

The nature and transport mechanism of hydrated hydro

Nature

417, 925-929

DOI: 10.1038/nature00797

Citation Report

#	ARTICLE	IF	CITATIONS
3	Ab initio molecular dynamics study of proton mobility in liquid methanol. Journal of Chemical Physics, 2002, 117, 4403-4413.	3.0	135
4	Solvation Structure and Mobility Mechanism of OH ⁻ : A Car ⁺ Parrinello Molecular Dynamics Investigation of Alkaline Solutions. Journal of Physical Chemistry B, 2002, 106, 12006-12016.	2.6	105
5	Ab Initio Molecular Dynamics Investigation of the Concentration Dependence of Charged Defect Transport in Basic Solutions via Calculation of the Infrared Spectrum. Journal of Physical Chemistry B, 2002, 106, 8009-8018.	2.6	78
6	Ab initio molecular dynamics: basic concepts, current trends and novel applications. Journal of Physics Condensed Matter, 2002, 14, R1297-R1355.	1.8	232
7	Argon predissociation infrared spectroscopy of the hydroxide-water complex (OH ⁻ ·H ₂ O). Chemical Physics Letters, 2002, 366, 412-416.	2.6	57
8	Das Transportverhalten hydratisierter Hydroxid-Ionen in Wasser. Angewandte Chemie, 2003, 115, 268-271.	2.0	10
9	Car ⁺ Parrinello Molecular Dynamics Study of the Rearrangement of the Valeramide Radical Cation. Chemistry - A European Journal, 2003, 9, 4396-4404.	3.3	8
10	New Insight into the Transport Mechanism of Hydrated Hydroxide Ions in Water. Angewandte Chemie - International Edition, 2003, 42, 258-260.	13.8	77
11	The hydration state of HO ⁺ (aq). Chemical Physics Letters, 2003, 380, 530-535.	2.6	59
12	Ab initio path integral study of isotope effect of hydronium ion. Chemical Physics Letters, 2003, 374, 229-234.	2.6	20
13	Stewart and beyond: New models of acid-base balance. Kidney International, 2003, 64, 777-787.	5.2	162
14	Hydrogen falls into line. Nature, 2003, 423, 595-596.	27.8	0
16	Phosphotransfer networks and cellular energetics. Journal of Experimental Biology, 2003, 206, 2039-2047.	1.7	432
17	Ab Initio Molecular Dynamics Computation of the Infrared Spectrum of Aqueous Uracil. Journal of Physical Chemistry B, 2003, 107, 10344-10358.	2.6	245
18	Solvation of hydroxyl ions in water. Journal of Chemical Physics, 2003, 119, 5001-5004.	3.0	76
19	Three-Fragment Counterpoise Correction of Potential Energy Curves for Proton-Transfer Reactions. Journal of Physical Chemistry A, 2003, 107, 7589-7596.	2.5	28
20	Hydrogen Bonding in Water. Physical Review Letters, 2003, 91, 215503.	7.8	284
21	The Mechanism of Proton Exclusion in the Aquaporin-1 Water Channel. Journal of Molecular Biology, 2003, 333, 279-293.	4.2	257

#	ARTICLE	IF	CITATIONS
22	Low resonant frequency storage and transfer in structured water cluster. , 0, , .		3
23	Nuclear Quantum Effects and Hydrogen Bonding in Liquids. Journal of the American Chemical Society, 2003, 125, 8992-8993.	13.7	70
24	From ab initio quantum chemistry to molecular dynamics: The delicate case of hydrogen bonding in ammonia. Journal of Chemical Physics, 2003, 119, 5965-5980.	3.0	153
25	Ammonia-chain clusters: Vibronic spectra of 7-hydroxyquinolineâ€¦(NH ₃) ₂ . Journal of Chemical Physics, 2003, 119, 3774-3784.	3.0	15
26	Spectroscopic Determination of the OH- Solvation Shell in the OH-middle dot(H ₂ O) _n Clusters. Science, 2003, 299, 1367-1372.	12.6	355
27	Algorithms and novel applications based on the isokinetic ensemble. II. Ab initio molecular dynamics. Journal of Chemical Physics, 2003, 118, 2527.	3.0	19
28	Quantum mechanical/molecular mechanical studies of a novel reaction catalyzed by proton transfers in ambient and supercritical states of water. Journal of Chemical Physics, 2003, 119, 7964-7971.	3.0	39
29	Hybrid quantum chemical studies for the methanol formation reaction assisted by the proton transfer mechanism in supercritical water: CH ₃ Cl+nH ₂ Oâ†’CH ₃ OH+HCl+(nâˆ’1)H ₂ O. Journal of Chemical Physics, 2003, 119, 8492-8499.	3.0	20
30	Torsional path integral Monte Carlo method for calculating the absolute quantum free energy of large molecules. Journal of Chemical Physics, 2003, 119, 68-76.	3.0	36
31	Voltage-Gated Proton Channels and Other Proton Transfer Pathways. Physiological Reviews, 2003, 83, 475-579.	28.8	635
33	H atom transfer along an ammonia chain: Tunneling and mode selectivity in 7-hydroxyquinolineâ€¦(NH ₃) ₃ . Journal of Chemical Physics, 2004, 121, 2578.	3.0	42
34	On-the-fly localization of electronic orbitals in Carâ€”Parrinello molecular dynamics. Journal of Chemical Physics, 2004, 120, 2169-2181.	3.0	42
35	From The Cover: Hydration and mobility of HO-(aq). Proceedings of the National Academy of Sciences of the United States of America, 2004, 101, 7229-7233.	7.1	145
36	Fracture of nanoporous thin-film glasses. Nature Materials, 2004, 3, 53-57.	27.5	77
37	On the Quantum Nature of an Excess Proton in Liquid Hydrogen Fluoride. ChemPhysChem, 2004, 5, 1569-1576.	2.1	19
38	Protonated Water Clusters: The Third Dimension. ChemPhysChem, 2004, 5, 1495-1497.	2.1	15
39	Scalable fine-grained parallelization of plane-wave-basedab initio molecular dynamics for large supercomputers. Journal of Computational Chemistry, 2004, 25, 2006-2022.	3.3	30
40	Ab initio molecular dynamics simulation of the OH radical in liquid water. Chemical Physics Letters, 2004, 398, 212-216.	2.6	50

#	ARTICLE	IF	CITATIONS
41	Formamide Hydrolysis Investigated by Multiple-Steering ab Initio Molecular Dynamics. Journal of Physical Chemistry B, 2004, 108, 369-375.	2.6	50
42	Structures, energetics, and spectra of hydrated hydroxide anion clusters. Journal of Chemical Physics, 2004, 121, 4657-4664.	3.0	70
43	Two-dimensional hydration shells of alkali metal ions at a hydrophobic surface. Journal of Chemical Physics, 2004, 121, 12572.	3.0	25
44	Ultrafast dynamics for electron photodetachment from aqueous hydroxide. Journal of Chemical Physics, 2004, 120, 11712-11725.	3.0	59
45	Clustered water and bio-signal networks. , 0, , .		0
46	Understanding the Hydration Structure of Square-Planar Aquaions: The [Pd(H ₂ O) ₄] ²⁺ Case. Journal of Physical Chemistry B, 2004, 108, 15851-15855.	2.6	56
47	Protons in Supercritical Water: A Multistate Empirical Valence Bond Study. Journal of the American Chemical Society, 2004, 126, 2125-2134.	13.7	46
48	Electronic Structure and Solvation of Copper and Silver Ions: A Theoretical Picture of a Model Aqueous Redox Reaction. Journal of the American Chemical Society, 2004, 126, 3928-3938.	13.7	196
49	Quantum corrections to classical time-correlation functions: Hydrogen bonding and anharmonic floppy modes. Journal of Chemical Physics, 2004, 121, 3973-3983.	3.0	302
50	Hydrothermal solution structure. , 2004, , 149-182.		19
51	Towards an assessment of the accuracy of density functional theory for first principles simulations of water. Journal of Chemical Physics, 2004, 120, 300-311.	3.0	489
52	Transport in Proton Conductors for Fuel-Cell Applications: Simulations, Elementary Reactions, and Phenomenology. Chemical Reviews, 2004, 104, 4637-4678.	47.7	1,952
53	Ions in water: The microscopic structure of concentrated NaOH solutions. Journal of Chemical Physics, 2004, 120, 10154-10162.	3.0	141
54	Zinc Solid-State NMR Spectroscopy of Human Carbonic Anhydrase: Implications for the Enzymatic Mechanism. Journal of the American Chemical Society, 2004, 126, 4735-4739.	13.7	78
55	Solvation shell of OH ⁻ ions in water. Journal of Molecular Liquids, 2005, 117, 81-84.	4.9	54
56	Dynamical properties and the proton transfer mechanism in the wetting water layer on Pt(111). Surface Science, 2005, 575, 300-306.	1.9	34
57	Steroid-based head-to-tail amphiphiles as effective iono- and protonophores. Tetrahedron, 2005, 61, 10689-10698.	1.9	10
58	The Shapes of Protons in Hydrogen Bonds Depend on the Bond Length. ChemPhysChem, 2005, 6, 1738-1741.	2.1	91

#	ARTICLE	IF	CITATIONS
59	Density and Temperature Dependence of Proton Diffusion in Water: A First-Principles Molecular Dynamics Study. <i>ChemPhysChem</i> , 2005, 6, 1775-1779.	2.1	52
60	A Tribute to Michele Parrinello: Publications in Peer-Reviewed Journals Including Review Articles (1971-2004). <i>ChemPhysChem</i> , 2005, 6, 1677-1684.	2.1	0
61	Toward a Monte Carlo program for simulating vapor-liquid phase equilibria from first principles. <i>Computer Physics Communications</i> , 2005, 169, 289-294.	7.5	29
62	Relative solvation and strength of polycyano- and polynitromethanes in water: a study with molecular dynamics simulations. <i>Journal of Physical Organic Chemistry</i> , 2005, 18, 128-133.	1.9	2
63	Calculation of heat capacities of light and heavy water by path-integral molecular dynamics. <i>Journal of Chemical Physics</i> , 2005, 123, 134502.	3.0	48
64	Dissolution dynamics of NaCl nanocrystal in liquid water. <i>Physical Review E</i> , 2005, 72, 012602.	2.1	29
65	Static and dynamical properties of heavy water at ambient conditions from first-principles molecular dynamics. <i>Journal of Chemical Physics</i> , 2005, 122, 204510.	3.0	191
66	A polarizable multistate empirical valence bond model for proton transport in aqueous solution. <i>Journal of Chemical Physics</i> , 2005, 122, 224507.	3.0	66
67	Ab initio molecular dynamics study of glycine intramolecular proton transfer in water. <i>Journal of Chemical Physics</i> , 2005, 122, 184506.	3.0	104
68	Thermodynamics and Proton Transport in Nafion. <i>Journal of the Electrochemical Society</i> , 2005, 152, A1548.	2.9	82
69	Solvation Structure of Hydroxyl Radical by Carà Parrinello Molecular Dynamics. <i>Journal of Physical Chemistry A</i> , 2005, 109, 378-386.	2.5	49
70	Finite-temperature properties of the muonium substituted ethyl radical CH ₂ MuCH ₂ : nuclear degrees of freedom and hyperfine splitting constants. <i>Molecular Physics</i> , 2005, 103, 2407-2436.	1.7	13
71	Circular Hydrogen Bond Networks on the Surface of β -Ribofuranose in Aqueous Solution. <i>Journal of Physical Chemistry B</i> , 2005, 109, 12603-12611.	2.6	10
72	Structural Fluctuation and Dynamics of Ribose Puckering in Aqueous Solution from First Principles. <i>Journal of Physical Chemistry B</i> , 2005, 109, 12997-13005.	2.6	7
73	Hydroxyl Radical and Hydroxide Ion in Liquid Water: A Comparative Electron Density Functional Theory Study. <i>Journal of Physical Chemistry B</i> , 2005, 109, 23605-23610.	2.6	48
74	Thermodynamics and Proton Transport in Nafion. <i>Journal of the Electrochemical Society</i> , 2005, 152, E123.	2.9	349
75	Mechanism of Pyridine Protonation in Water Clusters of Increasing Size. <i>Journal of Physical Chemistry A</i> , 2005, 109, 8341-8347.	2.5	32
76	Excited state hydrogen atom transfer in ammonia-wire and water-wire clusters. <i>International Reviews in Physical Chemistry</i> , 2005, 24, 457-488.	2.3	76

#	ARTICLE	IF	CITATIONS
77	Argon Predissociation Spectroscopy of the OH- \cdot H ₂ O and Cl- \cdot H ₂ O Complexes in the 1000-1900 cm ⁻¹ Region: Intramolecular Bending Transitions and the Search for the Shared-Proton Fundamental in the Hydroxide Monohydrate. Journal of Physical Chemistry A, 2005, 109, 571-575.	2.5	56
78	The Mechanism of Proton Transfer between Adjacent Sites Exposed to Water. Journal of Physical Chemistry B, 2005, 109, 11379-11388.	2.6	22
79	Photoreduction of 4,4'-Bipyridine by Amines in Acetonitrile-Water Mixtures: Influence of H-Bonding on the Ion-Pair Structure and Dynamics. Journal of Physical Chemistry A, 2005, 109, 10813-10823.	2.5	6
80	Geometrical H/D Isotope Effect on Hydrogen Bonds in Charged Water Clusters. Journal of the American Chemical Society, 2005, 127, 11908-11909.	13.7	86
81	Calculating Reversible Potentials for Pt-H and Pt-OH Bond Formation in Basic Solutions. Journal of Physical Chemistry B, 2005, 109, 7557-7563.	2.6	20
82	Fundamental Excitations of the Shared Proton in the H ₃ O ⁺ - and H ₅ O ²⁺ Complexes. Journal of Physical Chemistry A, 2005, 109, 1487-1490.	2.5	168
83	Observation of the Dynamical Change in a Water Monolayer Adsorbed on a ZnO Surface. Physical Review Letters, 2005, 95, 136101.	7.8	176
84	First-principles study of ferroelectricity and isotope effects in H-bonded KH ₂ PO ₄ crystals. Physical Review B, 2005, 71, .	3.2	100
85	Hydroxide and Proton Migration in Aquaporins. Biophysical Journal, 2005, 89, 1744-1759.	0.5	56
86	Dynamical effects on vibrational and electronic spectra of hydroperoxyl radical water clusters. Journal of Chemical Physics, 2005, 123, 084310.	3.0	47
87	Ions in water: The microscopic structure of concentrated hydroxide solutions. Journal of Chemical Physics, 2005, 122, 194509.	3.0	114
88	Molecular Dynamics Simulations of Atmospheric Oxidants at the Air-Water Interface: Solvation and Accommodation of OH and O ₃ . Journal of Physical Chemistry B, 2005, 109, 15876-15892.	2.6	121
89	A theoretical study on anomalous temperature dependence of pK _w of water. Journal of Chemical Physics, 2005, 122, 144504.	3.0	54
90	Comparison of CBS-QB3, CBS-APNO, G2, and G3 thermochemical predictions with experiment for formation of ionic clusters of hydronium and hydroxide ions complexed with water. Journal of Chemical Physics, 2005, 122, 024302.	3.0	57
91	Vibrational Analysis of the H ₅ O ²⁺ Infrared Spectrum Using Molecular and Driven Molecular Dynamics. Journal of Physical Chemistry A, 2006, 110, 2933-2939.	2.5	91
92	Prying Apart a Water Molecule with Anionic H-Bonding: A Comparative Spectroscopic Study of the X- \cdot H ₂ O (X = OH, O, F, Cl, and Br) Binary Complexes in the 600-3800 cm ⁻¹ Region. Journal of Physical Chemistry A, 2006, 110, 4943-4952.	2.5	157
93	Proton Conduction in Fuel Cells. , 0, , 709-736.		2
94	The mechanism of proton transfer between adjacent sites on the molecular surface. Biochimica Et Biophysica Acta - Bioenergetics, 2006, 1757, 931-941.	1.0	21

#	ARTICLE	IF	CITATIONS
95	Developing optimal Wertheim-like models of water for use in Statistical Associating Fluid Theory (SAFT) and related approaches. <i>Molecular Physics</i> , 2006, 104, 3561-3581.	1.7	170
96	Conformational Properties of and a Reorientation Triggered by Sugar's Water Vibrational Resonance in the Hydroxymethyl Group in Hydrated β -D-Glucopyranose. <i>Journal of Physical Chemistry B</i> , 2006, 110, 2405-2418.	2.6	26
97	Simulating Fluid-Phase Equilibria of Water from First Principles. <i>Journal of Physical Chemistry A</i> , 2006, 110, 640-646.	2.5	128
98	Excited-State Hydrogen-Atom Transfer along Solvent Wires: Water Molecules Stop the Transfer. <i>Journal of Physical Chemistry A</i> , 2006, 110, 1758-1766.	2.5	42
99	A Molecular Dynamics Investigation of Hydrolytic Polymerization in a Metal-Hydroxide Gel. <i>Journal of Physical Chemistry B</i> , 2006, 110, 7107-7112.	2.6	12
100	Structure of an $[\text{I}(\text{H}_2\text{O})_6]^-$ Anion Cluster in a 3D Anion Crystal Host $[\text{I}(\text{H}_2\text{O})_6\text{Fe}(\text{CN})_6]^{4-}$. <i>Inorganic Chemistry</i> , 2006, 45, 1168-1172.	4.0	22
101	Cluster Model for the Ionic Product of Water: Accuracy and Limitations of Common Density Functional Methods. <i>Journal of Physical Chemistry A</i> , 2006, 110, 9194-9199.	2.5	30
102	Ab Initio Molecular Dynamics Study of a Mixture of $\text{HF}(\text{aq})$ and $\text{HCl}(\text{aq})$. <i>Journal of Physical Chemistry B</i> , 2006, 110, 12699-12706.	2.6	8
103	Structure and Dynamics of $\text{OH}(\text{aq})$. <i>Accounts of Chemical Research</i> , 2006, 39, 151-158.	15.6	254
104	Insights into the Chemomechanical Coupling of the Myosin Motor from Simulation of Its ATP Hydrolysis Mechanism. <i>Biochemistry</i> , 2006, 45, 5830-5847.	2.5	55
105	Density Functional Theory Based Ab Initio Molecular Dynamics Using the Car-Parrinello Approach. , 2006, , 223-285.		9
107	Vapor-liquid equilibria of water from first principles: comparison of density functionals and basis sets. <i>Molecular Physics</i> , 2006, 104, 3619-3626.	1.7	79
108	Consideration of thermodynamic, transport, and mechanical properties in the design of polymer electrolyte membranes for higher temperature fuel cell operation. <i>Journal of Polymer Science, Part B: Polymer Physics</i> , 2006, 44, 2183-2200.	2.1	80
109	A multiscale systems approach to microelectronic processes. <i>Computers and Chemical Engineering</i> , 2006, 30, 1643-1656.	3.8	17
110	A QM/MM study combined with the theory of energy representation: Solvation free energies for anti/syn acetic acids in aqueous solution. <i>Chemical Physics Letters</i> , 2006, 419, 240-244.	2.6	25
111	Revisiting the free energy profile for the nucleophilic attack of hydroxide on formamide in aqueous solution. <i>Chemical Physics Letters</i> , 2006, 422, 210-217.	2.6	31
112	Multidimensional quantum dynamics and infrared spectroscopy of hydrogen bonds. <i>Physics Reports</i> , 2006, 430, 211-276.	25.6	133
113	Structure of liquid water at ambient temperature from ab initio molecular dynamics performed in the complete basis set limit. <i>Journal of Chemical Physics</i> , 2006, 125, 154507.	3.0	167

