

Water as an Active Constituent in Cell Biology

Chemical Reviews

108, 74-108

DOI: [10.1021/cr068037a](https://doi.org/10.1021/cr068037a)

Citation Report

#	ARTICLE	IF	CITATIONS
1	Hydration Profiles of Amyloidogenic Molecular Structures. <i>Journal of Biological Physics</i> , 2008, 34, 577-590.	0.7	8
3	Perspektiven der Biothermodynamik – I. Thermostatik und Thermodynamik irreversibler Prozesse. <i>Chemie-Ingenieur-Technik</i> , 2008, 80, 741-753.	0.4	2
4	Small-Angle X-Ray Scattering and Near-Infrared Vibrational Spectroscopy of Water Confined in Aerosol-OT Reverse Micelles. <i>ChemPhysChem</i> , 2008, 9, 2794-2801.	1.0	21
5	Hydration Dynamics of Water near an Amphiphilic Model Peptide at Low Hydration Levels: A Dielectric Relaxation Study. <i>ChemPhysChem</i> , 2008, 9, 2802-2808.	1.0	21
6	Water as a Biomolecule. <i>ChemPhysChem</i> , 2008, 9, 2677-2685.	1.0	109
7	Which Properties of a Spanning Network of Hydration Water Enable Biological Functions?. <i>ChemPhysChem</i> , 2008, 9, 2695-2702.	1.0	44
8	Compounds of Antibacterial Agent Ciprofloxacin and Magnesium - Crystal Structures and Molecular Modeling Calculations. <i>European Journal of Inorganic Chemistry</i> , 2008, 2008, 3718-3727.	1.0	35
9	Strong, Localized, and Directional Hydrogen Bonds Fluidize Ionic Liquids. <i>Angewandte Chemie - International Edition</i> , 2008, 47, 8731-8734.	7.2	386
11	Isn't self-assembly a misnomer? Multi-disciplinary arguments in favor of co-assembly. <i>Advances in Colloid and Interface Science</i> , 2008, 141, 37-47.	7.0	29
12	Effects of salts of the Hofmeister series on the hydrogen bond network of water. <i>Journal of Molecular Liquids</i> , 2008, 143, 160-170.	2.3	83
13	Down to atomic-scale intracellular water dynamics. <i>EMBO Journal</i> , 2008, 9, 543-547.	3.5	83
14	Water – an enduring mystery. <i>Nature</i> , 2008, 452, 291-292.	13.7	320
15	Dynamics of single-file water chains inside nanoscale channels: physics, biological significance and applications. <i>Journal Physics D: Applied Physics</i> , 2008, 41, 103002.	1.3	72
16	Hydrophobe-Water Interactions: Methane as a Model. <i>Biophysical Journal</i> , 2008, 95, 4241-4245.	0.2	12
17	Hemoglobin Dynamics in Red Blood Cells: Correlation to Body Temperature. <i>Biophysical Journal</i> , 2008, 95, 5449-5461.	0.2	85
18	Simulations of water at the interface with hydrophilic self-assembled monolayers (Review). <i>Biointerphases</i> , 2008, 3, FC13-FC22.	0.6	35
19	Water at polar and nonpolar solid walls (Review). <i>Biointerphases</i> , 2008, 3, FC23-FC39.	0.6	93
20	Water confined in reverse micelles – probe tool in biomedical informatics. <i>Physical Chemistry Chemical Physics</i> , 2008, 10, 4740.	1.3	5

#	ARTICLE	IF	CITATIONS
21	Nature of biological water: a femtosecond study. <i>Chemical Communications</i> , 2008, , 2848.	2.2	194
22	Force Trace Hysteresis and Temperature Dependence of Bridging Nanobubble Induced Forces between Hydrophobic Surfaces. <i>ACS Nano</i> , 2008, 2, 1817-1824.	7.3	36
23	Dissecting the Hydrogen Bond: A Quantum Monte Carlo Approach. <i>Journal of Chemical Theory and Computation</i> , 2008, 4, 1428-1434.	2.3	46
24	Integral Equation Study of the Hydrophobic Interaction between Graphene Plates. <i>Journal of Chemical Theory and Computation</i> , 2008, 4, 1928-1939.	2.3	29
25	Micelle formation in the presence of photosystem I. <i>Biochimica Et Biophysica Acta - Biomembranes</i> , 2008, 1778, 2298-2307.	1.4	27
26	Thermodynamics of water intrusion in nanoporous hydrophobic solids. <i>Physical Chemistry Chemical Physics</i> , 2008, 10, 4817.	1.3	103
27	Surface Protonation at the Rutile (110) Interface: Explicit Incorporation of Solvation Structure within the Refined MUSIC Model Framework. <i>Langmuir</i> , 2008, 24, 12331-12339.	1.6	88
28	Carbohydrate~Carbohydrate Interaction Prominence in 3D Supramolecular Self-Assembly. <i>Journal of Physical Chemistry B</i> , 2008, 112, 11595-11600.	1.2	17
29	Pyridine Ligand Rotation in Self-Assembled Trigonal Prisms. Evidence for Intracage Solvent Vapor Bubbles. <i>Journal of the American Chemical Society</i> , 2008, 130, 7629-7638.	6.6	41
30	Isostructural Self-Assembly of 2-Deoxyguanosine Derivatives in Aqueous and Organic Media. <i>Journal of the American Chemical Society</i> , 2008, 130, 10492-10493.	6.6	45
31	Polarization of Water in the First Hydration Shell of K ⁺ and Ca ²⁺ Ions. <i>Journal of Physical Chemistry B</i> , 2008, 112, 10786-10790.	1.2	41
32	Amino acids with an intermolecular proton bond as proton storage site in bacteriorhodopsin. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2008, 105, 19672-19677.	3.3	87
33	Interplay of local hydrogen-bonding and long-ranged dipolar forces in simulations of confined water. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2008, 105, 19136-19141.	3.3	59
34	Pairwise-additive hydrophobic effect for alkanes in water. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2008, 105, 9512-9515.	3.3	42
35	Cell water dynamics on multiple time scales. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2008, 105, 6266-6271.	3.3	177
36	Intrinsic thermal expansivity and hydrational properties of amyloid peptide A β ²⁴² in liquid water. <i>Journal of Chemical Physics</i> , 2008, 129, 195101.	1.2	30
37	Intrinsic Structure of Hydrophobic Surfaces: The Oil-Water Interface. <i>Physical Review Letters</i> , 2008, 101, 056102.	2.9	69
38	Unaffected microscopic dynamics of macroscopically arrested water in dilute clay gels. <i>Physical Review E</i> , 2008, 78, 061403.	0.8	11

