Impact of Solution Chemistry and Particle Anisotropy on the Collective Dynamics of Oriented Aggregation. <i>ACS Nano</i> , 2018 , 12, 10114-10122	16.7	28
87	A quantum statistical mechanical study of the enthalpy of formation of the water dimer. <i>Journal of Chemical Physics</i> , 1998 , 108, 6222-6232	3.9	27
86	Experimental and computational studies on collective hydrogen dynamics in ammonia borane: incoherent inelastic neutron scattering. <i>Journal of Chemical Physics</i> , 2009 , 130, 024507	3.9	25
85	Multicomponent dynamical nucleation theory and sensitivity analysis. <i>Journal of Chemical Physics</i> , 2004 , 120, 9133-41	3.9	25
84	Quantum Simulation of Aqueous Ionic Clusters. <i>The Journal of Physical Chemistry</i> , 1995 , 99, 13303-13306		25
83	Ab Initio Molecular Dynamics Reveal Spectroscopic Siblings and Ion Pairing as New Challenges for Elucidating Prenucleation Aluminum Speciation. <i>Journal of Physical Chemistry B</i> , 2018 , 122, 7394-7402	3.4	25

82	Self-consistent polarization neglect of diatomic differential overlap: application to water clusters. <i>Journal of Chemical Physics</i> , 2008 , 128, 164111	3.9	24
81	Quantifying the hydration structure of sodium and potassium ions: taking additional steps on Jacob's Ladder. <i>Physical Chemistry Chemical Physics</i> , 2020 , 22, 10641-10652	3.6	24
80	In Situ Al NMR Spectroscopy of Aluminate in Sodium Hydroxide Solutions above and below Saturation with Respect to Gibbsite. <i>Inorganic Chemistry</i> , 2018 , 57, 11864-11873	5.1	23
79	Classical and quantum mechanical studies of ice Ih near the melting temperature. <i>Journal of Chemical Physics</i> , 1996 , 104, 680-685	3.9	22
78	Quantum activated rate theory: Variational optimization of planar dividing surfaces. <i>Journal of Chemical Physics</i> , 1993 , 99, 8644-8653	3.9	22
77	Approximate path integral methods for partition functions. <i>Journal of Chemical Physics</i> , 1993 , 98, 4120-4127	3.9	22
76	Theory of photoinduced twisting dynamics in polar solvents: application to dimethylaminobenzonitrile in propanol at low temperatures. <i>Chemical Physics Letters</i> , 1991 , 176, 563-570	2.5	22
75	Semiempirical self-consistent polarization description of bulk water, the liquid-vapor interface, and cubic ice. <i>Journal of Physical Chemistry A</i> , 2011 , 115, 6046-53	2.8	21
74	The role of solvent heterogeneity in determining the dispersion interaction between nanoassemblies. <i>Journal of Physical Chemistry B</i> , 2015 , 119, 5873-81	3.4	20
73	Moving beyond the Solvent-Tip Approximation to Determine Site-Specific Variations of Interfacial Water Structure through 3D Force Microscopy. <i>Journal of Physical Chemistry C</i> , 2021 , 125, 1282-1291	3.8	20
72	Effects of Ionic Strength, Salt, and pH on Aggregation of Boehmite Nanocrystals: Tumbler Small-Angle Neutron and X-ray Scattering and Imaging Analysis. <i>Langmuir</i> , 2018 , 34, 15839-15853	4	20
71	Role of Solvents on the Thermodynamics and Kinetics of Forming Frustrated Lewis Pairs. <i>Journal of Physical Chemistry Letters</i> , 2012 , 3, 3312-3319	6.4	19
70	Self-consistent polarization density functional theory: application to argon. <i>Journal of Physical Chemistry A</i> , 2009 , 113, 2075-85	2.8	19
69	Pyroelectricity of water ice. <i>Journal of Physical Chemistry B</i> , 2008 , 112, 6379-89	3.4	18
68	Sensitivity analysis of thermodynamic properties of liquid water: a general approach to improve empirical potentials. <i>Journal of Physical Chemistry A</i> , 2006 , 110, 762-71	2.8	18
67	Water Lone Pair Delocalization in Classical and Quantum Descriptions of the Hydration of Model Ions. <i>Journal of Physical Chemistry B</i> , 2018 , 122, 3519-3527	3.4	17
66	Interaction of ClO radical with liquid water. <i>Journal of the American Chemical Society</i> , 2009 , 131, 14778-85	6.4	16
65	Modeling nanoscale hydrodynamics by smoothed dissipative particle dynamics. <i>Journal of Chemical Physics</i> , 2015 , 142, 194504	3.9	15