#	ARTICLE	IF	CITATIONS
114	Hyperfine interactions in aqueous solution of Cr ³⁺ : an ab initio molecular dynamics study. Theoretical Chemistry Accounts, 2006, 115, 190-195.	1.4	14
115	Ab initio simulation on the mechanism of proton transport in water. Journal of Power Sources, 2006, 161, 1420-1427.	7.8	27
116	Formamide Hydrolysis in Alkaline Aqueous Solution: Insight from Ab Initio Metadynamics Calculations. Angewandte Chemie - International Edition, 2006, 45, 2893-2897.	13.8	64
117	Proton Transfer 200 Years after von Grotthuss: Insights from Ab Initio Simulations. ChemPhysChem, 2006, 7, 1848-1870.	2.1	750
119	Electron-stimulated production of molecular oxygen in amorphous solid water on Pt(111): Precursor transport through the hydrogen bonding network. Journal of Chemical Physics, 2006, 125, 124702.	3.0	43
120	Proton Transfer at the Protein/Water Interface. , 0, , 1499-1526.		0
121	Conductivity of single-stranded and double-stranded deoxyribose nucleic acid under ambient conditions: The dominance of water. Applied Physics Letters, 2006, 88, 102102.	3.3	55
122	Structure of 2 molar NaOH in aqueous solution from neutron diffraction and empirical potential structure refinement. Physical Review B, 2006, 74, .	3.2	75
123	Infrared studies of ionic clusters: The influence of Yuan T. Lee. Journal of Chemical Physics, 2006, 125, 132302.	3.0	90
124	Gadolinium (III) ion in liquid water: Structure, dynamics, and magnetic interactions from first principles. Journal of Chemical Physics, 2007, 127, 084506.	3.0	49
125	Structures and spectral signatures of protonated water networks in bacteriorhodopsin. Proceedings of the National Academy of Sciences of the United States of America, 2007, 104, 6980-6985.	7.1	138
126	Raman and Infrared Spectroscopic Investigations on Aqueous Alkali Metal Phosphate Solutions and Density Functional Theory Calculations of Phosphate ²⁻ Water Clusters. Applied Spectroscopy, 2007, 61, 1312-1327.	2.2	93
127	On the geometry and entropy of non-Hamiltonian phase space. Journal of Statistical Mechanics: Theory and Experiment, 2007, 2007, P02013-P02013.	2.3	13
128	Explosive evolution of hydrogen abstraction of water on oxidized Ag(110) surfaces studied by scanning tunnelling microscopy. Physical Chemistry Chemical Physics, 2007, 9, 5274.	2.8	3
129	Hydrogen Bonding in Protonated Water Clusters: An Atoms-in-Molecules Perspective. Journal of Physical Chemistry A, 2007, 111, 13287-13290.	2.5	40
130	Hydrogen-Bonding between Pyrimidine and Water: A Vibrational Spectroscopic Analysis. Journal of Physical Chemistry A, 2007, 111, 5185-5191.	2.5	49
131	Can the Four-Coordinated, Penta-Valent Oxygen in Hydroxide Water Clusters Be Detected through Experimental Vibrational Spectroscopy?. Journal of Physical Chemistry A, 2007, 111, 4815-4820.	2.5	43
132	Dynamical properties of liquid water from ab initio molecular dynamics performed in the complete basis set limit. Journal of Chemical Physics, 2007, 126, 164501.	3.0	232

#	ARTICLE	IF	CITATIONS
133	Structural Investigation of Asymmetrical Dimer Radical Cation System (H ₂ O~H ₂ S)+:~ Proton-Transferred or Hemi-Bonded?. Journal of Physical Chemistry A, 2007, 111, 2362-2367.	2.5	22
134	Electron Detachment and Relaxation of OH-(aq). Journal of Physical Chemistry A, 2007, 111, 11410-11420.	2.5	22
135	Quantum Wavepacket Ab Initio Molecular Dynamics:~ An Approach for Computing Dynamically Averaged Vibrational Spectra Including Critical Nuclear Quantum Effects. Journal of Physical Chemistry A, 2007, 111, 10313-10324.	2.5	59
136	Connecting Solvation Shell Structure to Proton Transport Kinetics in Hydrogen~Bonded Networks via Population Correlation Functions. Physical Review Letters, 2007, 99, 145901.	7.8	157
137	Nature of the Aqueous Hydroxide Ion Probed by X-ray Absorption Spectroscopy. Journal of Physical Chemistry A, 2007, 111, 4776-4785.	2.5	63
138	Design of a Next Generation Force Field:~ The X-POL Potential. Journal of Chemical Theory and Computation, 2007, 3, 1890-1900.	5.3	209
139	Modeling Aqueous Silica Chemistry in Alkali Media. Journal of Physical Chemistry C, 2007, 111, 18155-18158.	3.1	70
140	AbInitioMolecular Dynamics Study of Carbon Dioxide and Bicarbonate Hydration and the Nucleophilic Attack of Hydroxide on CO ₂ . Journal of Physical Chemistry B, 2007, 111, 4453-4459.	2.6	87
141	Deprotonation Mechanism of NH ₄ ⁺ in the <i>Escherichia coli</i> Ammonium Transporter AmtB: Insight from QM and QM/MM Calculations. Angewandte Chemie - International Edition, 2007, 46, 6811-6815.	13.8	26
142	Water Dissociation in the Presence of Metal Ions. Angewandte Chemie - International Edition, 2007, 46, 7853-7855.	13.8	30
145	Global minimum structure searches via particle swarm optimization. Journal of Computational Chemistry, 2007, 28, 1177-1186.	3.3	147
146	Hydrogen-Bond-Induced Inclusion Complex in Aqueous Cellulose/LiOH/Urea Solution at Low Temperature. ChemPhysChem, 2007, 8, 1572-1579.	2.1	172
147	Proton Transfer 200 Years after von Grotthuss: Insights from Ab Initio Simulations. ChemPhysChem, 2007, 8, 209-210.	2.1	50
148	Cellobiose hydrolysis using organic~inorganic hybrid mesoporous silica catalysts. Applied Catalysis A: General, 2007, 327, 44-51.	4.3	89
149	Specific ion effects in physicochemical and biological systems: Simulations, theory and experiments. Colloids and Surfaces A: Physicochemical and Engineering Aspects, 2007, 303, 110-136.	4.7	78
150	A charged ring model for classical OH~(aq) simulations. Chemical Physics Letters, 2007, 442, 128-133.	2.6	46
151	Computer modeling of hydrogen and methane transport in cellular nanostructures of amorphous ice. Materials Science and Engineering C, 2007, 27, 1390-1392.	7.3	1
152	Study of basic biopolymer as proton membrane for fuel cell systems. Electrochimica Acta, 2007, 52, 3766-3778.	5.2	64

#	ARTICLE	IF	CITATIONS
153	Pressure dependence of ionic conductivity of hydrated and dehydrated zeolites A. <i>Physica B: Condensed Matter</i> , 2007, 390, 356-365.	2.7	19
154	Probing water dynamics with OH ⁺ . <i>Chemical Physics</i> , 2007, 336, 183-187.	1.9	37
155	Theoretical investigation of the electronic absorption spectrum of Piceatannol in methanolic solution. <i>Theoretical Chemistry Accounts</i> , 2008, 121, 147-153.	1.4	11
156	Structural and dynamical studies of all-trans and all-cis cyclo[(1R,3S)- β -Acc-Gly] ₃ peptides. <i>Journal of Molecular Modeling</i> , 2008, 14, 1147-1157.	1.8	6
157	Potentiometric titration behavior of poly(acrylic acid) within a cross-linked polymer network having amide groups. <i>Colloid and Polymer Science</i> , 2008, 286, 1425-1434.	2.1	10
158	Guest-dependent conformation of 18-crown-6 tetracarboxylic acid: Relation to chiral separation of racemic amino acids. <i>Chirality</i> , 2008, 20, 820-827.	2.6	29
159	A Single-Molecule Perspective on the Role of Solvent Hydrogen Bonds in Protein Folding and Chemical Reactions. <i>ChemPhysChem</i> , 2008, 9, 2836-2847.	2.1	39
160	Ab initio path integral ring polymer molecular dynamics: Vibrational spectra of molecules. <i>Chemical Physics Letters</i> , 2008, 451, 175-181.	2.6	55
161	Reorientation of hydroxide ions in water. <i>Chemical Physics Letters</i> , 2008, 466, 1-5.	2.6	25
162	Why Are Water's Hydrophobic Interfaces Charged?. <i>Journal of the American Chemical Society</i> , 2008, 130, 3915-3919.	13.7	204
163	Interaction between liquid water and hydroxide revealed by core-hole de-excitation. <i>Nature</i> , 2008, 455, 89-91.	27.8	177
165	Humidity Dependence of Charge Transport through DNA Revealed by Silicon-Based Nanotweezers Manipulation. <i>Biophysical Journal</i> , 2008, 94, 63-70.	0.5	68
166	The Study of Dynamically Averaged Vibrational Spectroscopy of Atmospherically Relevant Clusters Using Ab Initio Molecular Dynamics in Conjunction with Quantum Wavepackets. <i>Advances in Quantum Chemistry</i> , 2008, 55, 333-353.	0.8	7
167	The structure of aqueous sodium hydroxide solutions: A combined solution x-ray diffraction and simulation study. <i>Journal of Chemical Physics</i> , 2008, 128, 044501.	3.0	137
168	Effect of Water on the Ionothermal Synthesis of Molecular Sieves. <i>Journal of the American Chemical Society</i> , 2008, 130, 8120-8121.	13.7	111
169	Assessment of Multicoefficient Correlation Methods, Second-Order Møller-Plesset Perturbation Theory, and Density Functional Theory for H ₃ O ⁺ (H ₂ O) _n (n = 1-5) and OH-(H ₂ O) _n (n = 1-4). <i>Journal of Physical Chemistry B</i> , 2008, 112, 2372-2381.	2.6	29
170	Acidity constants from vertical energy gaps: density functional theory based molecular dynamics implementation. <i>Physical Chemistry Chemical Physics</i> , 2008, 10, 5238.	2.8	131
171	Fine-grained parallelization of the Car-Parrinello ab initio molecular dynamics method on the IBM Blue Gene/L supercomputer. <i>IBM Journal of Research and Development</i> , 2008, 52, 159-175.	3.1	36

#	ARTICLE	IF	CITATIONS
172	Trapping proton transfer intermediates in the disordered hydrogen-bonded network of cryogenic hydrofluoric acid solutions. <i>Physical Chemistry Chemical Physics</i> , 2008, 10, 4785.	2.8	20
173	On the Molecular Mechanism of Water Reorientation. <i>Journal of Physical Chemistry B</i> , 2008, 112, 14230-14242.	2.6	380
174	An Improved Multistate Empirical Valence Bond Model for Aqueous Proton Solvation and Transport. <i>Journal of Physical Chemistry B</i> , 2008, 112, 467-482.	2.6	228
175	Proton Translocation and Electronic Relaxation along a Hydrogen-Bonded Molecular Wire in a 6-Hydroxyquinoline/Acetic Acid Complex. <i>Journal of Physical Chemistry B</i> , 2008, 112, 8383-8386.	2.6	24
176	Hydrated Electron Production by Reaction of Hydrogen Atoms with Hydroxide Ions: A First-Principles Molecular Dynamics Study. <i>Journal of Physical Chemistry A</i> , 2008, 112, 7027-7034.	2.5	18
177	Systematic Approach for Computing Zero-Point Energy, Quantum Partition Function, and Tunneling Effect Based on Kleinert's Variational Perturbation Theory. <i>Journal of Chemical Theory and Computation</i> , 2008, 4, 1409-1422.	5.3	29
178	A first principles theoretical study of vibrational spectral diffusion and hydrogen bond dynamics in aqueous ionic solutions: D2O in hydration shells of Cl ⁻ ions. <i>Journal of Chemical Physics</i> , 2008, 129, 194512.	3.0	102
179	Investigation of the dominant hydration structures among the ionic species in aqueous solution: Novel quantum mechanics/molecular mechanics simulations combined with the theory of energy representation. <i>Journal of Chemical Physics</i> , 2008, 128, 064507.	3.0	21
180	Insights from first principles molecular dynamics studies toward infrared multiple-photon and single-photon action spectroscopy: Case study of the proton-bound dimethyl ether dimer. <i>Journal of Chemical Physics</i> , 2008, 128, 184308.	3.0	57
181	Combining quantum wavepacket <i>ab initio</i> molecular dynamics with QM/MM and QM/QM techniques: Implementation blending <i>ONIOM</i> and empirical valence bond theory. <i>Journal of Chemical Physics</i> , 2008, 129, 054109.	3.0	26
182	Proton Transfer in a Two-Dimensional Hydrogen-Bonding Network: Water and Hydroxyl on a Pt(111) Surface. <i>Physical Review Letters</i> , 2008, 100, 106101.	7.8	39
183	A molecular approach to understanding complex systems: computational statistical mechanics using state-of-the-art algorithms on terascale computational platforms. <i>Journal of Physics: Conference Series</i> , 2008, 125, 012014.	0.4	1
186	On the phase diagram of water with density functional theory potentials: The melting temperature of ice Ih with the Perdew-Burke-Ernzerhof and Becke-Lee-Yang-Parr functionals. <i>Journal of Chemical Physics</i> , 2009, 130, 221102.	3.0	203
187	Proton transfer and H/D isotopic exchange of water molecules mediated by hydroxide ions on ice film surfaces. <i>Journal of Chemical Physics</i> , 2009, 131, 044705.	3.0	13
188	Observation of a Zundel-like transition state during proton transfer in aqueous hydroxide solutions. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2009, 106, 15154-15159.	7.1	111
190	Efficient sampling for <i>ab initio</i> Monte Carlo simulation of molecular clusters using an interpolated potential energy surface. <i>Journal of Chemical Physics</i> , 2009, 130, 024107.	3.0	16
191	Pore-Water Morphological Transitions in Polymer Electrolyte of a Fuel Cell. <i>Journal of the Electrochemical Society</i> , 2009, 156, B1192.	2.9	17
192	On the applicability of centroid and ring polymer path integral molecular dynamics for vibrational spectroscopy. <i>Journal of Chemical Physics</i> , 2009, 130, 194510.	3.0	194

#	ARTICLE	IF	CITATIONS
193	Hydroxidionen bilden Wasserstoffbrücken. Chemie in Unserer Zeit, 2009, 43, 9-9.	0.1	0
194	110 Years of the Meyer-Overton Rule: Predicting Membrane Permeability of Gases and Other Small Compounds. ChemPhysChem, 2009, 10, 1405-1414.	2.1	193
195	Transition states for hydride-water (H ⁻)(H ₂ O) _n clusters, n=2-6, 20. Computational and Theoretical Chemistry, 2009, 916, 61-71.	1.5	5
196	Computing vibrational properties in hydrogen-bonded systems using quantum wavepacket ab initio molecular dynamics. International Journal of Quantum Chemistry, 2009, 109, 3798-3810.	2.0	11
197	Proton transfer in water-hydroxyl mixed overlayers on Pt(111): Combined approach of laser desorption and spatially-resolved X-ray photoelectron spectroscopy. Surface Science, 2009, 603, 1690-1695.	1.9	6
198	Liquid microjet for photoelectron spectroscopy. Nuclear Instruments and Methods in Physics Research, Section A: Accelerators, Spectrometers, Detectors and Associated Equipment, 2009, 601, 139-150.	1.6	129
199	Hydrogen bonding interaction in complexes of hydronium ion with selective chemical species. Chemical Physics Letters, 2009, 471, 36-40.	2.6	3
200	Hydroxide anion at the air-water interface. Chemical Physics Letters, 2009, 481, 2-8.	2.6	118
201	The reorientation mechanism of hydroxide ions in water: A molecular dynamics study. Chemical Physics Letters, 2009, 481, 9-16.	2.6	27
202	Ab Initio Molar Volumes and Gaussian Radii. Journal of Physical Chemistry A, 2009, 113, 1141-1150.	2.5	113
203	A multistate empirical valence bond model for solvation and transport simulations of OH ⁻ in aqueous solutions. Physical Chemistry Chemical Physics, 2009, 11, 9420.	2.8	45
204	Combined QM/MM MD Study of HCOO ⁻ Water Hydrogen Bonds in Aqueous Solution. Journal of Physical Chemistry A, 2009, 113, 3291-3298.	2.5	25
205	Ab Initio Molecular Dynamics Study of the Electronic Structure of Superoxide Radical Anion in Solution. Journal of Physical Chemistry A, 2009, 113, 800-804.	2.5	12
206	Investigating Hydroxide Anion Interfacial Activity by Classical and Multistate Empirical Valence Bond Molecular Dynamics Simulations. Journal of Physical Chemistry A, 2009, 113, 6356-6364.	2.5	44
207	Ab Initio Molecular Dynamics Studies of the Liquid-Vapor Interface of an HCl Solution. Journal of Physical Chemistry A, 2009, 113, 2144-2151.	2.5	45
208	Ground-State Proton Transfer of 7-Hydroxyquinoline Confined in Biologically Relevant Water Nanopools. Journal of Physical Chemistry C, 2009, 113, 16110-16115.	3.1	30
209	Urea, but not guanidinium, destabilizes proteins by forming hydrogen bonds to the peptide group. Proceedings of the National Academy of Sciences of the United States of America, 2009, 106, 2595-2600.	7.1	335
210	Ab Initio Molecular Dynamics Simulations of the Infrared Spectra of H ₃ O ⁺ and D ₃ O ⁺ . Journal of Chemical Theory and Computation, 2009, 5, 1328-1336.	5.3	22