#	ARTICLE	IF	CITATIONS
40	Dynamics of hydration water in proteins. <i>General Physiology and Biophysics</i> , 2009, 28, 168-173.	0.4	28
41	Stable Liquid Water Droplet on a Water Monolayer Formed at Room Temperature on Ionic Model Substrates. <i>Physical Review Letters</i> , 2009, 103, 137801.	2.9	238
42	On the phase diagram of water with density functional theory potentials: The melting temperature of ice Ih with the Perdewâ€“Burkeâ€“Ernzerhof and Beckeâ€“Leeâ€“Yangâ€“Parr functionals. <i>Journal of Chemical Physics</i> , 2009, 130, 221102.	1.2	203
43	Size-dependent hydrophobic to hydrophilic transition for nanoparticles: A molecular dynamics study. <i>Journal of Chemical Physics</i> , 2009, 131, 244706.	1.2	32
44	Solvation in protein (un)folding of melittin tetramerâ€“monomer transition. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2009, 106, 12593-12598.	3.3	53
45	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.	3.3	111
46	Water-mediated signal multiplication with Y-shaped carbon nanotubes. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2009, 106, 18120-18124.	3.3	120
47	Structural waters define a functional channel mediating activation of the GPCR, rhodopsin. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2009, 106, 14367-14372.	3.3	181
48	The Effects of Temperature and H/D Isotopic Dilution on the Transmission and Attenuated Total Reflection FTIR Spectra of Water. <i>Zeitschrift Fur Physikalische Chemie</i> , 2009, 223, 1011-1022.	1.4	7
49	Conserved waters mediate structural and functional activation of family A (rhodopsin-like) G protein-coupled receptors. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2009, 106, 8555-8560.	3.3	218
50	Crystallographic snapshots of iterative substrate translocations during nicotianamine synthesis in archaea. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2009, 106, 16180-16184.	3.3	17
51	Polyamorphism in Liquids and Amorphous Substances: An Analogue of Polymorphism in Crystalline Solids. <i>Transactions of the Indian Ceramic Society</i> , 2009, 68, 65-80.	0.4	6
52	The impact of hydration water on the dynamics of side chains of hydrophobic peptides: From dry powder to highly concentrated solutions. <i>Journal of Chemical Physics</i> , 2009, 130, 235101.	1.2	31
53	Molecular dynamics investigation of hydration of nanoscopic hydrophobic paraffin-like plates. <i>Journal of Chemical Physics</i> , 2009, 131, 014507.	1.2	15
54	Water structure, dynamics, and vibrational spectroscopy in sodium bromide solutions. <i>Journal of Chemical Physics</i> , 2009, 131, 144511.	1.2	135
55	Thermodynamic study of water confinement in hydrophobic zeolites by Monte Carlo simulations. <i>Molecular Simulation</i> , 2009, 35, 24-30.	0.9	27
56	Ordered water structure at hydrophobic graphite interfaces observed by 4D, ultrafast electron crystallography. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2009, 106, 4122-4126.	3.3	85
57	Atomic-scale dynamics inside living cells explored by neutron scattering. <i>Journal of the Royal Society Interface</i> , 2009, 6, S611-7.	1.5	6

#	ARTICLE	IF	CITATIONS
58	Coupled relaxations at the protein-water interface in the picosecond time scale. <i>Journal of the Royal Society Interface</i> , 2009, 6, S635-40.	1.5	21
59	Characterizing hydrophobicity of interfaces by using cavity formation, solute binding, and water correlations. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2009, 106, 15119-15124.	3.3	309
60	Insight into insoluble proteins with pure water. <i>FEBS Letters</i> , 2009, 583, 953-959.	1.3	51
61	Related Organocatalysts (2): Urea Derivatives. , 0, , 273-293.		3
62	Chiral configuration of the hydration layers of D - and L -alanine in water implied from dilution calorimetry. <i>Chirality</i> , 2010, 22, 587-592.	1.3	14
63	Perspektiven der Biothermodynamik IV. Hydratisierung von Proteinen. <i>Chemie-Ingenieur-Technik</i> , 2009, 81, 255-266.	0.4	0
64	Gated and Differently Functionalized (New) Porous Capsules Direct Encapsulates' Structures: Higher and Lower Density Water. <i>Chemistry - A European Journal</i> , 2009, 15, 1844-1852.	1.7	74
65	Have the primary structures of biomacromolecules been selected in a Darwinian fashion to adapt to the surrounding environments of our planet?. <i>IUBMB Life</i> , 2009, 61, 860-863.	1.5	3
66	Site-Dependent Excited-State Dynamics of a Fluorescent Probe Bound to Avidin and Streptavidin. <i>ChemPhysChem</i> , 2009, 10, 1517-1532.	1.0	17
67	Weakened Hydrogen Bonds in Water Confined between Lipid Bilayers: The Existence of a Long-Range Attractive Hydration Force. <i>ChemPhysChem</i> , 2009, 10, 1438-1441.	1.0	22
68	Strategies to model the near-solute solvent molecular density/polarization. <i>Journal of Computational Chemistry</i> , 2009, 30, 700-709.	1.5	12
70	Molecular Recognition at the Active Site of Catechol-O-Methyltransferase: Energetically Favorable Replacement of a Water Molecule Imported by a Bisubstrate Inhibitor. <i>Angewandte Chemie - International Edition</i> , 2009, 48, 9092-9096.	7.2	39
71	g_permute: Permutation-reduced phase space density compaction. <i>Computer Physics Communications</i> , 2009, 180, 455-458.	3.0	16
72	X-ray crystal structures of <i>Phanerochaete chrysosporium</i> Laminarinase 16A in complex with products from lichenin and laminarin hydrolysis. <i>FEBS Journal</i> , 2009, 276, 3858-3869.	2.2	30
73	Limits of life in hostile environments: no barriers to biosphere function?. <i>Environmental Microbiology</i> , 2009, 11, 3292-3308.	1.8	143
74	Collision-induced dissociation of protonated nanodroplets. <i>International Journal of Mass Spectrometry</i> , 2009, 279, 32-36.	0.7	7
75	Understanding dynamics of myoglobin in heterogeneous aqueous environments using coupled water fractions. <i>Advances in Colloid and Interface Science</i> , 2009, 150, 55-62.	7.0	3
76	The effect of hydrogen bonding on the solvent-mediated interaction of composite plates. <i>Journal of Colloid and Interface Science</i> , 2009, 336, 575-583.	5.0	6