64	Toward a First-Principles Framework for Predicting Collective Properties of Electrolytes. <i>Accounts of Chemical Research</i> , 2021 , 54, 2833-2843	24.3	14
63	Rate Theory of Ion Pairing at the Water Liquid-Vapor Interface. <i>Journal of Physical Chemistry C</i> , 2017 , 121, 10018-10026	3.8	13
62	Many-body decomposition of the binding energies for OH.(H ₂ O) ₂ and OH.(H ₂ O) ₃ complexes. <i>Journal of Chemical Physics</i> , 2008 , 128, 084307	3.9	13
61	Dependence of the Rate of LiF Ion-Pairing on the Description of Molecular Interaction. <i>Journal of Physical Chemistry B</i> , 2016 , 120, 1749-58	3.4	12
60	Variational solutions for the thermal and real time propagator using the McLachlan variational principle. <i>Journal of Chemical Physics</i> , 1994 , 100, 6570-6577	3.9	12
59	Semiconductor surface and interface dynamics from tight-binding molecular dynamics simulations. <i>Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films</i> , 1992 , 10, 2429-2435	2.9	12
58	Visualization of Aluminum Ions at the Mica Water Interface Links Hydrolysis State-to-Surface Potential and Particle Adhesion. <i>Journal of the American Chemical Society</i> , 2020 , 142, 6093-6102	16.4	11
57	Comment on "Quantum nature of the sign preference in ion-induced nucleation". <i>Physical Review Letters</i> , 2007 , 98, 109603; discussion 109604	7.4	11
56	Helium diffusion through H ₂ O and D ₂ O amorphous ice: observation of a lattice inverse isotope effect. <i>Physical Review Letters</i> , 2004 , 92, 198306	7.4	11
55	Nonequilibrium Solvation for an Aqueous-Phase Reaction. <i>ACS Symposium Series</i> , 1994 , 122-142	0.4	11
54	Solution of a new nonlinear equation for the distribution of charge carriers in a semiconductor. <i>Physical Review B</i> , 1986 , 34, 7063-7068	3.3	11
53	Al Pulsed Field Gradient, Diffusion-NMR Spectroscopy of Solvation Dynamics and Ion Pairing in Alkaline Aluminate Solutions. <i>Journal of Physical Chemistry B</i> , 2018 , 122, 10907-10912	3.4	11
52	Resolving local configurational contributions to X-ray and neutron radial distribution functions within solutions of concentrated electrolytes - a case study of concentrated NaOH. <i>Physical Chemistry Chemical Physics</i> , 2019 , 21, 6828-6838	3.6	10
51	Resolving Heterogeneous Dynamics of Excess Protons in Aqueous Solution with Rate Theory. <i>Journal of Physical Chemistry B</i> , 2020 , 124, 5665-5675	3.4	10
50	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. <i>Journal of Colloid and Interface Science</i> , 2020 , 576, 47-58	9.3	10
49	Understanding Vibrational Anharmonicity and Phonon Dispersion in Solid Ammonia Borane. <i>Journal of Physical Chemistry C</i> , 2012 , 116, 5926-5931	3.8	10
48	Activation energies and potentials of mean force for water cluster evaporation. <i>Journal of Chemical Physics</i> , 2008 , 128, 064306	3.9	10
47	Ab initio and analytical intermolecular potential for ClO-H ₂ O. <i>Journal of Chemical Physics</i> , 2007 , 126, 114304	3.9	10