#	ARTICLE	IF	CITATIONS
211	Functional Role of Asp160 and the Deprotonation Mechanism of Ammonium in the <i>Escherichia coli</i> Ammonia Channel Protein AmtB. <i>Journal of Physical Chemistry B</i> , 2009, 113, 4922-4929.	2.6	17
212	Spiers Memorial Lecture : Ions at aqueous interfaces. <i>Faraday Discussions</i> , 2009, 141, 9-30.	3.2	83
213	Benchmarking Polarizable Molecular Dynamics Simulations of Aqueous Sodium Hydroxide by Diffraction Measurements. <i>Journal of Physical Chemistry A</i> , 2009, 113, 4022-4027.	2.5	22
214	X-Ray photo- and resonant Auger-electron spectroscopy studies of liquid water and aqueous solutions. <i>Annual Reports on the Progress of Chemistry Section C</i> , 2009, 105, 174.	4.4	56
215	Quantum Effects on Vibrational and Electronic Spectra of Hydrazine Studied by "On-the-Fly" ab Initio Ring Polymer Molecular Dynamics. <i>Journal of Physical Chemistry A</i> , 2009, 113, 1985-1994.	2.5	50
216	Proton transport of water in acid-base reactions of 7-hydroxyquinoline. <i>Chemical Communications</i> , 2009, , 926.	4.1	44
217	Triple proton transfer of excited 7-hydroxyquinoline along a hydrogen-bonded water chain in ethers: secondary solvent effect on the reaction rate. <i>Photochemical and Photobiological Sciences</i> , 2009, 8, 1611.	2.9	38
218	Evaluation of B3LYP, X3LYP, and M06-Class Density Functionals for Predicting the Binding Energies of Neutral, Protonated, and Deprotonated Water Clusters. <i>Journal of Chemical Theory and Computation</i> , 2009, 5, 1016-1026.	5.3	326
219	An explanation for the charge on water's surface. <i>Physical Chemistry Chemical Physics</i> , 2009, 11, 10994.	2.8	145
220	Observation of Quasi-One Dimensional Proton Conductions in Molecular Porous Crystal [Co ^{III} (H ₂ bim) ₃](TMA)-20H ₂ O. <i>Journal of the Physical Society of Japan</i> , 2010, 79, 103601.	1.6	18
221	Negative differential resistance in hydrated deoxyribonucleic acid thin films mediated by diffusion-limited water redox reactions. <i>Applied Physics Letters</i> , 2010, 97, .	3.3	11
222	On the Formation of Proton-Shared and Contact Ion Pair Forms during the Dissociation of Moderately Strong Acids: An Ab Initio Molecular Dynamics Investigation. <i>Journal of Physical Chemistry B</i> , 2010, 114, 8147-8155.	2.6	11
223	Enol Tautomers of Watson-Crick Base Pair Models Are Metastable Because of Nuclear Quantum Effects. <i>Journal of the American Chemical Society</i> , 2010, 132, 11510-11515.	13.7	79
224	Experiments in a floating water bridge. <i>Experiments in Fluids</i> , 2010, 48, 121-131.	2.4	53
225	Traceability of electrolytic conductivity measurements to the International System of Units in the sub mS m ⁻¹ region and review of models of electrolytic conductivity cells. <i>Electrochimica Acta</i> , 2010, 55, 6323-6331.	5.2	27
228	Excited-State Prototropic Equilibrium Dynamics of 6-Hydroxyquinoline Encapsulated in Microporous Catalytic Faujasite Zeolites. <i>Chemistry - A European Journal</i> , 2010, 16, 12609-12615.	3.3	8
229	Two supramolecular microporous frameworks stabilized by hydroxyl anionic water cluster. <i>Journal of Molecular Structure</i> , 2010, 973, 136-143.	3.6	3
230	Low-concentration aqueous solutions of macrocyclic pyridine-pyrrole compound: Relationship between the parameters, physicochemical properties, and physiological activity of supramolecular nanosized associates. <i>Doklady Physical Chemistry</i> , 2010, 433, 142-146.	0.9	18

#	ARTICLE	IF	CITATIONS
231	Probing the Dynamics of Solvation and Structure of the OH ⁻ Ion in Aqueous Solution from Picosecond Transient Absorption Measurements. <i>Molecules</i> , 2010, 15, 3366-3377.	3.8	5
232	A statistical mechanical theory of proton transport kinetics in hydrogen-bonded networks based on population correlation functions with applications to acids and bases. <i>Journal of Chemical Physics</i> , 2010, 133, 124108.	3.0	69
233	Evaluation of the use of secondary energy for hydrogen generation. , 2010, , .		3
234	Capturing a DNA duplex under near-physiological conditions. <i>Applied Physics Letters</i> , 2010, 97, 163702.	3.3	6
235	Symmetric hydrogen bond in a water-hydroxyl complex on Cu(110). <i>Physical Review B</i> , 2010, 81, .	3.2	42
236	The behavior of NaOH at the air-water interface: A computational study. <i>Journal of Chemical Physics</i> , 2010, 133, 024705.	3.0	19
237	Hydration of cyanin dyes. <i>Journal of Chemical Physics</i> , 2010, 132, 114304.	3.0	8
238	Quantum wavepacket ab initio molecular dynamics: Generalizations using an extended Lagrangian treatment of diabatic states coupled through multireference electronic structure. <i>Journal of Chemical Physics</i> , 2010, 133, 184105.	3.0	14
239	Theoretical Investigation of Solvent Effects and Complex Systems: Toward the calculations of bioinorganic systems from ab initio molecular dynamics simulations and static quantum chemistry. <i>Advances in Inorganic Chemistry</i> , 2010, 62, 111-142.	1.0	9
240	Accumulated Proton-Donating Ability of Solvent Molecules in Proton Transfer. <i>Journal of the American Chemical Society</i> , 2010, 132, 297-302.	13.7	62
241	Comment on "An explanation for the charge on water's surface" by A. Gray-Weale and J. K. Beattie, <i>Phys. Chem. Chem. Phys.</i> , 2009, 11, 10994. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 14362.	2.8	12
242	Tuning Hydrated Nanoceria Surfaces: Experimental/Theoretical Investigations of Ion Exchange and Implications in Organic and Inorganic Interactions. <i>Langmuir</i> , 2010, 26, 7188-7198.	3.5	35
243	Local dynamics and structure of the solvated hydroxide ion in water. <i>Molecular Simulation</i> , 2010, 36, 69-73.	2.0	10
244	Density Functional Theory Study of Degradation of Tetraalkylammonium Hydroxides. <i>Journal of Physical Chemistry C</i> , 2010, 114, 11977-11983.	3.1	216
245	Dynamical Discrete/Continuum Linear Response Shells Theory of Solvation: Convergence Test for NH ₄ ⁺ and OH ⁻ Ions in Water Solution Using DFT and DFTB Methods. <i>Journal of Physical Chemistry B</i> , 2010, 114, 15941-15947.	2.6	20
246	Ab Initio Study of Water Polarization in the Hydration Shell of Aqueous Hydroxide: Comparison between Polarizable and Nonpolarizable Water Models. <i>Journal of Chemical Theory and Computation</i> , 2010, 6, 2888-2895.	5.3	16
247	Charge Reversal of Surfaces in Divalent Electrolytes: The Role of Ionic Dispersion Interactions. <i>Langmuir</i> , 2010, 26, 6430-6436.	3.5	83
248	Protonation of a Hydroxide Anion Bridging Two Divalent Magnesium Cations in Water Probed by First-Principles Metadynamics Simulation. <i>Journal of Physical Chemistry B</i> , 2010, 114, 11102-11109.	2.6	12

#	ARTICLE	IF	CITATIONS
249	Reply to the “Comment on “An explanation for the charge on water’s surface” by R. Vřıcha, D. Horinek, R. Buchner, B. Winter and P. Jungwirth, Phys. Chem. Chem. Phys., 2010, 12, DOI: 10.1039/c001492c. Physical Chemistry Chemical Physics, 2010, 12, 14364.	2.8	9
250	A classical molecular dynamics study of the anomalous ionic product in near-critical and supercritical water. Molecular Physics, 2010, 108, 193-203.	1.7	10
251	Many-body energies during proton transfer in an aqueous system. Journal of Molecular Modeling, 2010, 16, 1559-1566.	1.8	5
252	Simulation of Electrocatalytic Hydrogen Production by a Bioinspired Catalyst Anchored to a Pyrite Electrode. Journal of the American Chemical Society, 2010, 132, 8593-8601.	13.7	33
253	An <i>ab initio</i> molecular dynamics study of hydronium complexation in Na-montmorillonite. Philosophical Magazine, 2010, 90, 2459-2474.	1.6	33
254	Cobalt ^{II} Porphyrin Catalyzed Electrochemical Reduction of Carbon Dioxide in Water. 2. Mechanism from First Principles. Journal of Physical Chemistry A, 2010, 114, 10174-10184.	2.5	130
255	Aqueous Basic Solutions: Hydroxide Solvation, Structural Diffusion, and Comparison to the Hydrated Proton. Chemical Reviews, 2010, 110, 2174-2216.	47.7	414
256	Hydrolytic conversion of AsO ₄ ³⁻ to HAsO ₄ ²⁻ : a QMCF MD study. Physical Chemistry Chemical Physics, 2010, 12, 6244.	2.8	4
257	Hydrolysis of tetravalent group IV metal ions: an <i>ab initio</i> simulation study. Physical Chemistry Chemical Physics, 2010, 12, 12423.	2.8	10
258	Ionic mobility of the solvated proton and acid–base titration in a four-compartment capillary electrophoresis system. Analytical Methods, 2010, 2, 164-170.	2.7	34
259	Ground-state proton-transfer dynamics governed by configurational optimization. Physical Chemistry Chemical Physics, 2011, 13, 3730-3736.	2.8	13
260	Quantum fluctuations increase the self-diffusive motion of para-hydrogen in narrow carbon nanotubes. Physical Chemistry Chemical Physics, 2011, 13, 9824.	2.8	4
261	Comparison of Hydrated Hydroperoxide Anion (HOO ⁻)(H ₂ O) _n Clusters with Alkaline Hydrogen Peroxide (HOOH)(OH ⁻)(H ₂ O) _n Clusters, <i>n</i> = 1–8, 20: An <i>ab Initio</i> Study. Journal of Physical Chemistry A, 2011, 115, 6327-6338.	2.5	16
262	Hydroxide Hydrogen Bonding: Probing the Solvation Structure through Ultrafast Time Domain Raman Spectroscopy. Journal of Physical Chemistry Letters, 2011, 2, 1155-1160.	4.6	10
263	Insights into the Solvation and Mobility of the Hydroxyl Radical in Aqueous Solution. Journal of Chemical Theory and Computation, 2011, 7, 3725-3732.	5.3	28
264	Energy Relaxation Dynamics of the Hydration Complex of Hydroxide. Journal of Physical Chemistry A, 2011, 115, 14593-14598.	2.5	28
265	Path Integral Computation of Quantum Free Energy Differences Due to Alchemical Transformations Involving Mass and Potential. Journal of Chemical Theory and Computation, 2011, 7, 2358-2369.	5.3	36
266	On the Intramolecular Hydrogen Bond in Solution: Car–Parrinello and Path Integral Molecular Dynamics Perspective. Journal of Chemical Theory and Computation, 2011, 7, 3505-3513.	5.3	32

#	ARTICLE	IF	CITATIONS
267	Proton Transfer in Concentrated Aqueous Hydroxide Visualized Using Ultrafast Infrared Spectroscopy. <i>Journal of Physical Chemistry A</i> , 2011, 115, 3957-3972.	2.5	45
268	CH ₂ Cl ₂ + OH [•] Reaction in Aqueous Solution: A Combined Quantum Mechanical and Molecular Mechanics Study. <i>Journal of Physical Chemistry A</i> , 2011, 115, 1380-1384.	2.5	13
269	Path-Integral Calculations of Nuclear Quantum Effects in Model Systems, Small Molecules, and Enzymes via Gradient-Based Forward Corrector Algorithms. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 1273-1286.	5.3	31
270	Ultrafast Geminate Recombination after Photodetachment of Aqueous Hydroxide. <i>Journal of the American Chemical Society</i> , 2011, 133, 790-795.	13.7	22
271	Hybrid Quantum Mechanical/Molecular Mechanics Study of the S _N 2 Reaction of CH ₃ Cl+OH [•] in Water. <i>Journal of Physical Chemistry A</i> , 2011, 115, 12047-12052.	2.5	41
272	Shannon Entropy Based Time-Dependent Deterministic Sampling for Efficient "On-the-Fly" Quantum Dynamics and Electronic Structure. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 256-268.	5.3	15
273	Syntheses, Structural Characterization, and Properties of {[Cu(bpp) ₂ (H ₂ O) ₂](tp)·7H ₂ O} and {[Cu(bpp) ₂ (H ₂ O) ₂](ip)·7H ₂ O} Complexes. New Examples of the Organic Anionic Template Effect on Induced Assembly of Water Clusters (bpp =) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 492 Td (1,3-Bis(4	3.0	72
274	507-515. Proton Transport in Triflic Acid Pentahydrate Studied via Ab Initio Path Integral Molecular Dynamics. <i>Journal of Physical Chemistry A</i> , 2011, 115, 6112-6124.	2.5	35
275	Solvation Dynamics of Vaska's Complex by 2D-IR Spectroscopy. <i>Journal of Physical Chemistry C</i> , 2011, 115, 24813-24822.	3.1	31
276	Ions in solutions: Determining their polarizabilities from first-principles. <i>Journal of Chemical Physics</i> , 2011, 134, 014511.	3.0	67
277	A Partial Proton Transfer in Hydrogen Bond O~H···O in Crystals of Anhydrous Potassium and Rubidium Complex Chloranilates. <i>Journal of Physical Chemistry A</i> , 2011, 115, 3154-3166.	2.5	23
278	Dielectron Attachment and Hydrogen Evolution Reaction in Water Clusters. <i>Journal of Physical Chemistry A</i> , 2011, 115, 7378-7391.	2.5	37
279	HCO ₃ [•] Formation from CO ₂ at High pH: Ab Initio Molecular Dynamics Study. <i>Journal of Physical Chemistry B</i> , 2011, 115, 14683-14687.	2.6	39
280	Acidities of confined water in interlayer space of clay minerals. <i>Geochimica Et Cosmochimica Acta</i> , 2011, 75, 4978-4986.	3.9	32
281	Dynamical Screening and Ionic Conductivity in Water from Ab Initio Simulations. <i>Physical Review Letters</i> , 2011, 107, 185901.	7.8	41
282	A Theoretical Investigation of the Plausibility of Reactions between Ammonia and Carbonyl Species (Formaldehyde, Acetaldehyde, and Acetone) in Interstellar Ice Analogs at Ultracold Temperatures. <i>Journal of Physical Chemistry A</i> , 2011, 115, 5166-5183.	2.5	30
283	On the connection between proton transport, structural diffusion, and reorientation of the hydrated hydroxide ion as a function of temperature. <i>Chemical Physics Letters</i> , 2011, 511, 177-182.	2.6	43
284	An ab initio molecular dynamics study of supercritical aqueous ionic solutions: Hydrogen bonding, rotational dynamics and vibrational spectral diffusion. <i>Chemical Physics</i> , 2011, 387, 48-55.	1.9	16

#	ARTICLE	IF	CITATIONS
285	Protons migrate along interfacial water without significant contributions from jumps between ionizable groups on the membrane surface. Proceedings of the National Academy of Sciences of the United States of America, 2011, 108, 14461-14466.	7.1	100
286	Anion exchange membranes for alkaline fuel cells: A review. Journal of Membrane Science, 2011, 377, 1-35.	8.2	1,486
287	Quantum simulation of molecular interaction and dynamics at surfaces. Frontiers of Physics, 2011, 6, 294-308.	5.0	10
288	Theoretical studies on hydrogen bonding interactions: From small clusters to the liquid phase. International Journal of Quantum Chemistry, 2011, 111, 1256-1269. Hydration of NaHCO ₃ , KHCO ₃ , ($\text{http://www.w3.org/1998/Math/MathML}$) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 5	2.0	4
289	$\text{http://www.w3.org/1998/Math/MathML}$ altimg="si2.gif" overflow="scroll"> HCO_2 Chemical Physics Letters, 2011, 507, 89-95.	2.6	14
290	Polymer membranes for high temperature proton exchange membrane fuel cell: Recent advances and challenges. Progress in Polymer Science, 2011, 36, 813-843.	24.7	796
291	Quantum nuclear effects on the location of hydrogen above and below the palladium (100) surface. Surface Science, 2011, 605, 689-694.	1.9	13
292	Improving the convergence of closed and open path integral molecular dynamics via higher order Trotter factorization schemes. Journal of Chemical Physics, 2011, 135, 064104.	3.0	54
293	First-Principles Investigation on Ionization Strength, Volume Expansion, and Water Rotational Rigidity of Small Water Cluster Systems Formed around Sodium(I), Calcium(II), and Iron(II) Ions. Journal of the Physical Society of Japan, 2011, 80, 024601.	1.6	1
294	Characterization of polymer structures based on Burnside's lemma. Physical Review E, 2011, 84, 011805.	2.1	2
295	Inducing H/D Exchange in Ultrathin Ice Films by Proton Deficiency. Physical Review Letters, 2011, 107, 216101.	7.8	5
296	Proton Travel in Green Fluorescent Protein. Springer Series on Fluorescence, 2011, , 171-181.	0.8	1
297	Re-examining the properties of the aqueous vapor-liquid interface using dispersion corrected density functional theory. Journal of Chemical Physics, 2011, 135, 124712.	3.0	82
298	Proton transfer and the mobilities of the H ⁺ and OH ⁻ ions from studies of a dissociating model for water. Journal of Chemical Physics, 2011, 135, 124505.	3.0	170
299	Proton transport in a binary biomimetic solution revealed by molecular dynamics simulation. Journal of Chemical Physics, 2011, 135, 114502.	3.0	7
301	A first-principles theoretical study of hydrogen-bond dynamics and vibrational spectral diffusion in aqueous ionic solution: Water in the hydration shell of a fluoride ion. Pure and Applied Chemistry, 2012, 85, 27-40.	1.9	26
302	Natural polarizability and flexibility via explicit valency: The case of water. Journal of Chemical Physics, 2012, 136, 084109.	3.0	26
303	Eigen-like hydrated protons traveling with a local distortion through the water nanotube in new molecular porous crystals $\{[\text{M}(\text{H}_2\text{O})_3](\text{TMA})_n\}$ (M = Co, Rh, Ru). Journal of Chemical Physics, 2012, 137, 144503.	3.0	18

#	ARTICLE	IF	CITATIONS
304	A multilayered-representation quantum mechanical/molecular mechanics study of the SN2 reaction of CH3Br + OH ⁻ in aqueous solution. Journal of Chemical Physics, 2012, 137, 184501.	3.0	19
305	Direct Observation of Conformation-Dependent Pathways in the Excited-State Proton Transfer of 7-Hydroxyquinoline in Bulk Alcohols. Journal of Physical Chemistry B, 2012, 116, 14153-14158.	2.6	18
306	Exact Relation between Potential of Mean Force and Free-Energy Profile. Journal of Chemical Theory and Computation, 2012, 8, 3998-4003.	5.3	25
308	Proton Defect Solvation and Dynamics in Aqueous Acid and Base. Angewandte Chemie - International Edition, 2012, 51, 11029-11032.	13.8	31
309	Feasibility evaluation of the use of secondary energy for hydrogen generation. , 2012, , .		1
310	Excited-state hydrogen relay along a blended-alcohol chain as a model system of a proton wire: deuterium effect on the reaction dynamics. Physical Chemistry Chemical Physics, 2012, 14, 8885.	2.8	14
311	Hydroxide Ion Can Move Faster Than an Excess Proton through One-Dimensional Water Chains in Hydrophobic Narrow Pores. Journal of Physical Chemistry B, 2012, 116, 9744-9757.	2.6	37
312	Ultrafast charge delocalization dynamics in aqueous electrolytes: New insights from Auger electron spectroscopy. Chemical Physics Letters, 2012, 543, 1-11.	2.6	17
313	Ca ²⁺ solvation as a function of p, T, and pH from <i>ab initio</i> simulation. Journal of Chemical Physics, 2012, 137, 124502.	3.0	12
314	The mechanism of proton conduction in phosphoric acid. Nature Chemistry, 2012, 4, 461-466.	13.6	428
315	PVA-based hybrid membranes from cation exchange multisilicon copolymer for alkali recovery. Desalination, 2012, 304, 25-32.	8.2	37
316	A first principles molecular dynamics study of the solvation structure and migration kinetics of an excess proton and a hydroxide ion in binary water-ammonia mixtures. Journal of Chemical Physics, 2012, 136, 114509.	3.0	8
317	Mobility Mechanism of Hydroxyl Radicals in Aqueous Solution via Hydrogen Transfer. Journal of the American Chemical Society, 2012, 134, 532-538.	13.7	66
318	Developing a Systematic Approach for Ab Initio Path-Integral Simulations. , 0, , .		2
319	Energetics during proton transfer process in hydrated z ^{1/4} ndel ion complex. International Journal of Quantum Chemistry, 2012, 112, 1439-1448.	2.0	8
320	The Fuzzy Quantum Proton in the Hydrogen Chloride Hydrates. Journal of the American Chemical Society, 2012, 134, 8557-8569.	13.7	45
321	Proton transport in functionalised additives for PEM fuel cells: contributions from atomistic simulations. Chemical Society Reviews, 2012, 41, 5143.	38.1	27
322	Hydrogen bond dynamics and vibrational spectral diffusion in aqueous solution of acetone: A first principles molecular dynamics study#. Journal of Chemical Sciences, 2012, 124, 215-221.	1.5	20