#	ARTICLE	IF	CITATIONS
77	Hydration of biomolecules. <i>Chemical Physics Letters</i> , 2009, 480, 1-16.	1.2	81
78	Role of salts on the strength of pairwise hydrophobic interaction. <i>Chemical Physics Letters</i> , 2009, 483, 67-71.	1.2	26
79	Effect of Salt on the Excited-State Dynamics of Malachite Green in Bulk Aqueous Solutions and at Air/Water Interfaces: a Femtosecond Transient Absorption and Surface Second Harmonic Generation Study. <i>Journal of Physical Chemistry C</i> , 2009, 113, 11822-11829.	1.5	25
80	Supramolecular Gel Based on a Perylene Diimide Dye: Multiple Stimuli Responsiveness, Robustness, and Photofunction. <i>Journal of the American Chemical Society</i> , 2009, 131, 14365-14373.	6.6	205
81	Coherent neutron scattering study of confined water in nafion. <i>Physical Review B</i> , 2009, 80, .	1.1	9
82	Effect of Salt on the Dynamics of Aqueous Solution of Hydrophobic Solutes: A Molecular Dynamics Simulation Study. <i>Journal of Chemical & Engineering Data</i> , 2009, 54, 542-547.	1.0	9
83	Molecular Dynamics Simulations of Electrospayed Water Nanodroplets: Internal Potential Gradients, Location of Excess Charge Centers, and "Hopping" Protons. <i>Journal of Physical Chemistry B</i> , 2009, 113, 7071-7080.	1.2	12
84	Dynamics of Water and Ions Near DNA: Comparison of Simulation to Time-Resolved Stokes-Shift Experiments. <i>Journal of the American Chemical Society</i> , 2009, 131, 1724-1735.	6.6	86
85	Effect of Surface Polarity on the Structure and Dynamics of Water in Nanoscale Confinement. <i>Journal of Physical Chemistry B</i> , 2009, 113, 1438-1446.	1.2	143
86	Microscopic Wetting of Mixed Self-assembled Monolayers: A Molecular Dynamics Study. <i>Journal of Physical Chemistry B</i> , 2009, 113, 4161-4169.	1.2	40
87	Rotational Diffusion of Dihydroxy Coumarins: Effect of OH Groups and Their Relative Position on Solute-Solvent Interactions. <i>Journal of Physical Chemistry B</i> , 2009, 113, 8599-8606.	1.2	6
88	Dimerization Thermodynamics of Large Hydrophobic Plates: A Scaled Particle Theory Study. <i>Journal of Physical Chemistry B</i> , 2009, 113, 11232-11239.	1.2	66
89	Inhibition of Bubble Coalescence by Osmolytes: Sucrose, Other Sugars, and Urea. <i>Langmuir</i> , 2009, 25, 11406-11412.	1.6	30
90	Destabilization of the Hydrogen-Bond Structure of Water by the Osmolyte Trimethylamine N-Oxide. <i>Journal of Physical Chemistry B</i> , 2009, 113, 4038-4044.	1.2	64
91	Why Water Reorientation Slows without Iceberg Formation around Hydrophobic Solutes. <i>Journal of Physical Chemistry B</i> , 2009, 113, 2428-2435.	1.2	338
92	Vibrational Spectroscopy and Dynamics of Water Confined inside Reverse Micelles. <i>Journal of Physical Chemistry B</i> , 2009, 113, 15017-15028.	1.2	134
93	Hydrophobic Interactions of Hexane in Nanosized Water Droplets. <i>Journal of Physical Chemistry B</i> , 2009, 113, 12337-12342.	1.2	2
94	Interfacial Water at Hydrophobic and Hydrophilic Surfaces: Slip, Viscosity, and Diffusion. <i>Langmuir</i> , 2009, 25, 10768-10781.	1.6	433

#	ARTICLE	IF	CITATIONS
95	Manipulating Biomolecules with Aqueous Liquids Confined within Single-Walled Nanotubes. <i>Journal of the American Chemical Society</i> , 2009, 131, 2840-2845.	6.6	64
96	Fine Tuning of Electrostatics around the Internucleotidic Phosphate through Incorporation of Modified 2'-O-Methyl-Carbocyclic-LNAs and -ENAs Leads to Significant Modulation of Antisense Properties. <i>Journal of Organic Chemistry</i> , 2009, 74, 118-134.	1.7	44
97	Amphiphilic Organic Crystals. <i>Journal of the American Chemical Society</i> , 2009, 131, 17853-17859.	6.6	14
98	Water-protein interplay reveals the specificity of lytic protease. <i>Biochemical and Biophysical Research Communications</i> , 2009, 385, 165-169.	1.0	1
99	Dewetting and Hydrophobic Interaction in Physical and Biological Systems. <i>Annual Review of Physical Chemistry</i> , 2009, 60, 85-103.	4.8	423
100	Sequence-Specific Size, Structure, and Stability of Tight Protein Knots. <i>Biophysical Journal</i> , 2009, 96, 831-839.	0.2	40
101	From Powder to Solution: Hydration Dependence of Human Hemoglobin Dynamics Correlated to Body Temperature. <i>Biophysical Journal</i> , 2009, 96, 5073-5081.	0.2	40
102	Protein Hydration Dynamics and Molecular Mechanism of Coupled Water-Protein Fluctuations. <i>Journal of the American Chemical Society</i> , 2009, 131, 10677-10691.	6.6	182
103	Effect of Headgroup Size, Charge, and Solvent Structure on Polymer-Micelle Interactions, Studied by Molecular Dynamics Simulations. <i>Journal of Physical Chemistry B</i> , 2009, 113, 15170-15180.	1.2	28
104	Rattling in the Cage: Ions as Probes of Sub-picosecond Water Network Dynamics. <i>Journal of the American Chemical Society</i> , 2009, 131, 18512-18517.	6.6	147
105	NMR Studies of Structure and Dynamics of Liquid Molecules Confined in Extended Nanospaces. <i>Journal of Physical Chemistry B</i> , 2009, 113, 10808-10816.	1.2	95
106	Thermal Effects of Water Intrusion in Hydrophobic Nanoporous Materials. <i>Journal of the American Chemical Society</i> , 2009, 131, 9898-9899.	6.6	26
107	Anomalies of water and hydrogen bond dynamics in hydrophobic nanoconfinement. <i>Journal of Physics Condensed Matter</i> , 2009, 21, 504108.	0.7	30
108	Ultrafast Dynamics of Hydrogen Bond Exchange in Aqueous Ionic Solutions. <i>Journal of Physical Chemistry B</i> , 2009, 113, 7825-7835.	1.2	119
109	Capillary rise of water in hydrophilic nanopores. <i>Physical Review E</i> , 2009, 79, 067301.	0.8	157
110	Water co-encapsulation in an inverted molecular capsule. <i>Chemical Communications</i> , 2009, , 4191.	2.2	24
111	Protonated Arginine and Protonated Lysine: Hydration and Its Effect on the Stability of Salt-Bridge Structures. <i>Journal of Physical Chemistry B</i> , 2009, 113, 9995-10000.	1.2	43
112	Hydration of Protonated Aromatic Amino Acids: Phenylalanine, Tryptophan, and Tyrosine. <i>Journal of the American Chemical Society</i> , 2009, 131, 4695-4701.	6.6	62

#	ARTICLE	IF	CITATIONS
113	Evolution from Surface-Influenced to Bulk-Like Dynamics in Nanoscopically Confined Water. Journal of Physical Chemistry B, 2009, 113, 7973-7976.	1.2	97
114	Reinterpretation of the Liquid Water Quasi-Elastic Neutron Scattering Spectra Based on a Nondiffusive Jump Reorientation Mechanism. Journal of Physical Chemistry B, 2009, 113, 2684-2687.	1.2	59
115	¹³ C and ¹⁵ N NMR Study of the Hydration Response of T4 Lysozyme and β -Crystallin Internal Dynamics. Journal of Physical Chemistry B, 2009, 113, 10022-10034.	1.2	25
116	From shell to cell: neutron scattering studies of biological water dynamics and coupling to activity. Faraday Discussions, 2009, 141, 117-130.	1.6	82
117	Concerted orientation induced unidirectional water transport through nanochannels. Physical Chemistry Chemical Physics, 2009, 11, 9898.	1.3	57
118	Structural ultrafast dynamics of macromolecules: diffraction of free DNA and effect of hydration. Physical Chemistry Chemical Physics, 2009, 11, 10619.	1.3	11
119	Selective catalytic oxidation of hydrocarbons. New prospects. Russian Chemical Reviews, 2009, 78, 211-230.	2.5	39
120	Solvation Dynamics of Model Peptides Probed by Terahertz Spectroscopy. Observation of the Onset of Collective Network Motions. Journal of the American Chemical Society, 2009, 131, 3752-3755.	6.6	113
121	Heat-Induced Phase Transition and Crystallization of Hydrophobically End-Capped Poly(2-isopropyl-2-oxazoline)s in Water. Macromolecules, 2009, 42, 5818-5828.	2.2	76
123	Challenges for the Modern Science in its Descend Towards Nano Scale. Current Nanoscience, 2009, 5, 372-389.	0.7	22
124	Thermodynamics and structure of the {water + methanol} system viewed from three simple additive pair-wise intermolecular potentials based on the rigid molecule approximation. Collection of Czechoslovak Chemical Communications, 2010, 75, 617-635.	1.0	6
125	Water as a Biomolecule. , 2010, , 49-67.		0
127	The possible roles of water in the prebiotic chemical evolution of DNA. Physical Chemistry Chemical Physics, 2010, 12, 10147.	1.3	18
128	Geometric characteristics and energy landscapes of halogenâ€“waterâ€“hydrogen bridges at proteinâ€“ligand interfaces. Chemical Physics Letters, 2010, 485, 348-353.	1.2	13
129	Probing the hydrophobic effect of noncovalent complexes by mass spectrometry. Journal of the American Society for Mass Spectrometry, 2010, 21, 286-289.	1.2	53
130	Determination of water intrusion heat in hydrophobic microporous materials by high pressure calorimetry. Microporous and Mesoporous Materials, 2010, 134, 8-15.	2.2	8
131	Water reorientation in the hydration shells of hydrophilic and hydrophobic solutes. Science China: Physics, Mechanics and Astronomy, 2010, 53, 1068-1072.	2.0	11
132	Fluorescence Techniques for Determination of the Membrane Potentials in High Throughput Screening. Journal of Fluorescence, 2010, 20, 1139-1157.	1.3	15