46	Potentials of mean force with ab initio mixed Hamiltonian models of solvation. <i>Computational and Theoretical Chemistry</i> , 2003 , 632, 173-183		10
45	Quantum simulation of high-density amorphous ice. <i>Physical Review B</i> , 1996 , 54, 14873-14876	3.3	10
44	On the relation between Marcus theory and ultrafast spectroscopy of solvation kinetics. <i>Chemical Physics Letters</i> , 2018 , 692, 407-415	2.5	9
43	Experimental and theoretical study of molecular response of amine bases in organic solvents. <i>Journal of Physical Chemistry B</i> , 2014 , 118, 4883-8	3.4	9
42	Stimulated Desorption by Surface Electron Standing Waves. <i>Physical Review Letters</i> , 1999 , 82, 3348-3351	7.4	9
41	Method for Accurately Predicting Solvation Structure. <i>Journal of Chemical Theory and Computation</i> , 2020 , 16, 5401-5409	6.4	8
40	Silver Nanocube and Nanobar Growth via Anisotropic Monomer Addition and Particle Attachment Processes. <i>Langmuir</i> , 2018 , 34, 1466-1472	4	8
39	Dynamic solvent effects on activated chemical reactions Part II. Quantum mechanical effects. <i>Journal of the Chemical Society, Faraday Transactions</i> , 1997 , 93, 997-1009		8
38	Critical comparison of classical and quantum mechanical treatments of the phase equilibria of water. <i>Journal of Chemical Physics</i> , 2006 , 124, 114505	3.9	8
37	PageRank as a collective variable to study complex chemical transformations and their energy landscapes. <i>Journal of Chemical Physics</i> , 2019 , 150, 134102	3.9	7
36	Nanometer-Scale Correlations in Aqueous Salt Solutions. <i>Journal of Physical Chemistry Letters</i> , 2020 , 11, 2598-2604	6.4	7
35	Sculpting the Oil/Water Interface to Probe Ion Solvation. <i>Journal of Physical Chemistry B</i> , 2001 , 105, 2483-2498	3.4	7
34	Twisted intramolecular charge transfer and the torsional potential function of dimethylaminobenzonitrile. <i>Journal of Chemical Physics</i> , 1991 , 94, 7558-7559	3.9	7
33	Quasiclassical kinetic equation for charge-carrier transport in a semiconductor. <i>Journal of Applied Physics</i> , 1987 , 62, 177-184	2.5	7
32	Smoothed dissipative particle dynamics model for mesoscopic multiphase flows in the presence of thermal fluctuations. <i>Physical Review E</i> , 2016 , 94, 023304	2.4	7
31	Global topology of contact force networks: Insight into shear thickening suspensions. <i>Physical Review E</i> , 2019 , 99, 012607	2.4	7
30	Unraveling the spectral signatures of solvent ordering in K-edge XANES of aqueous Na. <i>Journal of Chemical Physics</i> , 2018 , 149, 124503	3.9	7
29	Molecular Dynamics Simulations and XAFS (MD-XAFS) 2017 , 251-270		6

28	Inference of principal species in caustic aluminate solutions through solid-state spectroscopic characterization. <i>Dalton Transactions</i> , 2020 , 49, 5869-5880	4.3	6
27	Effect of fine-tuning pore structures on the dynamics of confined water. <i>Journal of Chemical Physics</i> , 2019 , 150, 204706	3.9	5
26	Solvent exchange in liquid methanol and rate theory. <i>Chemical Physics Letters</i> , 2016 , 643, 142-148	2.5	5
25	On the determination of monomer dissociation energies of small water clusters from photoionization experiments. <i>Journal of Physical Chemistry A</i> , 2008 , 112, 1851-3	2.8	5
24	The Impact of Molecular Interactions on Atmospheric Aerosol Radiative Forcing. <i>Advances in Quantum Chemistry</i> , 2008 , 55, 429-447	1.4	5
23	Nanosurface enhanced Raman scattering fluctuation dynamics 2003 , 4962, 70		5
22	Heterolytic Scission of Hydrogen Within a Crystalline Frustrated Lewis Pair. <i>Inorganic Chemistry</i> , 2020 , 59, 15295-15301	5.1	5
21	Electron-phonon scattering contributions to metallic resistivity at 0 K. <i>Physical Review B</i> , 1996 , 54, 16591-16601	5.3	4
20	Unified equation of state for weakly and strongly coupled laboratory plasmas. <i>Physical Review A</i> , 1986 , 34, 3217-3220	2.6	4
19	Rate theory of ion pairing at the water liquid-vapor interface: A case of sodium iodide. <i>Journal of Chemical Physics</i> , 2018 , 148, 222820	3.9	4
18	Solvent reaction coordinate for an S ₂ reaction. <i>Journal of Chemical Physics</i> , 2020 , 153, 024103	3.9	4
17	Applying the scientific method to cybersecurity research 2016 ,		3
16	The oil-water interface: mapping the solvation potential. <i>Journal of the American Chemical Society</i> , 2009 , 131, 1037-42	16.4	3
15	Correlation function approach for diffusion in confined geometries. <i>Physical Review E</i> , 2020 , 102, 022129	2.4	3
14	Analytic distribution for charge carriers in a semiconductor dominated by equivalent intervalley scattering. <i>Physical Review B</i> , 1989 , 40, 5624-5631	3.3	2
13	Nonlinear electrical conductivity for a strongly coupled plasma. <i>Physics of Fluids</i> , 1987 , 30, 1789		2
12	Criterion for phase change in terms of oscillation of the pair distribution function. <i>Journal of Chemical Physics</i> , 1986 , 84, 7005-7008	3.9	2
11	Frustrated Coulombic and Cation Size Effects on Nanoscale Boehmite Aggregation: A Tumbler Small- and Ultra-Small-Angle Neutron Scattering Study. <i>Journal of Physical Chemistry C</i> , 2022 , 126, 4391-4414	2.8	2

10	Al ²⁷ NMR chemical shift of Al(OH) calculated from first principles: Assessment of error cancellation in chemically distinct reference and target systems. <i>Journal of Chemical Physics</i> , 2020 , 152, 134303	3.9	1
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