#	ARTICLE	IF	CITATIONS
323	Hydration structure and dynamics of a hydroxide ion in water clusters of varying size and temperature: Quantum chemical and ab initio molecular dynamics studies. <i>Chemical Physics</i> , 2012, 400, 154-164.	1.9	27
324	Research Progress in Ionothermal Synthesis of Molecular Sieves. <i>Chinese Journal of Catalysis</i> , 2012, 33, 39-50.	14.0	24
325	Multidimensional local mode calculations for the vibrational spectra of $\text{OH}^-(\text{H}_2\text{O})_2$ and $\text{OH}^-(\text{H}_2\text{O})_2\text{-Ar}$. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 14973.	2.8	16
326	Microscopic properties of liquid water from combined ab initio molecular dynamics and energy decomposition studies. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 15746.	2.8	55
327	Negative differential resistance in ZnO coated peptide nanotube. <i>Applied Physics A: Materials Science and Processing</i> , 2013, 112, 305-310.	2.3	5
328	Ab Initio Molecular Dynamics Study of the Very Short $\text{O}^-\cdots\text{H}\cdots\text{O}$ Hydrogen Bonds in the Condensed Phases. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 65-72.	5.3	11
329	Computational modeling of structure and OH-anion diffusion in quaternary ammonium polysulfone hydroxide "Polymer electrolyte for application in electrochemical devices. <i>Journal of Membrane Science</i> , 2013, 431, 79-85.	8.2	48
330	Proton transfer and the diffusion of H^+ and OH^- ions along water wires. <i>Journal of Chemical Physics</i> , 2013, 139, 124507.	3.0	30
331	First principles molecular dynamics study of proton dynamics and transport in phosphoric acid/imidazole (2:1) system. <i>Solid State Ionics</i> , 2013, 252, 34-39.	2.7	43
332	Lifetimes of Excess Protons in Water Using a Dissociative Water Potential. <i>Journal of Physical Chemistry B</i> , 2013, 117, 4089-4097.	2.6	32
333	Theoretical calculation of proton mobility for collective surface proton transport. <i>Physical Review E</i> , 2013, 87, 062908.	2.1	8
334	Proton transfer through the water gossamer. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2013, 110, 13723-13728.	7.1	320
335	How a Qualitative Study with Chemistry Instructors Informed Atomic Level Animation Design. <i>ACS Symposium Series</i> , 2013, , 205-239.	0.5	2
336	Role of the Membrane Dipole Potential for Proton Transport in Gramicidin A Embedded in a DMPC Bilayer. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 3826-3831.	5.3	17
337	Nature of proton transport in a water-filled carbon nanotube and in liquid water. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 6344.	2.8	51
338	Excited-State Tautomerization of 7-Azaindole in Nonpolar Solution: A Theoretical Study Based on Liquid-Phase Potential Surfaces of Mean Force. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 3557-3566.	5.3	6
339	The multigrid POTFIT (MGPF) method: Grid representations of potentials for quantum dynamics of large systems. <i>Journal of Chemical Physics</i> , 2013, 138, 014108.	3.0	95
340	The thermodynamics study on the dissolution mechanism of cellobiose in NaOH/urea aqueous solution. <i>Journal of Thermal Analysis and Calorimetry</i> , 2013, 111, 891-896.	3.6	10

#	ARTICLE	IF	CITATIONS
341	Characteristics of the “Hypercoordination” of hydroxide (OH ⁻) in water: A comparative study of HF/MM and B3LYP/MM MD simulations. <i>Journal of Molecular Liquids</i> , 2013, 188, 89-95.	4.9	4
343	Proton Conduction in Metal–Organic Frameworks and Related Modularly Built Porous Solids. <i>Angewandte Chemie - International Edition</i> , 2013, 52, 2688-2700.	13.8	658
344	Superadsorption of LiOH solution on chitosan as a new type of solvent for chitosan by freezing/blasting. <i>Carbohydrate Polymers</i> , 2013, 94, 430-435.	10.2	8
345	A qualitative study of the effect of a counterion and polar environment on the structure and spectroscopic signatures of a hydrated hydroxyl anion. <i>Theoretical Chemistry Accounts</i> , 2013, 132, 1.	1.4	22
346	Constant Pressure Path Integral Gibbs Ensemble Monte Carlo Method. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 2922-2929.	5.3	11
347	High efficiency photoelectrochemical water splitting and hydrogen generation using GaN nanowire photoelectrode. <i>Nanotechnology</i> , 2013, 24, 175401.	2.6	84
348	Intrinsic fluorescence properties of rhodamine cations in gas-phase: triplet lifetimes and dispersed fluorescence spectra. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 8162.	2.8	37
349	Model Studies of the Kinetics of Ester Hydrolysis under Stretching Force. <i>Angewandte Chemie - International Edition</i> , 2013, 52, 6992-6995.	13.8	49
350	Towards High Conductivity in Anion–Exchange Membranes for Alkaline Fuel Cells. <i>ChemSusChem</i> , 2013, 6, 1376-1383.	6.8	120
351	Solvation structures of protons and hydroxide ions in water. <i>Journal of Chemical Physics</i> , 2013, 138, 154506.	3.0	19
352	Temperature dependence on the structure of Zundel cation and its isotopomers. <i>Journal of Chemical Physics</i> , 2013, 138, 184307.	3.0	10
353	Theoretical Study of the Protonation of the One-Electron-Reduced Guanine–Cytosine Base Pair by Water. <i>Journal of Physical Chemistry B</i> , 2013, 117, 2096-2105.	2.6	14
354	Proton Transfer Dependence on Hydrogen-Bonding of Solvent to the Water Wire: A Theoretical Study. <i>Journal of Physical Chemistry B</i> , 2013, 117, 307-315.	2.6	23
355	Water's non-tetrahedral side. <i>Faraday Discussions</i> , 2013, 167, 529.	3.2	40
356	Understanding anion transport in an aminated trimethyl polyphenylene with high anionic conductivity. <i>Journal of Polymer Science, Part B: Polymer Physics</i> , 2013, 51, 1743-1750.	2.1	34
358	Large-scale atomistic and quantum-mechanical simulations of a Nafion membrane: Morphology, proton solvation and charge transport. <i>Beilstein Journal of Nanotechnology</i> , 2013, 4, 567-587.	2.8	64
360	Hybrid Proton and Electron Transport in Peptide Fibrils. <i>Advanced Functional Materials</i> , 2014, 24, 5873-5880.	14.9	58
361	Collective vibrations of water-solvated hydroxide ions investigated with broadband 2DIR spectroscopy. <i>Journal of Chemical Physics</i> , 2014, 140, 204508.	3.0	53

#	ARTICLE	IF	CITATIONS
362	Comparative Proton Transfer Efficiencies of Hydronium and Hydroxide in Aqueous Solution: Proton Transfer vs Brownian Motion. <i>Journal of Physical Chemistry B</i> , 2014, 118, 13671-13678.	2.6	18
363	Effect of quantum nuclear motion on hydrogen bonding. <i>Journal of Chemical Physics</i> , 2014, 140, 174508.	3.0	84
364	Chemistry of Materials™ 1k Club: Klaus-Dieter Kreuer. Establishing the Connection Between Materials and Proton Conductivity. <i>Chemistry of Materials</i> , 2014, 26, 6651-6652.	6.7	2
365	Properties of LiOH and LiCl at sub and supercritical water conditions. <i>Journal of Molecular Liquids</i> , 2014, 190, 30-33.	4.9	6
366	Aqueous solutions: state of the art in <i>ab initio</i> molecular dynamics. <i>Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences</i> , 2014, 372, 20120482.	3.4	121
367	Reactive molecular dynamics simulations of oxygen species in a liquid water layer of interest for plasma medicine. <i>Journal Physics D: Applied Physics</i> , 2014, 47, 025205.	2.8	97
368	Design and Synthesis of Hydroxide Ion-Conductive Metal-Organic Frameworks Based on Salt Inclusion. <i>Journal of the American Chemical Society</i> , 2014, 136, 1702-1705.	13.7	124
369	Constructing ionic highway in alkaline polymer electrolytes. <i>Energy and Environmental Science</i> , 2014, 7, 354-360.	30.8	439
370	Multiple time step integrators in <i>ab initio</i> molecular dynamics. <i>Journal of Chemical Physics</i> , 2014, 140, 084116.	3.0	33
371	An <i>ab initio</i> molecular dynamics study of the hydrogen bonded structure, dynamics and vibrational spectral diffusion of water in the ion hydration shell of a superoxide ion. <i>Chemical Physics</i> , 2014, 445, 105-112.	1.9	2
372	CO ₂ incorporation in hydroxide and hydroperoxide containing water clusters—a unifying mechanism for hydrolysis and protolysis. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 9371-9382.	2.8	2
373	A Dissociative Quantum Mechanical/Molecular Mechanical Molecular Dynamics Simulation and Infrared Experiments Reveal Characteristics of the Strongly Hydrolytic Arsenic(III). <i>Inorganic Chemistry</i> , 2014, 53, 11861-11870.	4.0	10
374	Nitrilic acid hexahydrate, a novel benchmark system of the Zundel cation in an intrinsically asymmetric environment: spectroscopic features and hydrogen bond dynamics characterised by experimental and theoretical methods. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 998-1007.	2.8	14
375	Limit of Metastability for Liquid and Vapor Phases of Water. <i>Physical Review Letters</i> , 2014, 112, 157802.	7.8	17
376	Quantum delocalization of benzene in the ring puckering coordinates. <i>International Journal of Quantum Chemistry</i> , 2014, 114, 534-542.	2.0	1
377	Why does the IR spectrum of hydroxide stretching vibration weaken with increase in hydration?. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 23143-23149.	2.8	19
378	Competition between excited state proton and OH [•] transport <i>via</i> a short water wire: solvent effects open the gate. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 13047-13051.	2.8	21
379	Nuclear Quantum Effects in Water: A Multiscale Study. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 816-824.	5.3	42

#	ARTICLE	IF	CITATIONS
380	Anion-exchange membranes in electrochemical energy systems. Energy and Environmental Science, 2014, 7, 3135-3191.	30.8	1,617
381	Ab Initio Molecular Dynamics Study of the Aqueous HOO ⁻ Ion. Journal of Physical Chemistry B, 2014, 118, 7937-7945.	2.6	7
382	A multilayered representation, quantum mechanical and molecular mechanics study of the CH ₃ F ₂ + ⁺ OH ⁻ reaction in water. Journal of Computational Chemistry, 2014, 35, 3.3 445-450.		13
383	Local and Collective Reaction Coordinates in the Transport of the Aqueous Hydroxide Ion. Journal of Physical Chemistry B, 2014, 118, 8062-8069.	2.6	12
384	Thermodynamics of hydronium and hydroxide surface solvation. Chemical Science, 2014, 5, 1745.	7.4	56
385	Elucidation of Aqueous Solvent-Mediated Hydrogen-Transfer Reactions by ab Initio Molecular Dynamics and Nudged Elastic-Band Studies of NaBH ₄ Hydrolysis. Journal of Physical Chemistry C, 2014, 118, 21385-21399.	3.1	37
386	Dynamical aspects of intermolecular proton transfer in liquid water and low-density amorphous ices. Physical Review E, 2014, 89, 052130.	2.1	7
387	Quantum Simulation of Collective Proton Tunneling in Hexagonal Ice Crystals. Physical Review Letters, 2014, 112, 148302.	7.8	63
388	Structurally modified aromatic sulfone polymer nanocomposites as polyelectrolyte membranes. High Performance Polymers, 2014, 26, 550-560.	1.8	3
389	Factors enabling high mobility of protons and water in perfluorosulfonate membranes under low hydration conditions1. International Journal of Hydrogen Energy, 2014, 39, 2795-2800.	7.1	27
390	The role of the umbrella inversion mode in proton diffusion. Chemical Physics Letters, 2014, 599, 133-138.	2.6	31
391	Theoretical investigation of local proton conductance in the proton exchange membranes. Chemical Physics Letters, 2014, 608, 11-16.	2.6	9
392	Lattice Boltzmann modeling of water-like fluids. Frontiers in Physics, 2014, 2, .	2.1	8
393	Proton transfer in liquid water confined inside graphene slabs. Physical Review E, 2015, 92, 032402.	2.1	6
394	Redox levels in aqueous solution: Effect of van der Waals interactions and hybrid functionals. Journal of Chemical Physics, 2015, 143, 244508.	3.0	62
395	Communication: Dynamical and structural analyses of solid hydrogen under vapor pressure. Journal of Chemical Physics, 2015, 143, 171102.	3.0	16
396	Proton tunneling in low dimensional cesium silicate LDS-1. Journal of Chemical Physics, 2015, 143, 024503.	3.0	5
397	Vibrational dynamics of aqueous hydroxide solutions probed using broadband 2DIR spectroscopy. Journal of Chemical Physics, 2015, 143, 194501.	3.0	26

#	ARTICLE	IF	CITATIONS
398	Water-Assisted Selective Hydrodeoxygenation of Lignin-Derived Guaiacol to Monooxygenates. <i>ChemCatChem</i> , 2015, 7, 2669-2674.	3.7	32
399	Unique Hydrogen-Bonded Complex of Hydronium and Hydroxide Ions. <i>Chemistry - A European Journal</i> , 2015, 21, 6350-6354.	3.3	10
400	Long-range proton relay shows an inverse linear free energy relationship depending on the pKa of the hydrogen-bonded wire. <i>RSC Advances</i> , 2015, 5, 2669-2676.	3.6	2
401	Helical peptide-polyamine and -polyether conjugates as synthetic ionophores. <i>Bioorganic and Medicinal Chemistry</i> , 2015, 23, 7386-7393.	3.0	4
402	Theoretical Description of the Structural Characteristics of the Quaternized SEBS Anion-Exchange Membrane Using DFT. <i>Journal of Physical Chemistry C</i> , 2015, 119, 28235-28246.	3.1	25
403	Electrically aligned ion channels in cation exchange membranes and their polarized conductivity. <i>Journal of Membrane Science</i> , 2015, 478, 19-24.	8.2	40
404	Excited-State Hydroxide Ion Transfer from a Model Xanthenol Photobase. <i>Journal of Physical Chemistry B</i> , 2015, 119, 2498-2506.	2.6	8
405	On-the-fly-coupled cluster path-integral molecular dynamics: impact of nuclear quantum effects on the protonated water dimer. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 14355-14359.	2.8	27
406	Proton transfer through hydrogen bonds in two-dimensional water layers: A theoretical study based on <i>ab initio</i> and quantum-classical simulations. <i>Journal of Chemical Physics</i> , 2015, 142, 044701.	3.0	20
407	Is the structure of hydroxide dihydrate $\text{OH}^-(\text{H}_2\text{O})_2$? An <i>ab initio</i> path integral molecular dynamics study. <i>Theoretical Chemistry Accounts</i> , 2015, 134, 1.	1.4	3
408	Nuclear quantum effects in chemical reactions via higher-order path-integral calculations. <i>Chemical Physics</i> , 2015, 450-451, 95-101.	1.9	6
409	An analysis of hydrated proton diffusion in <i>ab initio</i> molecular dynamics. <i>Journal of Chemical Physics</i> , 2015, 142, 014104.	3.0	63
411	Cubane-like $(\text{COO}^-)_2(\text{H}_2\text{O})_6$ anion water clusters: New building blocks of two trinodal supramolecular networks with mixed-connectivity. <i>Inorganic Chemistry Communication</i> , 2015, 55, 77-82.	3.9	3
412	Structure and Dynamics of the Instantaneous Water/Vapor Interface Revisited by Path-Integral and <i>Ab Initio</i> Molecular Dynamics Simulations. <i>Journal of Physical Chemistry B</i> , 2015, 119, 10079-10086.	2.6	61
413	Preparation of heterogeneous bipolar membranes and their performance evaluation for the regeneration of acid and alkali. <i>RSC Advances</i> , 2015, 5, 57632-57639.	3.6	9
414	Vibrational Signatures of Solvent-Mediated Deformation of the Ternary Core Ion in Size-Selected $[\text{MgSO}_4\text{Mg}(\text{H}_2\text{O})_n]^{2+}$ Clusters. <i>Journal of Physical Chemistry A</i> , 2015, 119, 8294-8302.	2.5	20
415	Ground and Excited States Of $\text{OH}^-(\text{H}_2\text{O})_n$ Clusters. <i>Journal of Physical Chemistry A</i> , 2015, 119, 8188-8201.	2.5	9
416	Acid-base dissociation mechanisms and energetics at the silica-water interface: An activationless process. <i>Journal of Colloid and Interface Science</i> , 2015, 451, 231-244.	9.4	96

#	ARTICLE	IF	CITATIONS
417	Challenges in the Interpretation of Protein H/D Exchange Data: A Molecular Dynamics Simulation Perspective. <i>Biochemistry</i> , 2015, 54, 2683-2692.	2.5	58
418	Competitive excited-state single or double proton transfer mechanisms for bis-2,5-(2-benzoxazolyl)-hydroquinone and its derivatives. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 11990-11999.	2.8	243
419	Metal-organic frameworks and their derived nanostructures for electrochemical energy storage and conversion. <i>Energy and Environmental Science</i> , 2015, 8, 1837-1866.	30.8	1,483
420	Theoretical investigation on the excited-state intramolecular proton transfer mechanism of 2-(2-benzofuryl)-3-hydroxychromone. <i>Journal of Physical Organic Chemistry</i> , 2015, 28, 596-601.	1.9	17
421	A Semi-Interpenetrating Network Approach for Dimensionally Stabilizing Highly-Charged Anion Exchange Membranes for Alkaline Fuel Cells. <i>ChemSusChem</i> , 2015, 8, 1472-1483.	6.8	40
422	A review on recent developments of anion exchange membranes for fuel cells and redox flow batteries. <i>RSC Advances</i> , 2015, 5, 37206-37230.	3.6	209
423	Anisotropic radio-chemically pore-filled anion exchange membranes for solid alkaline fuel cell (SAFC). <i>Journal of Membrane Science</i> , 2015, 495, 206-215.	8.2	26
424	Modeling pH variation in reverse osmosis. <i>Water Research</i> , 2015, 87, 328-335.	11.3	28
425	Nitrogen-Doped Carbon Nanocoil Array Integrated on Carbon Nanofiber Paper for Supercapacitor Electrodes. <i>ACS Applied Materials & Interfaces</i> , 2015, 7, 19370-19381.	8.0	64
426	Interplay between water uptake, ion interactions, and conductivity in an e-beam grafted poly(ethylene-co-tetrafluoroethylene) anion exchange membrane. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 4367-4378.	2.8	83
427	Theoretical vibrational spectra of OH ⁺ (H ₂ O) ₂ : the effect of quantum distribution and vibrational coupling. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 25505-25515.	2.8	11
428	Basic science of water: Challenges and current status towards a molecular picture. <i>Nano Research</i> , 2015, 8, 3085-3110.	10.4	27
429	The accurate calculation of the band gap of liquid water by means of GW corrections applied to plane-wave density functional theory molecular dynamics simulations. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 365-375.	2.8	54
430	Theoretical study on excited-state proton transfer via hydrogen-bonded ethanol (EtOH) wire for 7Al in the gas phase. <i>Theoretical Chemistry Accounts</i> , 2015, 134, 1.	1.4	8
431	Enhancing performance of hybrid liquid membrane process supported by porous anionic exchange membranes for removal of cadmium from wastewater. <i>Chemical Engineering Journal</i> , 2015, 264, 241-250.	12.7	33
432	Modular organization of cardiac energy metabolism: energy conversion, transfer and feedback regulation. <i>Acta Physiologica</i> , 2015, 213, 84-106.	3.8	43
433	Chemically Induced Proton Transfer: Enolate Oxyluciferin as the Firefly Bioluminophore. <i>Journal of Physical Chemistry B</i> , 2015, 119, 2140-2148.	2.6	27
434	Ionic Hydrogen Bonding Vibration in OH ⁺ ·(H ₂ O) ₂ ·4O ₂ . <i>Journal of Computer Chemistry Japan</i> , 2016, 15, 192-198.	0.1	2