#	ARTICLE	IF	CITATIONS
133	Interactions between Crown Ethers and Water, Methanol, Acetone, and Acetonitrile in Halogenated Solvents. <i>Journal of Solution Chemistry</i> , 2010, 39, 291-299.	0.6	17
134	Solubility of Thiophene-, Furan- and Pyrrole-2-Carboxaldehyde Phenylhydrazone Derivatives in 2.82 M Aqueous DMSO at 298.15 K, Inhibition of Lymphoproliferation and Tubulin Polymerization: A Study Based on the Scaled Particle Theory. <i>Journal of Solution Chemistry</i> , 2010, 39, 1099-1112.	0.6	8
135	What You Always Wanted to Know about Heat Capacities, but Were Afraid to Ask. <i>Journal of Solution Chemistry</i> , 2010, 39, 1777-1818.	0.6	30
136	Influence of polar solvents upon the complex formation of 18-crown-6 with cations in chloroform. <i>Journal of Inclusion Phenomena and Macrocyclic Chemistry</i> , 2010, 68, 411-416.	1.6	7
137	Maps of science as interdisciplinary discourse: co-citation contexts and the role of analogy. <i>Scientometrics</i> , 2010, 83, 835-849.	1.6	46
138	Major Challenges for the Modern Chemistry in Particular and Science in General. <i>Foundations of Science</i> , 2010, 15, 303-344.	0.4	7
141	In Silico Characterization of Ligand Binding Modes in the Human Histamine H ₄ Receptor and their Impact on Receptor Activation. <i>ChemBioChem</i> , 2010, 11, 1850-1855.	1.3	9
142	3D Stepwise Deconstruction of a Water Framework Templated by a Nanoporous Organic-Inorganic Hybrid Host. <i>Chemistry - A European Journal</i> , 2010, 16, 7741-7749.	1.7	14
145	Directional Proton Transfer in Membrane Proteins Achieved through Protonated Protein-Bound Water Molecules: A Proton Diode. <i>Angewandte Chemie - International Edition</i> , 2010, 49, 6889-6893.	7.2	54
146	Direct Three-Dimensional Imaging of the Buried Interfaces between Water and Superhydrophobic Surfaces. <i>Angewandte Chemie - International Edition</i> , 2010, 49, 9145-9148.	7.2	70
147	Temperature effects on the hydrophobic interaction of parallel plates in the framework of the probabilistic approach to hydrogen bonding. <i>Journal of Colloid and Interface Science</i> , 2010, 343, 510-521.	5.0	5
148	Role of hydration and water coordination in micellization of Pluronic block copolymers. <i>Journal of Colloid and Interface Science</i> , 2010, 352, 415-423.	5.0	27
149	Relation between the characteristic molecular volume and hydrophobicity of nonpolar molecules. <i>Journal of Chemical Thermodynamics</i> , 2010, 42, 1126-1130.	1.0	14
150	Aminocalix[4]arene: the effect of pH on the dynamics of gate and portals on the hydrophobic cavity. <i>Tetrahedron Letters</i> , 2010, 51, 6156-6160.	0.7	15
151	Water transportation across narrow channel of nanometer dimension. <i>Solid State Communications</i> , 2010, 150, 968-975.	0.9	8
152	Protein diffusion in crowded electrolyte solutions. <i>Biochimica Et Biophysica Acta - Proteins and Proteomics</i> , 2010, 1804, 68-75.	1.1	37
153	On the pairwise hydrophobic interaction of fullerene. <i>Chemical Physics Letters</i> , 2010, 499, 79-82.	1.2	26
154	Transferring electrons to water. <i>Nature Chemistry</i> , 2010, 2, 800-802.	6.6	5

#	ARTICLE	IF	CITATIONS
155	Dynamics in Biological Systems as seen by QENS. Zeitschrift Fur Physikalische Chemie, 2010, 224, 201-214.	1.4	0
156	Kinetics of water filling the hydrophobic channels of narrow carbon nanotubes studied by molecular dynamics simulations. Journal of Chemical Physics, 2010, 133, 204702.	1.2	21
157	Classical to Path-Integral Adaptive Resolution in Molecular Simulation: Towards a Smooth Quantum-Classical Coupling. Physical Review Letters, 2010, 104, 250201.	2.9	67
158	Dissecting the THz spectrum of liquid water from first principles via correlations in time and space. Proceedings of the National Academy of Sciences of the United States of America, 2010, 107, 12068-12073.	3.3	374
159	Assessing the thermodynamic signatures of hydrophobic hydration for several common water models. Journal of Chemical Physics, 2010, 132, 124504.	1.2	71
160	Anomalous dynamics of water confined in MCM-41 at different hydrations. Journal of Physics Condensed Matter, 2010, 22, 284102.	0.7	49
161	Phase transitions and dynamics of bulk and interfacial water. Journal of Physics Condensed Matter, 2010, 22, 284103.	0.7	16
162	Absence of a catalytic water confers resistance to the neurotoxin gabaculine. FASEB Journal, 2010, 24, 404-414.	0.2	8
163	Computational Analysis of Phosphopeptide Binding to the Polo-Box Domain of the Mitotic Kinase PLK1 Using Molecular Dynamics Simulation. PLoS Computational Biology, 2010, 6, e1000880.	1.5	24
164	Dynamics of water at the nanoscale hydrophobic confinement. Journal of Chemical Physics, 2010, 132, 064505.	1.2	30
165	Orientalional dynamics of water trapped between two nanoscopic hydrophobic solutes: A molecular dynamics simulation study. Journal of Chemical Physics, 2010, 133, 154515.	1.2	22
166	Hydration shells exchange charge with their protein. Journal of Physics Condensed Matter, 2010, 22, 365102.	0.7	0
167	The Role of Water Molecules in Computational Drug Design. Current Topics in Medicinal Chemistry, 2010, 10, 55-66.	1.0	155
168	Water: A Unique Solvent and Vital Component of Life. , 2010, , 389-408.		0
169	Hydrophobic Peptide Channels and Encapsulated Water Wires. Journal of the American Chemical Society, 2010, 132, 1075-1086.	6.6	60
170	New insights in the formation of silanol defects in silicalite-1 by water intrusion under high pressure. Physical Chemistry Chemical Physics, 2010, 12, 11454.	1.3	67
171	Nature of the Hydrogen Bond of Water in Solvents of Different Polarities. Journal of Physical Chemistry B, 2010, 114, 16997-17001.	1.2	38
172	Vibrational Spectroscopy as a Probe of Structure and Dynamics in Liquid Water. Chemical Reviews, 2010, 110, 1498-1517.	23.0	640

#	ARTICLE	IF	CITATIONS
173	Molecular simulation of water confined in nanoporous silica. <i>Journal of Physics Condensed Matter</i> , 2010, 22, 284110.	0.7	111
174	Prospects and Pits on the Path of Biomimetics: The Case of Tooth Enamel. <i>Journal of Biomimetics, Biomaterials, and Tissue Engineering</i> , 2010, 8, 45-78.	0.7	17
175	Ion Rejection Properties of Nanopores with Bipolar Fixed Charge Distributions. <i>Journal of Physical Chemistry B</i> , 2010, 114, 10143-10150.	1.2	46
176	Interfacial Free Energy Governs Single Polystyrene Chain Collapse in Water and Aqueous Solutions. <i>Journal of the American Chemical Society</i> , 2010, 132, 6530-6540.	6.6	90
177	Theoretical spectroscopy of floppy peptides at room temperature. A DFTMD perspective: gas and aqueous phase. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 3336.	1.3	158
178	Surface residues dynamically organize water bridges to enhance electron transfer between proteins. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2010, 107, 11799-11804.	3.3	50
179	Structural Properties of Hydration Shell Around Various Conformations of Simple Polypeptides. <i>Journal of Physical Chemistry B</i> , 2010, 114, 4536-4550.	1.2	35
180	Superacid Chemistry on Mildly Acidic Water. <i>Journal of Physical Chemistry Letters</i> , 2010, 1, 3488-3493.	2.1	70
181	Toward an Accurate Modeling of the Water~Zeolite Interaction: Calibrating the DFT Approach. <i>Journal of Physical Chemistry Letters</i> , 2010, 1, 763-768.	2.1	12
182	Are Long-Chain Alkanes Hydrophilic?. <i>Journal of Physical Chemistry B</i> , 2010, 114, 8646-8651.	1.2	32
183	Heme Proteins: The Role of Solvent in the Dynamics of Gates and Portals. <i>Journal of the American Chemical Society</i> , 2010, 132, 5156-5163.	6.6	23
184	Fluorescence Lifetime Probe for Solvent Microviscosity Utilizing Anilinonaphthalene Sulfonate. <i>Analytical Chemistry</i> , 2010, 82, 5470-5476.	3.2	24
185	The Link between Ion Specific Bubble Coalescence and Hofmeister Effects Is the Partitioning of Ions within the Interface. <i>Langmuir</i> , 2010, 26, 6478-6483.	1.6	76
186	Fluctuations in Number of Water Molecules Confined between Nanoparticles. <i>Journal of Physical Chemistry B</i> , 2010, 114, 13410-13414.	1.2	30
187	Direct Evidence of Angular Jumps During Water Reorientation Through Two-Dimensional Infrared Anisotropy. <i>Journal of Physical Chemistry Letters</i> , 2010, 1, 1511-1516.	2.1	40
188	Direct Interaction of Water Ice with Hydrophobic Methyl-Terminated Si(111). <i>Journal of Physical Chemistry C</i> , 2010, 114, 19004-19008.	1.5	7
189	Long-Range Effects of Confinement on Water Structure. <i>Journal of Physical Chemistry B</i> , 2010, 114, 4246-4251.	1.2	6
190	Iron-Nucleated Folding of a Metalloprotein in High Urea: Resolution of Metal Binding and Protein Folding Events. <i>Biochemistry</i> , 2010, 49, 6627-6634.	1.2	21

#	ARTICLE	IF	CITATIONS
191	Proteinâ€™water electrostatics and principles of bioenergetics. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 15335.	1.3	73
192	Influence of Concentration and Temperature on the Dynamics of Water in the Hydrophobic Hydration Shell of Tetramethylurea. <i>Journal of the American Chemical Society</i> , 2010, 132, 15671-15678.	6.6	124
193	Supramolecular Structures of Amyloid-Related Peptides in an Ambient Water Nanofilm. <i>Journal of Physical Chemistry B</i> , 2010, 114, 15759-15765.	1.2	18
194	Protein Denaturation by Ionic Liquids and the Hofmeister Series. <i>ACS Symposium Series</i> , 2010, , 107-117.	0.5	4
195	Dynamics of Water Clusters Confined in Proteins: A Molecular Dynamics Simulation Study of Interfacial Waters in a Dimeric Hemoglobin. <i>Journal of Physical Chemistry B</i> , 2010, 114, 16989-16996.	1.2	62
196	Comment on â€™The hydrophobic effect and its role in cold denaturationâ€™. <i>Cryobiology</i> 60 (2010) 91â€™99. <i>Cryobiology</i> , 2010, 60, 354-355.	0.3	5
197	Near infrared spectroscopy and aquaphotomics: Novel approach for rapid in vivo diagnosis of virus infected soybean. <i>Biochemical and Biophysical Research Communications</i> , 2010, 397, 685-690.	1.0	62
198	On the Origin of the Hydrophobic Water Gap: An X-ray Reflectivity and MD Simulation Study. <i>Journal of the American Chemical Society</i> , 2010, 132, 6735-6741.	6.6	103
199	Chemical complexityâ€™supramolecular self-assembly of synthetic and biological building blocks in water. <i>Chemical Society Reviews</i> , 2010, 39, 2806.	18.7	165
200	Topological Hydrogen-Bond Definition to Characterize the Structure and Dynamics of Liquid Water. <i>Journal of Physical Chemistry B</i> , 2010, 114, 16792-16810.	1.2	72
201	Dependence of the number of hydrogen bonds per water molecule on its distance to a hydrophobic surface and a thereupon-based model for hydrophobic attraction. <i>Journal of Chemical Physics</i> , 2010, 133, 194105.	1.2	13
202	Glycine in aqueous solution: solvation shells, interfacial water, and vibrational spectroscopy from <i>ab initio</i> molecular dynamics. <i>Journal of Chemical Physics</i> , 2010, 133, 114508.	1.2	61
203	Water Hydrogen-Bond Dynamics around Amino Acids: The Key Role of Hydrophilic Hydrogen-Bond Acceptor Groups. <i>Journal of Physical Chemistry B</i> , 2010, 114, 2083-2089.	1.2	113
204	Statistically Converged Properties of Water from Ab Initio Molecular Dynamics Simulations. , 2010, , 687-698.		1
205	Hosting anions. The energetic perspective. <i>Chemical Society Reviews</i> , 2010, 39, 3916.	18.7	119
206	Communication: On the locality of Hydrogen bond networks at hydrophobic interfaces. <i>Journal of Chemical Physics</i> , 2010, 133, 221101.	1.2	55
207	Can a Century Old Experiment Reveal Hidden Properties of Water?. <i>Water (Switzerland)</i> , 2010, 2, 381-410.	1.2	30
208	Long-distance correlations in molecular orientations of liquid water and shape-dependent hydrophobic force. <i>Physical Review E</i> , 2010, 81, 021201.	0.8	22