#	ARTICLE	IF	CITATIONS
435	Free-standing Functionalized Graphene Oxide Solid Electrolytes in Electrochemical Gas Sensors. <i>Advanced Functional Materials</i> , 2016, 26, 1729-1736.	14.9	110
436	Charge Transfer to LaAlO ₃ /SrTiO ₃ Interfaces Controlled by Surface Water Adsorption and Proton Hopping. <i>Advanced Functional Materials</i> , 2016, 26, 5453-5459.	14.9	19
437	Novel Processing of a Poly(phenyleneoxide) α -Poly(vinylbenzyltrimethylammonium) Copolymer Anion Exchange Membrane; The Effect On Mechanical And Transport Properties. <i>Electrochimica Acta</i> , 2016, 222, 1545-1554.	5.2	2
438	Microhydration of LiOH: Insight from electronic decays of core-ionized states. <i>Journal of Chemical Physics</i> , 2016, 144, 244302.	3.0	3
439	Proton diffusion dynamics along a diol as a proton-conducting wire in a photo-amphiprotic model system. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 32826-32839.	2.8	5
440	On the complex structural diffusion of proton holes in nanoconfined alkaline solutions within slit pores. <i>Nature Communications</i> , 2016, 7, 12625.	12.8	39
441	Zero-Gap Alkaline Water Electrolysis Using Ion-Solvating Polymer Electrolyte Membranes at Reduced KOH Concentrations. <i>Journal of the Electrochemical Society</i> , 2016, 163, F3125-F3131.	2.9	97
442	From Classical to Quantum and Back: A Hamiltonian Scheme for Adaptive Multiresolution Classical/Path-Integral Simulations. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 3030-3039.	5.3	20
443	Inverse Temperature Dependence of Nuclear Quantum Effects in DNA Base Pairs. <i>Journal of Physical Chemistry Letters</i> , 2016, 7, 2125-2131.	4.6	46
444	Nuclear Quantum Effects in Water and Aqueous Systems: Experiment, Theory, and Current Challenges. <i>Chemical Reviews</i> , 2016, 116, 7529-7550.	47.7	439
445	Ultrahigh humidity sensitivity of NaCl-added 3D mesoporous silica KIT-6 and its sensing mechanism. <i>RSC Advances</i> , 2016, 6, 38391-38398.	3.6	27
446	Proton Conductivity in Hydrogen Phosphate/Sulfates from a Coupled Molecular Dynamics/Lattice Monte Carlo (cMD/LMC) Approach. <i>Journal of Physical Chemistry C</i> , 2016, 120, 19913-19922.	3.1	11
447	DFT-TDDFT investigation of excited-state intramolecular proton transfer in 2-(2-hydroxyphenyl)benzimidazole derivatives: Effects of electron acceptor and donor groups. <i>Journal of Molecular Liquids</i> , 2016, 224, 83-88.	4.9	30
448	Base-hydration-resolved hydrogen-bond networking dynamics: Quantum point compression. <i>Journal of Molecular Liquids</i> , 2016, 223, 1277-1283.	4.9	26
449	Ab initio molecular dynamics study of Se(^{iv}) species in aqueous environment. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 26755-26763.	2.8	4
450	Proton Conductivity in Phosphoric Acid: The Role of Quantum Effects. <i>Physical Review Letters</i> , 2016, 117, 156001.	7.8	16
451	High performance aliphatic-heterocyclic benzyl-quaternary ammonium radiation-grafted anion-exchange membranes. <i>Energy and Environmental Science</i> , 2016, 9, 3724-3735.	30.8	215
452	Acidity Constant (pK_a) Calculation of Large Solvated Dye Molecules: Evaluation of Two Advanced Molecular Dynamics Methods. <i>ChemPhysChem</i> , 2016, 17, 3447-3459.	2.1	20

#	ARTICLE	IF	CITATIONS
453	Concentration-Dependent Proton Transfer Mechanisms in Aqueous NaOH Solutions: From Acceptor-Driven to Donor-Driven and Back. <i>Journal of Physical Chemistry Letters</i> , 2016, 7, 3302-3306.	4.6	66
454	Experimental and Theoretical Infrared Spectroscopic Study on Hydrated Nafion Membrane. <i>Macromolecules</i> , 2016, 49, 6621-6629.	4.8	58
455	Insight from Atomistic Simulations of Protonation Dynamics at the Nanoscale. <i>Fuel Cells</i> , 2016, 16, 682-694.	2.4	5
456	Combined Experimental and Theoretical Study of the Transient IR Spectroscopy of 7-Hydroxyquinoline in the First Electronically Excited Singlet State. <i>Journal of Physical Chemistry A</i> , 2016, 120, 9378-9389.	2.5	17
457	Origin of Acid-Base Catalytic Effects on Formaldehyde Hydration. <i>Journal of Physical Chemistry A</i> , 2016, 120, 9598-9606.	2.5	4
458	Nanoconfinement's Dramatic Impact on Proton Exchange between Glucose and Water. <i>Journal of Physical Chemistry Letters</i> , 2016, 7, 4597-4601.	4.6	14
459	Nuclear and Electron Wave Packet Molecular Dynamics Simulation Method and Its Application to Liquid, Solid and Supercooled Hydrogens. <i>Molecular Science</i> , 2016, 10, A0084.	0.2	0
460	High hydroxide conductivity in a chemically stable crystalline metal-organic framework containing a water-hydroxide supramolecular chain. <i>Chemical Communications</i> , 2016, 52, 8459-8462.	4.1	32
461	A Highly Hydroxide Conductive, Chemically Stable Anion Exchange Membrane, Poly(2,6 dimethyl 1,4) Tj ETQq0 0 0 rgBT /Overlock 10 Tf <i>Journal of the Electrochemical Society</i> , 2016, 163, H513-H520.	2.9	55
462	Protons and Hydroxide Ions in Aqueous Systems. <i>Chemical Reviews</i> , 2016, 116, 7642-7672.	47.7	358
463	Bicarbonate and chloride anion transport in anion exchange membranes. <i>Journal of Membrane Science</i> , 2016, 514, 125-134.	8.2	60
464	Ab Initio Molecular Dynamics Simulations of an Excess Proton in a Triethylene Glycol-Water Solution: Solvation Structure, Mechanism, and Kinetics. <i>Journal of Physical Chemistry B</i> , 2016, 120, 5223-5242.	2.6	5
465	Role of Presolvation and Anharmonicity in Aqueous Phase Hydrated Proton Solvation and Transport. <i>Journal of Physical Chemistry B</i> , 2016, 120, 1793-1804.	2.6	68
466	Synthesis of perfluorinated ionomers and their anion exchange membranes. <i>Journal of Membrane Science</i> , 2016, 515, 268-276.	8.2	24
467	Multistate empirical valence bond study of temperature and confinement effects on proton transfer in water inside hydrophobic nanochannels. <i>Journal of Computational Chemistry</i> , 2016, 37, 1935-1946.	3.3	4
468	Metal-Organic Frameworks Containing Missing-Linker Defects Leading to High Hydroxide-Ion Conductivity. <i>Chemistry - A European Journal</i> , 2016, 22, 1646-1651.	3.3	48
469	Hydroxide Solvation and Transport in Anion Exchange Membranes. <i>Journal of the American Chemical Society</i> , 2016, 138, 991-1000.	13.7	208
470	A facile functionalized routine for the synthesis of imidazolium-based anion-exchange membrane with excellent alkaline stability. <i>Journal of Membrane Science</i> , 2016, 505, 138-147.	8.2	63

#	ARTICLE	IF	CITATIONS
471	Effect of the bis-imidazolium-based poly(ionic liquid) on the microstructure and the properties of AAEMs based on polyvinyl alcohol. RSC Advances, 2016, 6, 25311-25318.	3.6	16
472	Alkaline anion exchange membranes based on KOH-treated multilayer graphene oxide. Journal of Membrane Science, 2016, 508, 51-61.	8.2	69
473	Anisotropic structure and dynamics of the solvation shell of a benzene solute in liquid water from ab initio molecular dynamics simulations. Physical Chemistry Chemical Physics, 2016, 18, 6132-6145.	2.8	20
474	Directed Assembly of Soft Colloids through Rapid Solvent Exchange. ACS Nano, 2016, 10, 1425-1433.	14.6	61
475	Synthesis, crystal and electronic structure, and optical properties of two new chalcogenide-iodides: Ba ₃ Q ₄ I ₂ (Q = S, Se). Inorganic Chemistry Frontiers, 2016, 3, 306-312.	6.0	5
476	Solid acid catalyzed synthesis of furans from carbohydrates. Catalysis Reviews - Science and Engineering, 2016, 58, 36-112.	12.9	111
477	Modeling quantum nuclei with perturbed path integral molecular dynamics. Chemical Science, 2016, 7, 1368-1372.	7.4	31
478	Divide-and-Conquer-Type Density-Functional Tight-Binding Simulations of Hydroxide Ion Diffusion in Bulk Water. Journal of Physical Chemistry B, 2017, 121, 1362-1371.	2.6	38
479	Significant Enhancement of Proton Transport in Bioinspired Peptide Fibrils by Single Acidic or Basic Amino Acid Mutation. Advanced Functional Materials, 2017, 27, 1604624.	14.9	38
480	The improved ion clustering and conductivity of a di-quaternized poly(arylene ether ketone) Tj ETQq1 1 0.784314 rgBT /Overlock 10 TES	4.9	10
481	Resolving H(Cl, Br, I) capabilities of transforming solution hydrogen-bond and surface-stress. Chemical Physics Letters, 2017, 678, 233-240.	2.6	31
482	Hybrid Energy Storage of Ni(OH) ₂ -coated N-doped Graphene Aerogel//N-doped Graphene Aerogel for the Replacement of NiCd and NiMH Batteries. Scientific Reports, 2017, 7, 1124.	3.3	35
483	Click mediated high-performance anion exchange membranes with improved water uptake. Journal of Materials Chemistry A, 2017, 5, 1022-1027.	10.3	39
484	Experimental evidence of a 3-centre, 2-electron covalent bond character of the central Oâ€“Hâ€“O fragment on the Zundel cation in crystals of Zundel nitranilate tetrahydrate. CrystEngComm, 2017, 19, 3898-3901.	2.6	11
485	What makes aromatic polyamide membranes superior: New insights into ion transport and membrane structure. Journal of Membrane Science, 2017, 540, 120-128.	8.2	45
486	Elaborating the excited-state proton transfer behaviors for novel 3H-MC and P2H-CH. Organic Chemistry Frontiers, 2017, 4, 1935-1942.	4.5	31
487	Importance of a Fully Anharmonic Treatment of Equilibrium Isotope Fractionation Properties of Dissolved Ionic Species As Evidenced by Li ⁺ (aq). Accounts of Chemical Research, 2017, 50, 1597-1605.	15.6	31
488	Waterâ€™chromophore electron transfer determines the photochemistry of cytosine and cytidine. Physical Chemistry Chemical Physics, 2017, 19, 17531-17537.	2.8	21

#	ARTICLE	IF	CITATIONS
489	Pitfall in Free-Energy Simulations on Simplest Systems. <i>ChemistrySelect</i> , 2017, 2, 4398-4418.	1.5	0
490	Second-Generation ReaxFF Water Force Field: Improvements in the Description of Water Density and OH-Anion Diffusion. <i>Journal of Physical Chemistry B</i> , 2017, 121, 6021-6032.	2.6	87
491	Role of solvation structure in the shuttling of the hydrated excess proton. <i>Journal of Chemical Sciences</i> , 2017, 129, 1045-1051.	1.5	4
492	HCl, KCl and KOH solvation resolved solute-solvent interactions and solution surface stress. <i>Applied Surface Science</i> , 2017, 422, 475-481.	6.1	20
493	A DFT/TDDFT Study on Excited State Process of a Novel Probe 4-Fluoroflavinol. <i>Journal of Cluster Science</i> , 2017, 28, 2449-2460.	3.3	9
494	Comparing hydroxide and hydronium at the instantaneous air-water interface using polarizable multi-state empirical valence bond models. <i>Computational and Theoretical Chemistry</i> , 2017, 1116, 64-72.	2.5	11
495	Proton Exchange in a Paramagnetic Chemical Exchange Saturation Transfer Agent from Experimental Studies and <i>ab Initio</i> Metadynamics Simulation. <i>Inorganic Chemistry</i> , 2017, 56, 4317-4323.	4.0	15
496	Proton-Transfer-Driven Water Exchange Mechanism in the Na ⁺ Solvation Shell. <i>Journal of Physical Chemistry B</i> , 2017, 121, 4184-4190.	2.6	18
497	The Hydrated Electron. <i>Annual Review of Physical Chemistry</i> , 2017, 68, 447-472.	10.8	136
499	Proton-Transfer Mechanisms at the Water-ZnO Interface: The Role of Presolvation. <i>Journal of Physical Chemistry Letters</i> , 2017, 8, 1476-1483.	4.6	106
500	Concerted Mechanisms of Excited-State Proton Intramolecular Transfer for Bis-2,4-(2-benzoxazolyl)-hydroquinone and Its Derivatives. <i>Journal of Physical Chemistry A</i> , 2017, 121, 8217-8226.	2.5	6
501	Proton mobility in aqueous systems: combining <i>ab initio</i> accuracy with millisecond timescales. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 28604-28609.	2.8	8
502	How Water's Properties Are Encoded in Its Molecular Structure and Energies. <i>Chemical Reviews</i> , 2017, 117, 12385-12414.	47.7	284
503	Direct Observation of Double Hydrogen Transfer via Quantum Tunneling in a Single Porphycene Molecule on a Ag(110) Surface. <i>Journal of the American Chemical Society</i> , 2017, 139, 12681-12687.	13.7	49
504	Theoretical Investigation of the H ₂ O ₂ -Induced Degradation Mechanism of Hydrated Nafion Membrane via Ether-Linkage Dissociation. <i>ACS Omega</i> , 2017, 2, 4053-4064.	3.5	29
505	Friction Regimes of Water-Lubricated Diamond (111): Role of Interfacial Ether Groups and Tribo-Induced Aromatic Surface Reconstructions. <i>Physical Review Letters</i> , 2017, 119, 096101.	7.8	63
506	Exploring the excited state behavior for 2-(phenyl)imidazo[4,5-c]pyridine in methanol solvent. <i>Scientific Reports</i> , 2017, 7, 11728.	3.3	22
507	Predicting the Ionic Product of Water. <i>Scientific Reports</i> , 2017, 7, 10244.	3.3	40

#	ARTICLE	IF	CITATIONS
508	Quantum Nuclear Dynamics of Protons within Layered Hydroxides at High Pressure. Scientific Reports, 2017, 7, 4842.	3.3	6
509	Nanoconfinement in Slit Pores Enhances Water Self-Dissociation. Physical Review Letters, 2017, 119, 056002.	7.8	70
510	Charge Effects on the Efflorescence in Single Levitated Droplets. Journal of Physical Chemistry A, 2017, 121, 6790-6799.	2.5	4
511	Combined multi-level quantum mechanics theories and molecular mechanics study of water-induced transition state of $\text{OH}^+ + \text{CO}_2$ reaction in aqueous solution. Chinese Physics B, 2017, 26, 103401.	1.4	0
512	Towards a dissociative SPC-like water model “probing the impact of intramolecular Coulombic contributions. Physical Chemistry Chemical Physics, 2017, 19, 31910-31920.	2.8	15
513	Partial Molar Volumes of Aqua Ions from First Principles. Journal of Chemical Theory and Computation, 2017, 13, 3427-3431.	5.3	7
514	Surface modification of PVDF membrane by radiation-induced graft polymerization for novel membrane bioreactor. Journal of Industrial and Engineering Chemistry, 2017, 46, 103-110.	5.8	44
515	Structure of aqueous NaOH solutions: insights from neural-network-based molecular dynamics simulations. Physical Chemistry Chemical Physics, 2017, 19, 82-96.	2.8	64
516	Potentials of mean force in acidic proton transfer reactions in constrained geometries. Molecular Simulation, 2017, 43, 134-140.	2.0	0
517	Collective proton transfer in ordinary ice: local environments, temperature dependence and deuteration effects. Physical Chemistry Chemical Physics, 2017, 19, 2623-2635.	2.8	33
518	Molecular modeling of OH^- transport in poly(arylene ether sulfone ketone)s containing quaternized ammonio-substituted fluorenyl groups as anion exchange membranes. Journal of Membrane Science, 2017, 522, 237-244.	8.2	44
519	Cation Hydration in Supercritical NaOH and HCl Aqueous Solutions. Journal of Physical Chemistry B, 2017, 121, 11383-11389.	2.6	11
520	Anomalous thermal properties of water. Journal of Water Chemistry and Technology, 2017, 39, 331-338.	0.6	2
521	From classical to quantum and back: Hamiltonian adaptive resolution path integral, ring polymer, and centroid molecular dynamics. Journal of Chemical Physics, 2017, 147, 244104.	3.0	13
522	Polarized Neutron Reflectometry of Metal Consumption and Passive Film Growth on Nickel Exposed to an Alkaline Deuterium Oxide (D_2O) Solution. Journal of the Electrochemical Society, 2017, 164, C699-C707.	2.9	4
523	Ground-State Long-Range Proton Transfer Controlled by Proton-Accepting Ability of Hydrogen-Bonded Chains: A Theoretical Study. Progress in Reaction Kinetics and Mechanism, 2017, 42, 384-396.	2.1	0
524	The effect of SiO_2 additives on solid hydroxide ion-conducting polymer electrolytes: a Raman microscopy study. Physical Chemistry Chemical Physics, 2018, 20, 7148-7155.	2.8	10
525	Nuclear quantum effects enter the mainstream. Nature Reviews Chemistry, 2018, 2, .	30.2	271

#	ARTICLE	IF	CITATIONS
526	Acid resistant sulphonated poly(vinylidene fluoride-co-hexafluoropropylene)/graphene oxide composite cation exchange for water splitting by iodine-sulfur bunsen process for hydrogen production. Journal of Membrane Science, 2018, 552, 377-386.	8.2	21
527	Effect of CO ₂ absorption on ion and water mobility in an anion exchange membrane. Journal of Power Sources, 2018, 380, 64-75.	7.8	53
528	Permutationally Invariant Potential Energy Surfaces. Annual Review of Physical Chemistry, 2018, 69, 151-175.	10.8	152
529	The Effect of Ambient Carbon Dioxide on Anion-Exchange Membrane Fuel Cells. ChemSusChem, 2018, 11, 1136-1150.	6.8	137
530	Different ESIPT Mechanisms for Angular-Shaped Quinacridone in Toluene and Dimethyl Formamide (DMF) Solvents: A Theoretical Study. Journal of the Chinese Chemical Society, 2018, 65, 667-673.	1.4	2
531	Nuclear quantum effects on the vibrational dynamics of liquid water. Journal of Chemical Physics, 2018, 148, 102328.	3.0	27
532	Synthesis and Properties of Symmetric Side-Chain Quaternized Poly(Arylene Ether Sulfone)s for Anion Exchange Membrane Fuel Cells. Macromolecular Chemistry and Physics, 2018, 219, 1700416.	2.2	4
533	Performance of an environmentally benign acid base flow battery at high energy density. International Journal of Energy Research, 2018, 42, 1524-1535.	4.5	42
534	(H, Li)Br and LiOH Solvation Bonding Dynamics: Molecular Nonbond Interactions and Solute Extraordinary Capabilities. Journal of Physical Chemistry B, 2018, 122, 1228-1238.	2.6	28
535	Theoretical study on the substituent effect of halogen atom at different position of 7-azaindole-water derivatives: relative stability and excited-state proton-transfer mechanism. Structural Chemistry, 2018, 29, 1341-1350.	2.0	8
536	Local initiation conditions for water autoionization. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, E4569-E4576.	7.1	52
537	Assessing Many-Body Effects of Water Self-Ions. I: OH ⁻ (H ₂ O) _n Clusters. Journal of Chemical Theory and Computation, 2018, 14, 1982-1997.	5.3	38
538	Selectivity of ion exchange membranes: A review. Journal of Membrane Science, 2018, 555, 429-454.	8.2	722
539	Solvent-controlled tautomerism of malononitrile-naphthalimide via intramolecular proton transfer. Dyes and Pigments, 2018, 155, 121-125.	3.7	8
540	The critical relation between chemical stability of cations and water in anion exchange membrane fuel cells environment. Journal of Power Sources, 2018, 375, 351-360.	7.8	179
541	Theoretical Study on the Substituent Effect on the Excited-State Proton Transfer in the 7-Azaindole-Water Derivatives. Photochemistry and Photobiology, 2018, 94, 27-35.	2.5	7
542	Accuracy of Potfit-based potential representations and its impact on the performance of (ML-)MCTDH. Chemical Physics, 2018, 509, 116-130.	1.9	11
543	Perturbed path integrals in imaginary time: Efficiently modeling nuclear quantum effects in molecules and materials. Journal of Chemical Physics, 2018, 148, 102325.	3.0	10

#	ARTICLE	IF	CITATIONS
544	Influence of the hydrogen bond quantum nature in liquid water and heavy water on stimulated Raman scattering. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2018, 199, 462-464.	3.9	9
545	Nuclear Quantum Effect and H/D Isotope Effect on Hydrogen-Bonded Systems with Path Integral Simulation. , 2018, , 377-399.		1
546	Liquidâ€“Vapor Phase Diagram of RPBE-D3 Water: Electronic Properties along the Coexistence Curve and in the Supercritical Phase. <i>Journal of Physical Chemistry B</i> , 2018, 122, 3318-3329.	2.6	33
547	Exploring excitedâ€“state proton transfer mechanism for 9,10â€“dihydroxybenzo[h]quinolone. <i>Journal of Physical Organic Chemistry</i> , 2018, 31, e3756.	1.9	3
548	Microtopographic control on the ground thermal regime in ice wedge polygons. <i>Cryosphere</i> , 2018, 12, 1957-1968.	3.9	34
549	Hydroxide Transport in Anion-Exchange Membranes for Alkaline Fuel Cells. , 0, , .		4
550	Coupled Multimodal Dynamics of Hydrogen-Containing Ion Networks in Water-Deficient, Sodium Hydroxide-Aluminate Solutions. <i>Journal of Physical Chemistry B</i> , 2018, 122, 12097-12106.	2.6	12
551	Aqueous charge injection: solvation bonding dynamics, molecular nonbond interactions, and extraordinary solute capabilities. <i>International Reviews in Physical Chemistry</i> , 2018, 37, 363-558.	2.3	26
552	Binary Alkoxide Ionic Liquids. <i>ACS Sustainable Chemistry and Engineering</i> , 2018, 6, 13676-13680.	6.7	19
553	Nuclear Quantum Effects in Sodium Hydroxide Solutions from Neural Network Molecular Dynamics Simulations. <i>Journal of Physical Chemistry B</i> , 2018, 122, 10158-10171.	2.6	29
554	A Highly Conductive and Mechanically Robust OH ^{âˆ’} Conducting Membrane for Alkaline Water Electrolysis. <i>Chemistry of Materials</i> , 2018, 30, 6420-6430.	6.7	43
555	Density functional theory studies on the external OH ^{âˆ’} -induced barrierless proton dissociation mechanism for the forced hydrolysis reaction of Al ³⁺ (aq). <i>International Journal of Quantum Chemistry</i> , 2018, 118, e25682.	2.0	4
556	Sulfonated Nanobamboo Fiber-Reinforced Quaternary Ammonia Poly(ether ether ketone) Membranes for Alkaline Polymer Electrolyte Fuel Cells. <i>ACS Applied Materials & Interfaces</i> , 2018, 10, 33581-33588.	8.0	24
557	Investigation of hydroxide ion-conduction in solid polymer electrolytes via electrochemical impedance spectroscopy. <i>Electrochimica Acta</i> , 2018, 288, 1-11.	5.2	4
558	Aqueous sodium hydroxide (NaOH) solutions at high pressure and temperature: insights from <i>in situ</i> Raman spectroscopy and <i>ab initio</i> molecular dynamics simulations. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 21629-21639.	2.8	15
559	Anionic Water Cluster Polymers [(H ₂ O) ₁₈ (OH) ₂] _n Is Stabilized by Bis(2,2â€“bipyridine) Cupric Chloride [Cu(bipy) ₂ Cl] ^{âˆ’} . <i>Molecules</i> , 2018, 23, 195.	3.8	6
560	Entangled trajectories Hamiltonian dynamics for treating quantum nuclear effects. <i>Journal of Chemical Physics</i> , 2018, 148, 144106.	3.0	3
561	Molecular Simulation of Quaternary Ammonium Solutions at Low Hydration Levels. <i>Journal of Physical Chemistry C</i> , 2018, 122, 11204-11213.	3.1	43

#	ARTICLE	IF	CITATIONS
562	Unusual Proton Transfer Kinetics in Water at the Temperature of Maximum Density. Physical Review Letters, 2018, 121, 076001.	7.8	6
563	Benchmark Electronic Structure Calculations for H_3O^+ (H_2O) n , $n = 0-5$, Clusters and Tests of an Existing 1,2,3-Body Potential Energy Surface with a New 4-Body Correction. Journal of Chemical Theory and Computation. 2018, 14, 4553-4566.	5.3	39
564	Electronic state and optical response in a hydrogen-bonded molecular conductor. Physical Review B, 2018, 97, .	3.2	5
565	Structural aspects of the topological model of the hydrogen bond in water on auto-dissociation <i>via</i> proton transfer. Physical Chemistry Chemical Physics, 2018, 20, 16414-16427.	2.8	13
566	The Case of Formic Acid on Anatase TiO_2 (101): Where is the Acid Proton?. Angewandte Chemie, 2019, 131, 12561-12564.	2.0	10
567	Specific Reaction Parameter Multigrid POTFIT (SRP-MGPF): Automatic Generation of Sum-of-Products Form Potential Energy Surfaces for Quantum Dynamical Calculations. Frontiers in Chemistry, 2019, 7, 576.	3.6	6
568	An ab initio molecular dynamics study of benzene in water at supercritical conditions: Structure, dynamics, and polarity of hydration shell water and the solute. Journal of Chemical Physics, 2019, 151, 044508.	3.0	6
569	High-Level VSCF/VCI Calculations Decode the Vibrational Spectrum of the Aqueous Proton. Journal of Physical Chemistry B, 2019, 123, 7214-7224.	2.6	23
570	The Case of Formic Acid on Anatase TiO_2 (101): Where is the Acid Proton?. Angewandte Chemie - International Edition, 2019, 58, 12431-12434.	13.8	59
571	DPD simulations of anion exchange membrane: The effect of an alkyl spacer on the hydrated morphology. Solid State Ionics, 2019, 339, 115012.	2.7	18
572	Superionic conduction along ordered hydroxyl networks in molecular-thin nanosheets. Materials Horizons, 2019, 6, 2087-2093.	12.2	22
574	Lewis Basic and H_2O_2 Solutions: $\text{O}^{\bullet-}:\text{O}$ Compression. Springer Series in Chemical Physics, 2019, , 103-127.	0.2	0
575	DPD simulations of anion exchange membranes functionalized with various cationic groups and associated anions. Solid State Ionics, 2019, 340, 115011.	2.7	20
576	Proton diffusion facilitated by indirect interactions between proton donors through several hydrogen bonds. Chemical Physics Letters, 2019, 731, 136627.	2.6	10
577	Hydroxide Ion Diffusion in Anion-Exchange Membranes at Low Hydration: Insights from Ab Initio Molecular Dynamics. Chemistry of Materials, 2019, 31, 5778-5787.	6.7	64
578	Lewis Acidic Solutions: H^+H Fragilization. Springer Series in Chemical Physics, 2019, , 85-102.	0.2	0
579	Water Plays a Cocatalytic Role in Epoxide Ring Opening Reaction in Aspartate Proteases: A QM/MM Study. Journal of Physical Chemistry B, 2019, 123, 7955-7964.	2.6	10
580	Light, temperature, and pH control of aqueous azopyridine-terminated poly(N-isopropylacrylamide) solutions. Polymer Chemistry, 2019, 10, 5080-5086.	3.9	14

#	ARTICLE	IF	CITATIONS
581	Ultrafast Proton Transport between a Hydroxy Acid and a Nitrogen Base along Solvent Bridges Governed by the Hydroxide/Methoxide Transfer Mechanism. <i>Journal of the American Chemical Society</i> , 2019, 141, 14581-14592.	13.7	26
582	Structural modifications and ionic transport of PVA-KOH hydrogels applied in Zn/Air batteries. <i>Journal of Electroanalytical Chemistry</i> , 2019, 850, 113380.	3.8	66
583	Structure of the aqueous electron. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 20538-20565.	2.8	54
584	Hiding in the Crowd: Spectral Signatures of Overcoordinated Hydrogen-Bond Environments. <i>Journal of Physical Chemistry Letters</i> , 2019, 10, 6067-6073.	4.6	22
585	Ultraviolet-photon exposure stimulates negative current conductivity in amorphous ice below 50â€°K. <i>Chemical Physics Letters</i> , 2019, 737, 136820.	2.6	6
586	The effect of different environments on excited-state intramolecular proton transfer in 4â€²-methoxy-3-hydroxyflavone. <i>Organic Chemistry Frontiers</i> , 2019, 6, 218-225.	4.5	28
587	One-dimensional vs. two-dimensional proton transport processes at solidâ€“liquid zinc-oxideâ€“water interfaces. <i>Chemical Science</i> , 2019, 10, 1232-1243.	7.4	39
588	Diffusion-free Grotthuss topochemistry for high-rate and long-life proton batteries. <i>Nature Energy</i> , 2019, 4, 123-130.	39.5	446
589	Kinetic Significance of Protonâ€“Electron Transfer during Condensed Phase Reduction of Carbonyls on Transition Metal Clusters. <i>ACS Catalysis</i> , 2019, 9, 1763-1778.	11.2	45
590	Unprecedented O:â†”:O compression and Hâ†”H fragilization in Lewis solutions. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 2234-2250.	2.8	27
591	Proton transfer in hydrogen-bonded degenerate systems of water and ammonia in metalâ€“organic frameworks. <i>Chemical Science</i> , 2019, 10, 16-33.	7.4	224
592	Resolving local configurational contributions to X-ray and neutron radial distribution functions within solutions of concentrated electrolytes â€“ a case study of concentrated NaOH. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 6828-6838.	2.8	14
593	Effect of CO ₂ on the properties of anion exchange membranes for fuel cell applications. <i>Journal of Membrane Science</i> , 2019, 586, 140-150.	8.2	61
594	Effect of Carbonate Anions on Quaternary Ammonium-Hydroxide Interaction. <i>Journal of Physical Chemistry C</i> , 2019, 123, 15956-15962.	3.1	17
595	<i>Ab initio</i> molecular dynamics studies of hydroxide coordination of alkaline earth metals and uranyl. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 13809-13820.	2.8	6
596	Evaluation of the electrical and dielectric behavior of hybrid materials based on layered zinc hydroxide and benzoate. <i>Ionics</i> , 2019, 25, 5391-5399.	2.4	1
597	Investigation of the Structure of Concentrated NaOH Aqueous Solutions by Combining Molecular Dynamics and Wide-Angle X-ray Scattering. <i>Journal of Physical Chemistry B</i> , 2019, 123, 5121-5130.	2.6	11
598	Preparation of Polysulfone anion exchange membranes incorporated with Gemini cationic molecules. <i>Journal of Polymer Research</i> , 2019, 26, 1.	2.4	3

#	ARTICLE	IF	CITATIONS
599	Multiscale water dynamics in model Anion Exchange Membranes for Alkaline Membrane Fuel Cells. Journal of Membrane Science, 2019, 586, 240-247.	8.2	10
600	Discovery of precise pH-controlled biomimetic catalysts: defective zirconium metal-organic frameworks as alkaline phosphatase mimics. Nanoscale, 2019, 11, 11270-11278.	5.6	29
601	Counter Cations Affect Transport in Aqueous Hydroxide Solutions with Ion Specificity. Journal of the American Chemical Society, 2019, 141, 6930-6936.	13.7	18
602	A Quasielastic Neutron Scattering Study of Water Diffusion in Model Anion Exchange Membranes over Localized and Extended Volume Increments. Journal of Physical Chemistry C, 2019, 123, 14195-14206.	3.1	18
603	Water in zeolite L and its MOF mimic. Zeitschrift Fur Kristallographie - Crystalline Materials, 2019, 234, 495-511.	0.8	10
604	Ionized water confined in graphene nanochannels. Physical Chemistry Chemical Physics, 2019, 21, 9285-9295.	2.8	10
605	The quantum nature of hydrogen. International Reviews in Physical Chemistry, 2019, 38, 35-61.	2.3	18
606	Advances and issues in developing salt-concentrated battery electrolytes. Nature Energy, 2019, 4, 269-280.	39.5	1,026
607	Cation exchange membrane based on side chain grafted sulfonic acid with poly(vinylidene) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 427 Td Science, 2019, 580, 134-142.	8.2	8
608	A Roadmap to Low-Cost Hydrogen with Hydroxide Exchange Membrane Electrolyzers. Advanced Materials, 2019, 31, e1805876.	21.0	184
609	Exploring Side-Chain Designs for Enhanced Ion Conductivity of Anion-Exchange Membranes by Mesoscale Simulations. Journal of Physical Chemistry C, 2019, 123, 10802-10815.	3.1	36
610	Versatile electrification of two-dimensional nanomaterials in water. Nature Communications, 2019, 10, 1656.	12.8	66
611	Possible low-energy isomers of OH (H ₂ O) ₄ (n = 0, ±1) clusters via the particle swarm optimization algorithm: An ab initio study. Computational and Theoretical Chemistry, 2019, 1155, 20-30.	2.5	1
612	pH-Dependent Morphology and Photoresponse of Azopyridine-Terminated Poly(<i>N</i> -isopropylacrylamide) Nanoparticles in Water. Macromolecules, 2019, 52, 2939-2948.	4.8	17
613	Theoretical study on kinetics of ammonia-catalyzed ground-state tautomerization in 2-pyridone: effect of chemical modification. Chemical Papers, 2019, 73, 1561-1569.	2.2	4
614	Ab Initio Molecular Dynamics Study of Hydroxide Diffusion Mechanisms in Nanoconfined Structural Mimics of Anion Exchange Membranes. Journal of Physical Chemistry C, 2019, 123, 4638-4653.	3.1	43
615	Quantum nature of the hydrogen bond from ambient conditions down to ultra-low temperatures. Physical Chemistry Chemical Physics, 2019, 21, 24967-24975.	2.8	15
616	Modeling chemical reactions on surfaces: The roles of chemical bonding and van der Waals interactions. Progress in Surface Science, 2019, 94, 100561.	8.3	39

#	ARTICLE	IF	CITATIONS
617	Recycling of isopropanol for cost-effective, environmentally friendly production of carboxymethylated cellulose nanofibrils. Carbohydrate Polymers, 2019, 208, 365-371.	10.2	5
618	Robust High Thermoelectric Harvesting Under a Self-Humidifying Bilayer of Metal Organic Framework and Hydrogel Layer. Advanced Functional Materials, 2019, 29, 1807549.	14.9	64
619	Characterization of transport through polymers for fracking fluid treatment and organic acid concentration in extractive membrane bioreactors. Journal of Chemical Technology and Biotechnology, 2019, 94, 690-700.	3.2	5
620	Molecular dynamics simulation on the effect of water uptake on hydrogen bond network for OH ⁺ conduction in imidazolium-g-PPO membrane. International Journal of Hydrogen Energy, 2019, 44, 3760-3770.	7.1	30
621	The theoretical study about the ESIPT mechanism for 2,4-bis(benzooxazol-2-yl)hydroquinone: Single or double?. Journal of Physical Organic Chemistry, 2019, 32, e3903.	1.9	7
622	Effects of different oxygen-containing anions on the structure of water clusters. Supramolecular Chemistry, 2019, 31, 283-287.	1.2	2
623	Recent advances in quantum-mechanical molecular dynamics simulations of proton transfer mechanism in various water-based environments. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2020, 10, e1419.	14.6	10
624	Preparation of click-driven cross-linked anion exchange membranes with low water uptake. Particology, 2020, 48, 65-73.	3.6	13
625	Phosphoric acid doped triazole-containing cross-linked polymer electrolytes with enhanced stability for high-temperature proton exchange membrane fuel cells. Journal of Membrane Science, 2020, 595, 117508.	8.2	45
626	Pressure-dependent electronic structure calculations using integral equation-based solvation models. Biophysical Chemistry, 2020, 257, 106258.	2.8	14
627	Theoretical exploration about the ESIPT mechanism and hydrogen bonding interaction for 2-(3,5-dichloro-2-hydroxyphenyl)-benzoxazole-6-carboxylic acid. Journal of Physical Organic Chemistry, 2020, 33, e4020.	1.9	3
628	Hydroxide ion conducting polymer electrolytes and their applications in solid supercapacitors: A review. Energy Storage Materials, 2020, 24, 6-21.	18.0	108
629	Temperature effects on the ionic conductivity in concentrated alkaline electrolyte solutions. Physical Chemistry Chemical Physics, 2020, 22, 10426-10430.	2.8	25
630	Physical principles of the formation of a nanoparticle electric double layer in metal hydrosols. Colloid and Polymer Science, 2020, 298, 1-7.	2.1	4
631	In-depth understanding of the CO ₂ limitation of air fed anion exchange membrane fuel cells. Sustainable Energy and Fuels, 2020, 4, 1801-1811.	4.9	8
632	Membranes for zinc-air batteries: Recent progress, challenges and perspectives. Journal of Power Sources, 2020, 475, 228689.	7.8	58
633	The Role of Protons and Hydrides in the Catalytic Hydrogenolysis of Guaiacol at the Ruthenium Nanoparticle-Water Interface. ACS Catalysis, 2020, 10, 12310-12332.	11.2	29
634	Stabilization of Hydroxide Ions at the Interface of a Hydrophobic Monolayer on Water via Reduced Proton Transfer. Physical Review Letters, 2020, 125, 156803.	7.8	21