#	ARTICLE	IF	CITATIONS
209	Solvation theory to provide a molecular interpretation of the hydrophobic entropy loss of noble-gas hydration. <i>Journal of Physics Condensed Matter</i> , 2010, 22, 284108.	0.7	26
210	Ultrafast Dynamics and Hydrogen-Bond Structure in Aqueous Solutions of Model Peptides. <i>Journal of Physical Chemistry B</i> , 2010, 114, 10684-10691.	1.2	64
211	Water Hydrogen Bond Dynamics in Aqueous Solutions of Amphiphiles. <i>Journal of Physical Chemistry B</i> , 2010, 114, 3052-3059.	1.2	106
212	Variations of water's local-structure induced by solvation of NaCl. <i>Chinese Physics B</i> , 2010, 19, 036101.	0.7	2
213	Can Salting-In/Salting-Out Ions be Classified as Chaotropes/Kosmotropes?. <i>Journal of Physical Chemistry B</i> , 2010, 114, 643-650.	1.2	153
215	Temperature-Induced Water Release and Uptake in Organic Porous Networks. <i>Journal of Physical Chemistry B</i> , 2010, 114, 5694-5699.	1.2	10
216	High Performance Computing in Science and Engineering, Garching/Munich 2009. , 2010, , .		3
217	Pore size dependent dynamics of confined water probed by FIR spectroscopy. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 6928.	1.3	13
218	Signal transmission, conversion and multiplication by polar molecules confined in nanochannels. <i>Nanoscale</i> , 2010, 2, 1976.	2.8	33
219	Hydration of nucleic acid bases: a Carâ€Parrinello molecular dynamics approach. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 3363.	1.3	28
220	Controlled ionic condensation at the surface of a native extremophile membrane. <i>Nanoscale</i> , 2010, 2, 222-229.	2.8	18
221	Specific cellular water dynamics observed in vivo by neutron scattering and NMR. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 10154.	1.3	49
222	On the Role of Water in Peroxidase Catalysis: A Theoretical Investigation of HRP Compound I Formation. <i>Journal of Physical Chemistry B</i> , 2010, 114, 5161-5169.	1.2	89
223	Thermodynamic Properties of <i>N</i> -Isopropylacrylamide in Water: Solubility Transition, Phase Separation of Supersaturated Solution, and Glass Formation. <i>Journal of Physical Chemistry B</i> , 2010, 114, 14995-15002.	1.2	16
224	Nuclear Quantum Effects in the Reorientation of Water. <i>Journal of Physical Chemistry Letters</i> , 2010, 1, 2316-2321.	2.1	62
225	Hydration Structure of the Quaternary Ammonium Cations. <i>Journal of Physical Chemistry B</i> , 2010, 114, 15018-15028.	1.2	31
226	Structural Determinants Underlying Photoprotection in the Photoactive Orange Carotenoid Protein of Cyanobacteria. <i>Journal of Biological Chemistry</i> , 2010, 285, 18364-18375.	1.6	152
227	State-resolved THz spectroscopy and dynamics of crystalline peptideâ€water systems. <i>Faraday Discussions</i> , 2011, 150, 175.	1.6	16

#	ARTICLE	IF	CITATIONS
228	Shared solvation of sodium ions in alcohol-water solutions explains the non-ideality of free energy of solvation. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 15423.	1.3	5
229	Computational probe of cavitation events in protein systems. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 19902.	1.3	9
230	Reduced coupling of water molecules near the surface of reverse micelles. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 19355.	1.3	9
231	Non-monotonic dependence of water reorientation dynamics on surface hydrophilicity: competing effects of the hydration structure and hydrogen-bond strength. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 19911.	1.3	60
232	Adhesive water networks facilitate binding of protein interfaces. <i>Nature Communications</i> , 2011, 2, 261.	5.8	132
233	Dynamics of Encapsulated Water inside Molecular Cages. <i>Journal of Physical Chemistry B</i> , 2011, 115, 5980-5992.	1.2	28
234	Viscosity of Aqueous Solutions and Local Microscopic Structure. <i>Journal of Physical Chemistry B</i> , 2011, 115, 14008-14013.	1.2	45
235	Understanding the Mechanisms of Bioprotection: A Comparative Study of Aqueous Solutions of Trehalose and Maltose upon Supercooling. <i>Journal of Physical Chemistry Letters</i> , 2011, 2, 977-982.	2.1	49
236	Mapping the Hydration Dynamics of Ubiquitin. <i>Journal of the American Chemical Society</i> , 2011, 133, 12326-12329.	6.6	103
237	Dissecting the Energetics of Hydrophobic Hydration of Polypeptides. <i>Journal of Physical Chemistry B</i> , 2011, 115, 14859-14865.	1.2	34
238	Entrapment of a Water Wire in a Hydrophobic Peptide Channel with an Aromatic Lining. <i>Journal of Physical Chemistry B</i> , 2011, 115, 9236-9243.	1.2	25
239	Effect of Hydrogen Bonding between Water Molecules on Their Density Distribution near a Hydrophobic Surface. <i>Journal of Physical Chemistry Letters</i> , 2011, 2, 1382-1386.	2.1	18
240	Hydrogen-Bond-Assisted Excited-State Deactivation at Liquid/Water Interfaces. <i>Langmuir</i> , 2011, 27, 4645-4652.	1.6	23
241	Fluoroalkyl and Alkyl Chains Have Similar Hydrophobicities in Binding to the "Hydrophobic Wall" of Carbonic Anhydrase. <i>Journal of the American Chemical Society</i> , 2011, 133, 14017-14026.	6.6	87
242	Low-Frequency Modes of Aqueous Alkali Halide Solutions: An Ultrafast Optical Kerr Effect Study. <i>Journal of Physical Chemistry B</i> , 2011, 115, 1863-1873.	1.2	63
243	Molecular Dynamics Simulation Study of Interaction between Model Rough Hydrophobic Surfaces. <i>Journal of Physical Chemistry A</i> , 2011, 115, 6059-6067.	1.1	13
244	Molecular Dynamics and Neutron Scattering Study of Glucose Solutions Confined in MCM-41. <i>Journal of Physical Chemistry B</i> , 2011, 115, 910-918.	1.2	37
245	Solid-Solid and Solid-Fluid Equilibria of the Most Popular Models of Methanol Obtained by Computer Simulation. <i>Journal of Physical Chemistry B</i> , 2011, 115, 3522-3530.	1.2	9