#	ARTICLE	IF	CITATIONS
635	Hydration structure of As ^{III} aqueous solutions from ab initio molecular dynamics simulations. Journal of Molecular Liquids, 2020, 318, 114056.	4.9	0
636	Hydroxide-Enhanced Superexchange Magnetic Couplings in Ionic Clathrate Hydrates. Journal of Physical Chemistry C, 2020, 124, 25455-25464.	3.1	0
637	Adding salt to expand voltage window of humid ionic liquids. Nature Communications, 2020, 11, 5809.	12.8	60
638	Tuning water reduction through controlled nanoconfinement within an organic liquid matrix. Nature Catalysis, 2020, 3, 656-663.	34.4	91
639	Investigation of Itaconic Acid Separation by Operating a Commercialized Electrodialysis Unit with Bipolar Membranes. Processes, 2020, 8, 1031.	2.8	3
640	Slowing Down of the Molecular Reorientation of Water in Concentrated Alkaline Solutions. Journal of Physical Chemistry B, 2020, 124, 8309-8316.	2.6	6
641	Synthesis, characterization, thermal properties and biological activity of diazine-ring containing hydrazones and their metal complexes. Journal of Thermal Analysis and Calorimetry, 2022, 147, 229-242.	3.6	1
642	Controlling Keto-Enol Tautomerism of Ureidopyrimidinone to Generate a Single-Quadruple AADD-DDAA Dimeric Array. Organic Letters, 2020, 22, 7305-7309.	4.6	6
643	Recent Advances in Bipolar Membrane Design and Applications. Chemistry of Materials, 2020, 32, 8060-8090.	6.7	96
644	Mechanistic Insights into the Hydrogen Oxidation Reaction on PtNi Alloys in Alkaline Media: A First-Principles Investigation. ACS Applied Materials & Interfaces, 2020, 12, 40248-40260.	8.0	33
645	How Can Protons Migrate in Extremely Compressed Liquid Water?. Physical Review Letters, 2020, 125, 086001.	7.8	3
646	Reactive Molecular Dynamics at Constant Pressure via Nonreactive Force Fields: Extending the Empirical Valence Bond Method to the Isothermal-Isobaric Ensemble. Journal of Physical Chemistry A, 2020, 124, 7585-7597.	2.5	3
647	Through-Plane Conductivity of Anion Exchange Membranes at Sub-Freezing Temperatures- Hydroxide vs (Bi-)Carbonate Ions. Journal of the Electrochemical Society, 2020, 167, 084513.	2.9	8
648	Hydration Properties of H_nPO_4 ($n = 1-3$) From Ab Initio Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2020, 124, 5454-5464.	2.6	4
649	Unexpected hydroxide ion structure and properties at low hydration. Journal of Molecular Liquids, 2020, 313, 113485.	4.9	25
650	ABEEM/MM OH ⁻ Models for OH ⁻ (H ₂ O) _n Clusters and Aqueous OH ⁻ : Structures, Charge Distributions, and Binding Energies. Journal of Physical Chemistry A, 2020, 124, 5963-5978.	2.5	7
651	Water Layering Affects Hydroxide Diffusion in Functionalized Nanoconfined Environments. Journal of Physical Chemistry Letters, 2020, 11, 5087-5091.	4.6	25
652	Ultrafast Proton Transfer Dynamics on the Repulsive Potential of the Ethanol Dication: Roaming-Mediated Isomerization versus Coulomb Explosion. Journal of Physical Chemistry A, 2020, 124, 2785-2791.	2.5	27

#	ARTICLE	IF	CITATIONS
653	Simulation study of the effects of phase separation on hydroxide solvation and transport in anion exchange membranes. <i>Journal of Chemical Physics</i> , 2020, 152, 094903.	3.0	9
654	Hybrid Solvation Model with First Solvation Shell for Calculation of Solvation Free Energy. <i>ChemPhysChem</i> , 2020, 21, 762-769.	2.1	5
655	Ion conduction switching between H^{+} and OH^{-} induced by pH in graphene oxide. <i>Chemical Communications</i> , 2020, 56, 4364-4367.	4.1	14
656	Theoretical insights into excited-state hydrogen bonding effects and intramolecular proton transfer (ESIPT) mechanism for BTS system. <i>Scientific Reports</i> , 2020, 10, 5119.	3.3	22
657	Dynamics of Water in the Solvation Shell of an Iodate Ion: A Born–Oppenheimer Molecular Dynamics Study. <i>Journal of Physical Chemistry B</i> , 2020, 124, 2618-2631.	2.6	3
658	Experimental Approach to Physicochemical Hydrogen Processes on Cosmic Ice Dust. <i>Journal of the Physical Society of Japan</i> , 2020, 89, 051015.	1.6	6
659	A comprehensive review on water management strategies and developments in anion exchange membrane fuel cells. <i>International Journal of Hydrogen Energy</i> , 2020, 45, 19642-19663.	7.1	51
660	Hydrogen Bond Dynamics in the Solvation Shell on Proton Transfer in Aqueous Solution. <i>Journal of Physical Chemistry B</i> , 2020, 124, 1817-1823.	2.6	9
661	DFT modelling of explicit solid–solid interfaces in batteries: methods and challenges. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 10412-10425.	2.8	44
662	PiNN: A Python Library for Building Atomic Neural Networks of Molecules and Materials. <i>Journal of Chemical Information and Modeling</i> , 2020, 60, 1184-1193.	5.4	48
663	Designing Anion Exchange Membranes with Enhanced Hydroxide Ion Conductivity by Mesoscale Simulations. <i>Journal of Physical Chemistry C</i> , 2020, 124, 4470-4482.	3.1	34
664	Zeolite Synthesis under Nonconventional Conditions: Reagents, Reactors, and <i>Modi Operandi</i> . <i>Chemistry of Materials</i> , 2020, 32, 4884-4919.	6.7	45
665	Revealing and comparing different excited-state intramolecular proton transfer processes for 3-ethyl-2-quinolinecarboxylic acid. <i>Journal of Physical Chemistry A</i> , 2020, 124, 1367-1373.	1.4	0
666	Description of Hydroxide Ion Structural Diffusion in a Quaternized SEBS Anion Exchange Membrane Using Ab Initio Molecular Dynamics. <i>Journal of Physical Chemistry C</i> , 2020, 124, 9834-9851.	3.1	13
667	Effective ion mobility in anion exchange ionomers: Relations with hydration, porosity, tortuosity, and percolation. <i>Journal of Membrane Science</i> , 2021, 617, 118622.	8.2	33
668	Interplay of the functional units of a binder in the oxygen reduction process of zinc-air battery. <i>Catalysis Today</i> , 2021, 370, 66-74.	4.4	9
669	Hydroxide promotes ion pairing in the $NaNO_2$ – $NaOH$ – H_2O system. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 112-122.	2.8	8
670	Rejection of harsh pH saline solutions using graphene membranes. <i>Carbon</i> , 2021, 171, 240-247.	10.3	9

#	ARTICLE	IF	CITATIONS
671	Super-ions of sodium cations with hydrated hydroxide anions: inorganic structure-directing agents in zeolite synthesis. <i>Materials Horizons</i> , 2021, 8, 2576-2583.	12.2	16
672	Distinct molecular dynamics dividing liquid-like and gas-like supercritical hydrogens. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 22110-22118.	2.8	7
673	Proton transfer in bulk water using the full adaptive QM/MM method: integration of solute- and solvent-adaptive approaches. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 8344-8360.	2.8	7
674	Hydronium ion diffusion in model proton exchange membranes at low hydration: insights from <i>ab initio</i> molecular dynamics. <i>Journal of Materials Chemistry A</i> , 2021, 9, 2448-2458.	10.3	25
675	Electron Density Change in Semiconductor by Ion Adsorption at Solid-Liquid Interface. <i>Advanced Materials</i> , 2021, 33, e2007581.	21.0	11
676	Emerging Porous Solid Electrolytes for Hydroxide Ion Transport. <i>Advanced Functional Materials</i> , 2021, 31, 2100083.	14.9	27
677	Conductive and Stable Crosslinked Anion Exchange Membranes Based on Poly(arylene ether sulfone). <i>Macromolecular Research</i> , 2021, 29, 157-163.	2.4	7
678	Confining Water in Ionic and Organic Solvents to Tune Its Adsorption and Reactivity at Electrified Interfaces. <i>Accounts of Chemical Research</i> , 2021, 54, 1034-1042.	15.6	21
679	Designing anion exchange membranes for CO ₂ electrolyzers. <i>Nature Energy</i> , 2021, 6, 339-348.	39.5	209
680	Switching between Proton Vacancy and Excess Proton Transfer Pathways in the Reaction between 7-Hydroxyquinoline and Formate. <i>Journal of Physical Chemistry A</i> , 2021, 125, 1845-1859.	2.5	10
681	Self-interaction correction in water-ion clusters. <i>Journal of Chemical Physics</i> , 2021, 154, 094302.	3.0	16
682	Mesoscale Simulation on the Hydrated Morphologies of SPEEK Membrane. <i>Macromolecular Theory and Simulations</i> , 2021, 30, 2100006.	1.4	4
683	First-Principles Grand-Canonical Simulations of Water Adsorption in Proton-Exchanged Zeolites. <i>Journal of Physical Chemistry C</i> , 2021, 125, 6090-6098.	3.1	11
684	A Triad Fluorenone Derivative Bearing Two Imidazole Groups That Switches between Three States by Base and Acid Stimuli. <i>Chemistry Letters</i> , 2021, 50, 1363-1367.	1.3	0
685	Identifying the structural relaxation dynamics in a strongly asymmetric binary glass former. <i>Journal of Chemical Physics</i> , 2021, 154, 144504.	3.0	5
686	OH ⁻ and H ₃ O ⁺ Diffusion in Model AEMs and PEMs at Low Hydration: Insights from Ab Initio Molecular Dynamics. <i>Membranes</i> , 2021, 11, 355.	3.0	11
687	Metallopolymer as a Solid Electrolyte for Rechargeable Zn-Metal Alkaline Batteries. , 2021, 3, 799-806.		9
688	Progress in neutron techniques: towards improved polymer electrolyte membranes for energy devices. <i>Journal of Physics Condensed Matter</i> , 2021, 33, 264005.	1.8	3

#	ARTICLE	IF	CITATIONS
689	The hopping mechanism of the hydrated excess proton and its contribution to proton diffusion in water. <i>Journal of Chemical Physics</i> , 2021, 154, 194506.	3.0	12
690	Mapping the Design of Electrolyte Materials for Electrically Rechargeable Zinc–Air Batteries. <i>Advanced Materials</i> , 2021, 33, e2006461.	21.0	63
691	Magnetic field-induced capacitance change in aqueous carbon-based supercapacitors. <i>Cell Reports Physical Science</i> , 2021, 2, 100455.	5.6	13
692	Investigating the suitability of poly tetraarylphosphonium based anion exchange membranes for electrochemical applications. <i>Scientific Reports</i> , 2021, 11, 13841.	3.3	11
693	Structure, Kinetics, and Thermodynamics of Water and Its Ions at the Interface with Monoclinic ZrO ₂ Resolved via Ab Initio Molecular Dynamics. <i>Journal of Physical Chemistry C</i> , 2021, 125, 15233-15242.	3.1	3
694	Parameterization of classical nonpolarizable force field for hydroxide toward the large-scale molecular dynamics simulation of cellulose in pre-cooled alkali/urea aqueous solution. <i>Journal of Applied Polymer Science</i> , 2021, 138, 51477.	2.6	4
695	Multiblock Copolymer Anion-Exchange Membranes Derived from Vinyl Addition Polynorbornenes. <i>ACS Applied Energy Materials</i> , 2021, 4, 10273-10279.	5.1	15
696	Characterizing and Contrasting Structural Proton Transport Mechanisms in Azole Hydrogen Bond Networks Using Ab Initio Molecular Dynamics. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 8749-8756.	4.6	2
697	Theoretical study of the alkaline hydrogen oxidation reaction on Ni-Based nanocluster Catalysts: Effects of graphene supports and dopants. <i>Applied Surface Science</i> , 2021, 567, 150895.	6.1	7
698	Investigation of OH radical in the water nanodroplet during vapor freezing process: An ab initio molecular dynamics study. <i>Journal of Molecular Liquids</i> , 2021, 343, 117597.	4.9	6
699	Delivery of Electrons by Proton-Hole Transfer in Ice at 10 K: Role of Surface OH Radicals. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 704-710.	4.6	6
700	Ion-conductive metal–organic frameworks. <i>Dalton Transactions</i> , 2021, 50, 5385-5397.	3.3	33
701	A rechargeable aqueous proton battery based on a dipyrrophenazine anode and an indium hexacyanoferrate cathode. <i>Chemical Communications</i> , 2021, 57, 4307-4310.	4.1	29
703	Structure and Properties of Water. , 0, , 29-59.		4
704	Advanced Car–Parrinello Techniques: Path Integrals and Nonadiabaticity in Condensed Matter Simulations. , 2006, , 507-539.		11
705	6.3 Mitochondria-Nucleus Energetic Communication: Role for Phosphotransfer Networks in Processing Cellular Information. , 2007, , 641-666.		5
706	Dielectric Spectroscopy of Solutions. , 2004, , 265-288.		13
707	Proton Transfer in Aqueous Solution: Exploring the Boundaries of Adaptive QM/MM. Challenges and Advances in Computational Chemistry and Physics, 2015, , 51-91.	0.6	17

#	ARTICLE	IF	CITATIONS
708	Ab Initio Path Integral Molecular Dynamics Simulations of F ₂ H ⁺ and F ₂ H ₃ ⁺ . Progress in Theoretical Chemistry and Physics, 2012, , 207-216.	0.2	2
709	The possible implications of magnetic field effect on understanding the reactant of water splitting. Chinese Journal of Catalysis, 2022, 43, 148-157.	14.0	31
711	Mesoscale Simulations of Anion Exchange Membranes Based on Quaternary Ammonium Tethered Triblock Copolymers. Macromolecules, 2017, 50, 4397-4405.	4.8	62
712	Carbon dioxide, bicarbonate and carbonate ions in aqueous solutions under deep Earth conditions. Physical Chemistry Chemical Physics, 2020, 22, 10717-10725.	2.8	10
713	Formation and migration of H ₃ O ⁺ and OH ⁻ ions at the water/silica and water/vapor interfaces under the influence of a static electric field: a molecular dynamics study. Physical Chemistry Chemical Physics, 2020, 22, 22537-22548.	2.8	4
714	Ab initio metadynamics calculations of dimethylamine for probing pK _b variations in bulk vs. surface environments. Physical Chemistry Chemical Physics, 2020, 22, 26265-26277.	2.8	17
715	Unveiling two deuteration effects on hydrogen-bond breaking process of water isotopomers. Physical Review Materials, 2019, 3, .	2.4	14
716	Molecular Dynamics Simulation Study of the Ionic Mobility of OH ⁻ Using the OSS2 Model. Bulletin of the Korean Chemical Society, 2006, 27, 1154-1158.	1.9	6
717	Precise control of water and wastewater treatment systems with non-ideal heterogeneous mixing models and high-fidelity sensing. Chemical Engineering Journal, 2022, 430, 132819.	12.7	5
718	Dynamics and Surface Propensity of H ⁺ and OH ⁻ within Rigid Interfacial Water: Implications for Electrocatalysis. Journal of Physical Chemistry Letters, 2021, 12, 10128-10134.	4.6	4
719	Accelerated Vibrational Energy Relaxation of Water in Alkaline Environments. Journal of Physical Chemistry B, 2021, 125, 11980-11986.	2.6	2
720	Basic Concepts and Trends in ab Initio Molecular Dynamics. , 2004, , 53-91.		0
721	Electrochemistry, 2014, 14, 1-14.		0
722	Transport Mechanism in the Escherichia coli Ammonia Channel AmtB: A Computational Study. Challenges and Advances in Computational Chemistry and Physics, 2010, , 397-429.	0.6	0
723	Water-Hydroxyl Complexes: Direct Observation of a Symmetric Hydrogen Bond. Springer Theses, 2012, , 101-113.	0.1	0
725	Organization in Brain for Complementary Communication - Role of Astrocytes Endfoot Processes in Brain Synergy and Cognitive Coherence. SSRN Electronic Journal, 0, , .	0.4	0
726	Numerical Studies of the Tunneling Splitting of Malonaldehyde and the Eigenstates of Hydrated Hydroxide Anion Using MCTDH. , 2013, , 201-218.		0
727	- Polymer Electrolyte Membranes. , 2014, , 100-195.		0

#	ARTICLE	IF	CITATIONS
728	Geochemical rate models: an introduction to geochemical kinetics. Choice Reviews, 2014, 52, 52-0858-52-0858.	0.2	2
729	A Theoretical Model of Overpotential at Interfaces in Polymer Electrolyte Fuel Cells. International Journal of Chemical Engineering and Applications (IJCEA), 2015, 6, 243-249.	0.3	0
730	Chapter 2. Molecular Dynamics Simulations: Principles and Applications for the Study of Membrane Proteins. RSC Theoretical and Computational Chemistry Series, 2016, , 19-58.	0.7	0
731	Microwave Radiation Effects on the Process of Escherichia coli Cultivation. Microbiology and Biotechnology Letters, 2019, 47, 372-380.	0.4	2
732	Theoretical investigation of excited state charge and proton transfer mechanism for the novel 10-methylindolo[2,3-a]indolo[2,3-a]acridone molecule. Journal of Physical Organic Chemistry, 2020, 33, e4075.	3.0	3
733	Bayesian Estimation of the Hydroxyl Radical Diffusion Coefficient at Low Temperature and High Pressure from Atomistic Molecular Dynamics. Journal of Chemical Physics, 2021, 155, 194504.	3.0	1
734	The Energy as a Determinant Factor in the Ethiopathogeny of Chromosomal Abnormalities. The Unsuspected Bioenergetic Role of Melanin. , 0, , .		0
735	Hydration and Hydrogen Bond Order of Octadecanoic Acid and Octadecanol Films on Water at 21 and 1 Å°C. Journal of Physical Chemistry A, 2021, 125, 10065-10078.	2.5	8
736	Enabling high-energy-density aqueous batteries with hydrogen bond-anchored electrolytes. Matter, 2022, 5, 162-179.	10.0	98
737	Kinetic Oxygen Isotope Fractionation between Water and Aqueous OH ⁻ during Hydroxylation of CO ₂ . ACS Earth and Space Chemistry, 0, , .	2.7	1
738	The degradation effect on proton dissociation and transfer in perfluorosulfonic acid membranes. Physical Chemistry Chemical Physics, 2022, 24, 3007-3016.	2.8	3
739	Decoupling polymer, water and ion transport dynamics in ion-selective membranes for fuel cell applications. Journal of Non-Crystalline Solids: X, 2022, 13, 100073.	1.2	3
740	Ni, Co Hydroxide Modified by Partial Substitution of OH ⁻ with Cl ⁻ for Boosting Ultra-Fast Redox Kinetics up to 500 mV s ⁻¹ in Supercapacitors. Advanced Functional Materials, 2022, 32, .	14.9	18
741	Breviarium de Motu Simulato Ad Atomos Pertinenti. Israel Journal of Chemistry, 2022, 62, .	2.3	3
742	Electrocatalysis in Alkaline Media and Alkaline Membrane-Based Energy Technologies. Chemical Reviews, 2022, 122, 6117-6321.	47.7	195
743	A DFT Mechanistic Study on Base-Catalyzed Cleavage of the 1 ² -O-4 Ether Linkage in Lignin: Implications for Selective Lignin Depolymerization. Frontiers in Chemistry, 2022, 10, 793759.	3.6	1
744	Non-Monotonic Temperature Dependence of Hydroxide Ion Diffusion in Anion Exchange Membranes. Chemistry of Materials, 2022, 34, 2133-2145.	6.7	25
745	Controlling Hydronium Diffusivity in Model Proton Exchange Membranes. Journal of Physical Chemistry Letters, 2022, 13, 2245-2253.	4.6	7