#	ARTICLE	IF	CITATIONS
246	Microscopic Wetting of Self-Assembled Monolayers with Different Surfaces: A Combined Molecular Dynamics and Quantum Mechanics Study. <i>Langmuir</i> , 2011, 27, 8611-8620.	1.6	34
247	Monovalent Cation Size and DNA Conformational Stability. <i>Biochemistry</i> , 2011, 50, 3084-3094.	1.2	63
248	Role of Hydration Force in the Self-Assembly of Collagens and Amyloid Steric Zipper Filaments. <i>Journal of the American Chemical Society</i> , 2011, 133, 11766-11773.	6.6	18
249	The Role of Hydrophobic Surfaces in Altering Water-Mediated Peptide~Peptide Interactions in an Aqueous Environment. <i>Journal of Physical Chemistry A</i> , 2011, 115, 6088-6092.	1.1	0
250	New Insights into the Structure of the Vapor/Water Interface from Large-Scale First-Principles Simulations. <i>Journal of Physical Chemistry Letters</i> , 2011, 2, 105-113.	2.1	126
251	Evaluating How Discrete Water Molecules Affect Protein~DNA ~ and ~+~ Stacking and T-Shaped Interactions: The Case of Histidine-Adenine Dimers. <i>Journal of Physical Chemistry B</i> , 2011, 115, 10990-11003.	1.2	24
252	Dynamics of Weak, Bifurcated, and Strong Hydrogen Bonds in Lithium Nitrate Trihydrate. <i>Journal of Physical Chemistry Letters</i> , 2011, 2, 1633-1638.	2.1	13
253	Enhanced small-angle scattering connected to the Widom line in simulations of supercooled water. <i>Journal of Chemical Physics</i> , 2011, 134, 214506.	1.2	67
254	A Possible Role of Water in the Protein Folding Process. <i>Journal of Physical Chemistry B</i> , 2011, 115, 14280-14294.	1.2	44
255	Role of Hydration in Collagen Recognition by Bacterial Adhesins. <i>Biophysical Journal</i> , 2011, 100, 2253-2261.	0.2	26
256	Do Hydration Dynamics Follow the Structural Perturbation during Thermal Denaturation of a Protein: A Terahertz Absorption Study. <i>Biophysical Journal</i> , 2011, 101, 925-933.	0.2	70
257	Solution behavior of copolymers with poly(ethylene oxide) as the ~hydrophobic~block. <i>Soft Matter</i> , 2011, 7, 9956.	1.2	15
258	Molecular Docking with Ligand Attached Water Molecules. <i>Journal of Chemical Information and Modeling</i> , 2011, 51, 909-917.	2.5	67
259	Local Order and Mobility of Water Molecules around Ambivalent Helices. <i>Journal of Physical Chemistry B</i> , 2011, 115, 12257-12265.	1.2	8
260	Specific Salt Effects on Poly(ethylene oxide) Electrolyte Solutions. <i>Macromolecules</i> , 2011, 44, 1719-1727.	2.2	54
261	Onset of Hydrogen Bonded Collective Network of Water in 1,4-Dioxane. <i>Journal of Physical Chemistry A</i> , 2011, 115, 14462-14469.	1.1	24
262	Three-Dimensional Water Channel Embedded in an β -Cyclic Octapeptide-Derived Organic Porous Material. <i>Crystal Growth and Design</i> , 2011, 11, 3351-3357.	1.4	5
263	Hydrogen bond dynamics in heavy water studied with quantum dynamical simulations. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 19865.	1.3	16

#	ARTICLE	IF	CITATIONS
264	Temperature-Dependent Infrared Spectroscopy of Water from a First-Principles Approach. <i>Journal of Physical Chemistry A</i> , 2011, 115, 6861-6871.	1.1	25
265	Possible Origin of the Inverse and Direct Hofmeister Series for Lysozyme at Low and High Salt Concentrations. <i>Langmuir</i> , 2011, 27, 9504-9511.	1.6	119
266	Dynamics of Water in Concentrated Solutions of Amphiphiles: Key Roles of Local Structure and Aggregation. <i>Journal of Physical Chemistry B</i> , 2011, 115, 3254-3262.	1.2	70
267	Vibrational spectroscopy of water in hydrated lipid multi-bilayers. I. Infrared spectra and ultrafast pump-probe observables. <i>Journal of Chemical Physics</i> , 2011, 135, 075101.	1.2	50
268	Exploring hydrophobicity by THz absorption spectroscopy of solvated amino acids. <i>Faraday Discussions</i> , 2011, 150, 193.	1.6	63
269	THz Spectra and Dynamics of Aqueous Solutions Studied by the Ultrafast Optical Kerr Effect. <i>Journal of Physical Chemistry B</i> , 2011, 115, 2563-2573.	1.2	66
270	Role of hydration on the functionality of a proteolytic enzyme $\hat{\iota}$ -chymotrypsin under crowded environment. <i>Biochimie</i> , 2011, 93, 1424-1433.	1.3	41
271	Effect of Surface Morphology on the Ordered Water Layer at Room Temperature. <i>Journal of Physical Chemistry C</i> , 2011, 115, 3018-3024.	1.5	52
272	Water in the Active Site of Ketosteroid Isomerase. <i>Biochemistry</i> , 2011, 50, 6689-6700.	1.2	7
273	New Theoretical Method for Rapid Prediction of Solvation Free Energy in Water. <i>Journal of Physical Chemistry B</i> , 2011, 115, 6971-6975.	1.2	60
274	Control of Unidirectional Transport of Single-File Water Molecules through Carbon Nanotubes in an Electric Field. <i>ACS Nano</i> , 2011, 5, 351-359.	7.3	171
275	Comparison of Tetrahedral Order, Liquid State Anomalies, and Hydration Behavior of mTIP3P and TIP4P Water Models. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 3354-3367.	2.3	52
276	Derivation of Equations Describing Distance Solute Oscillation of Induced Solvent Polarization. <i>Bulletin of the Chemical Society of Japan</i> , 2011, 84, 58-69.	2.0	8
277	Measurements of Microproperties of Water Utilizing Charge-Transfer Dye Anilinonaphthalene Sulfonate. <i>Bunseki Kagaku</i> , 2011, 60, 11-18.	0.1	0
278	Interpretation of the water surface vibrational sum-frequency spectrum. <i>Journal of Chemical Physics</i> , 2011, 135, 044701.	1.2	118
279	A recyclable supramolecular membrane for size-selective separation of nanoparticles. <i>Nature Nanotechnology</i> , 2011, 6, 141-146.	15.6	212
280	Site-resolved measurement of water-protein interactions by solution NMR. <i>Nature Structural and Molecular Biology</i> , 2011, 18, 245-249.	3.6	212
281	The variation of the number of hydrogen bonds per water molecule in the vicinity of a hydrophobic surface and its effect on hydrophobic interactions. <i>Current Opinion in Colloid and Interface Science</i> , 2011, 16, 272-284.	3.4	19