#	ARTICLE	IF	CITATIONS
746	Solid Electrolyte Interface Regulated by Solventâ€inâ€Water Electrolyte Enables Highâ€Voltage and Stable Aqueous Mgâ€MnO ₂ Batteries. Advanced Energy Materials, 2022, 12, .	19.5	14
747	Ruthenium hydrides encapsulated in solâ€gel glasses exhibit new ultrafast vibrational dynamics. Journal of Chemical Physics, 2022, 156, 124502.	3.0	1
748	Disentangling water, ion and polymer dynamics in an anion exchange membrane. Nature Materials, 2022, 21, 555-563.	27.5	32
749	Structural proton transfer rates in pure water according to Marcus theory and TD-DFT computations. Journal of Molecular Liquids, 2022, 357, 119048.	4.9	3
755	The impact of carbonation on hydroxide diffusion in nano-confined anion exchange membranes. Journal of Materials Chemistry A, 2022, 10, 11137-11149.	10.3	6
756	A review on process design and bilayer electrolyte materials of bipolar membrane fuel cell. International Journal of Energy Research, 2022, 46, 11620-11639.	4.5	4
757	A new insight into the interaction of hydroxyl radical with supercooled nanodroplet in the atmosphere. Journal of Molecular Liquids, 2022, 359, 119261.	4.9	4
758	Quantum mechanical effects in acidâ€base chemistry. Chemical Science, 2022, 13, 6998-7006.	7.4	8
759	Ion hydration controls self-diffusion in multicomponent aqueous electrolyte solutions of NaNO ₂ -NaOH-H ₂ O. Journal of Molecular Liquids, 2022, 360, 119441.	4.9	3
760	Structural and Dynamic Properties of Solvated Hydroxide and Hydronium Ions in Water from Ab Initio Modeling. Journal of Chemical Physics, 0, , .	3.0	8
761	Ultrafast charge transfer coupled to quantum proton motion at molecule/metal oxide interface. Science Advances, 2022, 8, .	10.3	21
762	Inherent Promotion of Ionic Conductivity via Collective Vibrational Strong Coupling of Water with the Vacuum Electromagnetic Field. Journal of the American Chemical Society, 2022, 144, 12177-12183.	13.7	21
763	Constructing dual active sites for synergistic electrocatalysis of hydrogen oxidation: single-metal-atoms anchored on WC ₂ O ₂ MXene. Materials Chemistry Frontiers, 2022, 6, 2458-2467.	5.9	3
764	Development of energy-related functions of metalâ€organic frameworks and metal/MOF composites. Bulletin of Japan Society of Coordination Chemistry, 2022, 79, 88-99.	0.2	0
765	Anion Exchange Membranes for Fuel Cells Based on Quaternized Polystyrene-b-poly(ethylene-co-butylene)-b-polystyrene Triblock Copolymers with Spacer-Sidechain Design. Polymers, 2022, 14, 2860.	4.5	4
766	Ion-Selective Graphene Oxide/Polyvinyl Alcohol Composite Membranes for Rechargeable Alkaline Zinc Manganese Dioxide Batteries. ACS Applied Energy Materials, 0, , .	5.1	4
767	Accurate diffusion coefficients of the excess proton and hydroxide in water via extensive <i>ab initio</i> simulations with different schemes. Journal of Chemical Physics, 2022, 157, .	3.0	2
768	Formation and Dissolution of Surface Metal Carbonate Complexes: Implications for Interfacial Carbon Mineralization in Metal Silicates. Journal of Physical Chemistry C, 2022, 126, 11574-11584.	3.1	6

#	ARTICLE	IF	CITATIONS
769	Oxygen and Proton Transport in Flooded Graphene Pores with N-Dopants and Defects. Journal of Physical Chemistry C, 2022, 126, 11447-11456.	3.1	2
771	Molecular dynamics insight into phase separation and transport in anion-exchange membranes: Effect of hydrophobicity of backbones. Journal of Membrane Science, 2022, 661, 120922.	8.2	28
772	Anion Exchange Membranes for Alkaline Polymer Electrolyte Fuel Cellsâ€”A Concise Review. Materials, 2022, 15, 5601.	2.9	12
773	Structure and reactivity of sodium aluminate complexes in alkaline solutions. Journal of Molecular Liquids, 2022, 367, 120379.	4.9	2
774	How membrane characteristics influence the performance of CO ₂ and CO electrolysis. Energy and Environmental Science, 2022, 15, 4440-4469.	30.8	40
775	Challenges and prospects of high-voltage aqueous electrolytes for energy storage applications. Physical Chemistry Chemical Physics, 2022, 24, 20674-20688.	2.8	3
776	Clean power generation from salinity gradient using reverse electrodialysis technologies: Recent advances, bottlenecks, and future direction. Chemical Engineering Journal, 2023, 452, 139482.	12.7	22
777	Stabilizing the Unstable: Chromium Coating on NiMo Electrode for Enhanced Stability in Intermittent Water Electrolysis. ACS Applied Materials & Interfaces, 2022, 14, 40822-40833.	8.0	8
778	Water Uptake in an Anion Exchange Membrane Based on Polyamine: A First-Principles Study. Journal of Physical Chemistry B, 2022, 126, 7418-7428.	2.6	5
779	Fast Hydroxide Conduction via Hydrogen-Bonding Network Confined in Benzimidazolium-Functionalized Covalent Organic Frameworks. ACS Applied Materials & Interfaces, 2022, 14, 43861-43867.	8.0	3
780	Limiting Conductivities of Strong Acids and Bases in D ₂ O and H ₂ O: Deuterium Isotope Effects on Proton Hopping over a Wide Temperature Range. Journal of Physical Chemistry B, 2022, 126, 8791-8803.	2.6	4
781	Hydroxide Chemoselectivity Changes with Water Microsolvation. Journal of Physical Chemistry Letters, 2022, 13, 10216-10221.	4.6	8
782	Anion-exchange membrane water electrolyzers and fuel cells. Chemical Society Reviews, 2022, 51, 9620-9693.	38.1	93
783	A Template Editing Strategy to Create Interlayerâ€”Confined Active Species for Efficient and Durable Oxygen Evolution Reaction. Advanced Materials, 2023, 35, .	21.0	15
784	Recent developments in ion conductive membranes for CO ₂ electrochemical reduction. Chemical Engineering Journal, 2023, 456, 140942.	12.7	7
785	Theoretical insights into the hydrogen oxidation reaction on single metal atoms anchored on the edge of MoS ₂ nanosheets. Computational Materials Science, 2023, 218, 111921.	3.0	0
786	Recent developments of membranes and electrocatalysts for the hydrogen production by anion exchange membrane water electrolyzers: A review. Arabian Journal of Chemistry, 2023, 16, 104451.	4.9	18
787	Comprehensive H ₂ O Molecules Regulation via Deep Eutectic Solvents for Ultraâ€”Stable Zinc Metal Anode. Angewandte Chemie, 2023, 135, .	2.0	1

#	ARTICLE	IF	CITATIONS
788	Comprehensive H ₂ O Molecules Regulation via Deep Eutectic Solvents for Ultra-Stable Zinc Metal Anode. <i>Angewandte Chemie - International Edition</i> , 2023, 62, .	13.8	63
789	Exploring the Dynamical Nature of Intermolecular Hydrogen Bonds in Benzamide, Quinoline and Benzoic Acid Derivatives. <i>Molecules</i> , 2022, 27, 8847.	3.8	3
790	A cellulose-derived supramolecule for fast ion transport. <i>Science Advances</i> , 2022, 8, .	10.3	25
791	Fluorinated Poly(aryl piperidinium) Membranes for Anion Exchange Membrane Fuel Cells. <i>Advanced Materials</i> , 2023, 35, .	21.0	40
792	Optimization of a Perovskite Oxide-Based Cathode Catalyst Layer on Performance of Direct Ammonia Fuel Cells. <i>ACS Applied Materials & Interfaces</i> , 2023, 15, 1029-1041.	8.0	3
793	A Covalent Organic Framework as a Long-Life and High-Rate Anode Suitable for Both Aqueous Acidic and Alkaline Batteries. <i>Angewandte Chemie</i> , 2023, 135, .	2.0	4
794	A Covalent Organic Framework as a Long-Life and High-Rate Anode Suitable for Both Aqueous Acidic and Alkaline Batteries. <i>Angewandte Chemie - International Edition</i> , 2023, 62, .	13.8	26
795	Rational Design of Flexible Zn-Based Batteries for Wearable Electronic Devices. <i>ACS Nano</i> , 2023, 17, 1764-1802.	14.6	50
796	Ion Concentration Influences the Charge Transfer Due to a Water-Air Contact Line Moving over a Hydrophobic Surface: Charge Measurements and Theoretical Models. <i>Langmuir</i> , 2023, 39, 1826-1837.	3.5	8
797	Flexible Zinc-Air Batteries with Ampere-Hour Capacities and Wide-Temperature Adaptabilities. <i>Advanced Materials</i> , 2023, 35, .	21.0	40
798	Steering CO ₂ electroreduction selectivity towards CH ₄ and C ₂ H ₄ on a tannic acid-modified Cu electrode. <i>Materials Chemistry Frontiers</i> , 2023, 7, 1395-1402.	5.9	3
799	Hydroxide Diffusion in Functionalized Cylindrical Nanopores as Idealized Models of Anion Exchange Membrane Environments: An Ab Initio Molecular Dynamics Study. <i>Journal of Physical Chemistry C</i> , 2023, 127, 2792-2804.	3.1	3
801	Surface Hydroxyl-Ion Diffusion and Hierarchical Structure of Adsorbed Water on Hydrated Layered Double Hydroxides. <i>Journal of Physical Chemistry C</i> , 2023, 127, 6045-6053.	3.1	0
802	Hybrid Aqueous/Non-aqueous Electrolytes for Lithium-Ion and Zinc-Ion Batteries: A Mini-Review. <i>Batteries and Supercaps</i> , 2023, 6, .	4.7	3
803	Molecular insight into the GaP(110)-water interface using machine learning accelerated molecular dynamics. <i>Journal of Energy Chemistry</i> , 2023, 82, 239-247.	12.9	7
804	The primary gas phase hydration shell of hydroxide. <i>Science Advances</i> , 2023, 9, .	10.3	1
805	Functional groups in anion exchange membranes: Insights from Ab initio molecular dynamics. <i>Journal of Membrane Science</i> , 2023, 678, 121638.	8.2	3
806	The Role of Silicate Enrichment on the Discharge Duration of Silicon-Air Batteries. <i>ChemSusChem</i> , 2023, 16, .	6.8	2

#	ARTICLE	IF	CITATIONS
807	Search for a Grotthuss mechanism through the observation of proton transfer. Communications Chemistry, 2023, 6, .	4.5	13
808	Investigating percolation and clustering effects on aquivion and nafion membranes at the molecular scale. International Journal of Hydrogen Energy, 2023, 48, 33283-33296.	7.1	2
809	A stochastic description of pH within nanoscopic water pools. Cell Reports Physical Science, 2023, 4, 101458.	5.6	0
810	New generation radiation-grafted PVDF-g-VBC based dual-fiber electrospun anion exchange membranes. International Journal of Hydrogen Energy, 2024, 51, 1390-1401.	7.1	1
811	Quantum Behaviors of H in Water. , 2023, , 303-312.		0
812	Hydrated Ions on Surfaces. , 2023, , 243-251.		0
813	Theoretical Approaches. , 2023, , 41-75.		0
814	Understanding the Structure and Function of Water at the Molecular Scale. , 2023, , 21-40.		0
815	Water Adsorption on Metal Surfaces. , 2023, , 161-199.		0
816	Derivation of parameter sets for the ReaxFF+ method for modeling an electrochemical machining process. Procedia CIRP, 2023, 117, 231-236.	1.9	1
817	Characterizing Structure-Dependent $\text{TiS}_{2\text{H}_2\text{O}}$ Interfaces Using Deep-Neural-Network-Assisted Molecular Dynamics. Journal of Physical Chemistry C, 2023, 127, 9750-9758.	3.1	2
818	Microscopic Mechanism of Proton Transfer in Pure Water under Ambient Conditions. Journal of Chemical Theory and Computation, 2023, 19, 4243-4254.	5.3	3
819	Strengthening Aqueous Electrolytes without Strengthening Water. Angewandte Chemie - International Edition, 2023, 62, .	13.8	4
820	Understanding hydrogen electrocatalysis by probing the hydrogen-bond network of water at the electrified Pt H^+ solution interface. Nature Energy, 2023, 8, 859-869.	39.5	16
821	Strengthening Aqueous Electrolytes without Strengthening Water. Angewandte Chemie, 2023, 135, .	2.0	0
822	A chemically interlocked bipolar membrane achieving stable water dissociation for high output ammonia electrosynthesis. Energy and Environmental Science, 2023, 16, 3815-3824.	30.8	2
823	Coexistence of Cationic and Anionic Phosphate Moieties in Solids: Unusual but Not Impossible. Journal of Physical Chemistry Letters, 2023, 14, 7249-7255.	4.6	0
824	Ab Initio Molecular Dynamics Study of the Proton Transfer in Hydroxyl Ion-Induced Hydrolysis of Aluminum Monomers. Journal of Physical Chemistry B, 2023, 127, 7342-7351.	2.6	0

#	ARTICLE	IF	CITATIONS
825	Developing machine-learned potentials to simultaneously capture the dynamics of excess protons and hydroxide ions in classical and path integral simulations. <i>Journal of Chemical Physics</i> , 2023, 159, .	3.0	1
826	Ionovoltaics in energy harvesting and applications: A journey from early development to current state-of-the-art. <i>EcoMat</i> , 2023, 5, .	11.9	2
827	Preferred planar crystal growth and uniform solid electrolyte interfaces enabled by anion receptors for stable aqueous Zn batteries. <i>Energy and Environmental Science</i> , 2023, 16, 4572-4583.	30.8	17
828	Advances in high performance anion exchange membranes: Molecular design, preparation methods, and ion transport dynamics. <i>Journal of Environmental Chemical Engineering</i> , 2023, 11, 110749.	6.7	1
829	Ir Strangelove, or How to Learn to Stop Worrying and Love the PEM Water Electrolysis. <i>Energy & Fuels</i> , 2023, 37, 12558-12569.	5.1	1
830	Unveiling the structure and ion dynamics of amorphous Na ₃ VO ₄ antiperovskite electrolytes by first-principles molecular dynamics. <i>Journal of Materials Chemistry A</i> , 0, , .	10.3	0
831	A Bio-Inspired Methylation Approach to Salt-Concentrated Hydrogel Electrolytes for Long-Life Rechargeable Batteries. <i>Angewandte Chemie</i> , 2023, 135, .	2.0	1
832	A Bio-Inspired Methylation Approach to Salt-Concentrated Hydrogel Electrolytes for Long-Life Rechargeable Batteries. <i>Angewandte Chemie - International Edition</i> , 2023, 62, .	13.8	1
833	Fast Ionic Actuators with Silver-Silver Chloride Electrodes and a Mixed Ionic Liquid Electrolyte. <i>Advanced Engineering Materials</i> , 2024, 26, .	3.5	0
834	Unlimiting ionic conduction: manipulating hydration dynamics through vibrational strong coupling of water. <i>Chemical Science</i> , 2023, 14, 11441-11446.	7.4	2
835	Mechanistic Insights into Water Autoionization through Metadynamics Simulation Enhanced by Machine Learning. <i>Physical Review Letters</i> , 2023, 131, .	7.8	0
836	Mineralization of Poly(vinyl alcohol) by Ozone Microbubbles under a Wide Range of pH Conditions. <i>Langmuir</i> , 2023, 39, 15215-15221.	3.5	1
837	Ultrafast Geminate Recombination Facilitated by Hydrogen-Atom Transfer in Charge Transfer Reactions from Hydroxide and Methoxide Ions. <i>Journal of Physical Chemistry Letters</i> , 2023, 14, 10463-10468.	4.6	0
838	Consistent density functional theory-based description of ion hydration through density-corrected many-body representations. <i>Journal of Chemical Physics</i> , 2023, 159, .	3.0	2
839	A kinetic study of ex-situ soil remediation by nickel extraction using natural deep eutectic solvent. <i>Environmental Technology (United Kingdom)</i> , 0, , 1-14.	2.2	0
840	Theoretical Examination of the Hydroxide Transport in Cobaltocenium-Containing Polyelectrolytes. <i>Journal of Physical Chemistry B</i> , 2023, 127, 10129-10141.	2.6	0
841	Comprehensive Understandings of Hydrogen Bond Chemistry in Aqueous Batteries. <i>Advanced Materials</i> , 0, , .	21.0	1
842	Accurate modeling of aqueous chemistry at the nano-/micro-scale. <i>Scientia Sinica Chimica</i> , 2024, 54, 93-111.	0.4	1

#	ARTICLE	IF	CITATIONS
843	Probing the self-ionization of liquid water with ab initio deep potential molecular dynamics. Proceedings of the National Academy of Sciences of the United States of America, 2023, 120, .	7.1	0
844	Modeling nuclear quantum effects on long-range electrostatics in nonuniform fluids. Journal of Chemical Physics, 2023, 159, .	3.0	2
845	Computational Modeling of Hydrated Polyamine-Based Anion Exchange Membranes via Molecular Dynamics Simulation. Journal of Physical Chemistry C, 0, , .	3.1	0
847	Ions and electron conductive porous coordination polymers for energy applications. , 2024, , 237-272.		0
850	Efficient acid/alkali recovery enabled by only one negatively charged microporous polymer membrane. AIChE Journal, 2024, 70, .	3.6	0
851	Nuclear Quantum Effects in Hydroxide Hydrate Along the H-Bond Bifurcation Pathway. Journal of Physical Chemistry A, 2024, 128, 1600-1610.	2.5	0
852	Characterization of iron(III) in aqueous and alkaline environments with <i>ab initio</i> and ReaxFF potentials. Journal of Chemical Physics, 2024, 160, .	3.0	0
853	Energy storage devices based on flexible and self-healable hydrogel electrolytes: Recent advances and future prospects. Journal of Energy Storage, 2024, 85, 110961.	8.1	0
854	Exploiting Cation Structure and Water Content in Modulating the Acidity of Ammonium Hydrogen Sulfate Protic Ionic Liquids. Journal of Physical Chemistry Letters, 2024, 15, 2311-2318.	4.6	0
855	Evaluation of Iron Chlorin e6 disappearance and hydrolysis in soil and garlic using salting-out assisted liquid-liquid extraction coupled with high-performance liquid chromatography and ultraviolet-visible detection. Food Chemistry, 2024, 447, 138960.	8.2	0
856	Decoding Electrochemical Processes of Lithium-Ion Batteries by Classical Molecular Dynamics Simulations. Advanced Energy Materials, 0, , .	19.5	0
857	Revealing the Molecular Origin of Anisotropy around Chloride Ions in Bulk Water. Journal of Physical Chemistry Letters, 2024, 15, 3037-3042.	4.6	0
858	Art, fact and artifact: reflections on the cross-talk between theory and experiment. Physical Chemistry Chemical Physics, 2024, 26, 9848-9855.	2.8	0