#	ARTICLE	IF	CITATIONS
282	Evidence for water structuring forces between surfaces. <i>Current Opinion in Colloid and Interface Science</i> , 2011, 16, 551-556.	3.4	37
283	Local polarity excess at the interface of water with a nonpolar solute. <i>Chemical Physics Letters</i> , 2011, 511, 256-261.	1.2	28
284	In situ molecular dynamics analysis of the water hydrogen bond at biomolecular sites: Hydrophobicity enhances dynamics heterogeneity. <i>Chemical Physics Letters</i> , 2011, 517, 80-85.	1.2	5
285	Perspective on the structure of liquid water. <i>Chemical Physics</i> , 2011, 389, 1-34.	0.9	289
286	Supramolecular Assembly and Binding in Aqueous Solution: Useful Tips Regarding the Hofmeister and Hydrophobic Effects. <i>Israel Journal of Chemistry</i> , 2011, 51, 798-806.	1.0	32
287	Hydrophobicity of Proteins and Interfaces: Insights from Density Fluctuations. <i>Annual Review of Chemical and Biomolecular Engineering</i> , 2011, 2, 147-171.	3.3	192
288	Semiempirical Self-Consistent Polarization Description of Bulk Water, the Liquid-Vapor Interface, and Cubic Ice. <i>Journal of Physical Chemistry A</i> , 2011, 115, 6046-6053.	1.1	22
289	Reorientation and Allied Dynamics in Water and Aqueous Solutions. <i>Annual Review of Physical Chemistry</i> , 2011, 62, 395-416.	4.8	310
290	Adaptive Supramolecular Nanomaterials Based on Strong Noncovalent Interactions. <i>ACS Nano</i> , 2011, 5, 6791-6818.	7.3	413
291	Restructuring of Hydrophobic Surfaces Created by Surfactant Adsorption to Mica Surfaces. <i>Langmuir</i> , 2011, 27, 11737-11741.	1.6	22
292	Evaluating the contribution of solvophobic effects to the Gibbs energy of solvation in methanol. <i>Russian Journal of Physical Chemistry A</i> , 2011, 85, 621-626.	0.1	4
293	Liquid and Glass Polymorphism in a Monatomic System with Isotropic, Smooth Pair Interactions. <i>Journal of Physical Chemistry B</i> , 2011, 115, 14229-14239.	1.2	41
294	Optimization of NMR spectroscopy of encapsulated proteins dissolved in low viscosity fluids. <i>Journal of Biomolecular NMR</i> , 2011, 50, 421-30.	1.6	20
295	The evolution of Photosystem II: insights into the past and future. <i>Photosynthesis Research</i> , 2011, 107, 71-86.	1.6	57
296	What is the best density functional to describe water clusters: evaluation of widely used density functionals with various basis sets for (H ₂ O) _n (n=1-10). <i>Theoretical Chemistry Accounts</i> , 2011, 130, 341-352.	0.5	46
297	A Nuclear Magnetic Resonance study of the reversible denaturation of hydrated lysozyme. <i>Physica A: Statistical Mechanics and Its Applications</i> , 2011, 390, 2904-2908.	1.2	16
298	Ordered water monolayer at room temperature. <i>Rendiconti Lincei</i> , 2011, 22, 5-16.	1.0	9
299	Hydration sites of unpaired RNA bases: a statistical analysis of the PDB structures. <i>BMC Structural Biology</i> , 2011, 11, 41.	2.3	10

#	ARTICLE	IF	CITATIONS
300	Solvophobic effects and relationships between the Gibbs energy and enthalpy for the solvation process. <i>Journal of Physical Organic Chemistry</i> , 2011, 24, 1088-1094.	0.9	43
301	Nanosized hydroxyapatite and other calcium phosphates: Chemistry of formation and application as drug and gene delivery agents. <i>Journal of Biomedical Materials Research - Part B Applied Biomaterials</i> , 2011, 96B, 152-191.	1.6	438
302	Discrepancy in the near-solute electric dipole moment calculated from the electric field. <i>Journal of Computational Chemistry</i> , 2011, 32, 2783-2799.	1.5	10
303	Pathway-Dependent Self-Assembly of Perylene Diimide/Peptide Conjugates in Aqueous Medium. <i>Chemistry - A European Journal</i> , 2011, 17, 6068-6075.	1.7	171
304	Noncovalent Water-Based Materials: Robust yet Adaptive. <i>Chemistry - A European Journal</i> , 2011, 17, 9016-9026.	1.7	107
305	Structure of hydration water in proteins: A comparison of molecular dynamics simulations and database analysis. <i>Biophysical Chemistry</i> , 2011, 158, 73-80.	1.5	32
306	Intermolecular hydrogen bonding interactions of furan, isoxazole and oxazole with water. <i>Computational and Theoretical Chemistry</i> , 2011, 963, 71-75.	1.1	37
307	Biological water: A critique. <i>Chemical Physics Letters</i> , 2011, 503, 1-11.	1.2	259
308	Electronic properties of a methane-water solution. <i>Chemical Physics Letters</i> , 2011, 506, 183-189.	1.2	12
309	Effect of nanotube-length on the transport properties of single-file water molecules: Transition from bidirectional to unidirectional. <i>Journal of Chemical Physics</i> , 2011, 134, 244513.	1.2	27
310	Strong water-mediated friction asymmetry and surface dynamics of zwitterionic solids at ambient conditions: L-alanine as a case study. <i>Journal of Chemical Physics</i> , 2011, 134, 124705.	1.2	8
311	Isotope effects in liquid water by infrared spectroscopy. V. A sea of OH ₂ of C _{2v} symmetry. <i>Journal of Chemical Physics</i> , 2011, 134, 164502.	1.2	18
312	Multiscale Approaches and Perspectives to Modeling Aqueous Electrolytes and Polyelectrolytes. <i>Topics in Current Chemistry</i> , 2011, 307, 251-294.	4.0	9
313	Vibrational spectroscopy of water in hydrated lipid multi-bilayers. II. Two-dimensional infrared and peak shift observables within different theoretical approximations. <i>Journal of Chemical Physics</i> , 2011, 135, 164506.	1.2	26
314	Prediction and interpretation of the hydration entropies of monovalent cations and anions. <i>Molecular Physics</i> , 2011, 109, 37-48.	0.8	26
315	Mechanism of the hydrophobic effect in the biomolecular recognition of arylsulfonamides by carbonic anhydrase. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2011, 108, 17889-17894.	3.3	304
316	Electrostatic interaction forces in aqueous salt solutions of variable concentration and valency. <i>Nanotechnology</i> , 2011, 22, 305706.	1.3	65
317	Predicting what extra-terrestrials will be like: and preparing for the worst. <i>Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences</i> , 2011, 369, 555-571.	1.6	16

#	ARTICLE	IF	CITATIONS
318	From Water and Ions to Crowded Biomacromolecules: <i>In Vivo</i> Structuring of a Prokaryotic Cell. <i>Microbiology and Molecular Biology Reviews</i> , 2011, 75, 491-506.	2.9	63
319	The "Autothixotropic" Phenomenon of Water and its Role in Proton Transfer. <i>International Journal of Molecular Sciences</i> , 2011, 12, 7481-7494.	1.8	14
320	Oriental relaxation dynamics in aqueous ionic solution: Polarization-selective two-dimensional infrared study of angular jump-exchange dynamics in aqueous 6M NaClO ₄ . <i>Journal of Chemical Physics</i> , 2011, 134, 044516.	1.2	42
321	DNA-Based Soft Phases. <i>Topics in Current Chemistry</i> , 2011, 318, 225-279.	4.0	29
322	Two-dimensional infrared spectral signature and hydration of the oxalate dianion. <i>Journal of Chemical Physics</i> , 2011, 135, 204502.	1.2	32
323	Structure and dynamics of protein waters revealed by radiolysis and mass spectrometry. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2012, 109, 14882-14887.	3.3	44
324	Stressing Lipid Membranes: Effects of Polymers on Membrane Structural Integrity. <i>Materials Research Society Symposia Proceedings</i> , 2012, 1480, 1.	0.1	1
325	Microscopic probing of the size dependence in hydrophobic solvation. <i>Journal of Chemical Physics</i> , 2012, 136, 074507.	1.2	30
326	Relaxation and jump dynamics of water at the mica interface. <i>Journal of Chemical Physics</i> , 2012, 136, 194701.	1.2	37
327	Dynamics of two-dimensional monolayer water confined in hydrophobic and charged environments. <i>Journal of Chemical Physics</i> , 2012, 137, 114510.	1.2	12
328	Semiquantal molecular dynamics simulations of hydrogen-bond dynamics in liquid water using multi-dimensional Gaussian wave packets. <i>Journal of Chemical Physics</i> , 2012, 137, 174503.	1.2	10
329	Solvated dissipative electro-elastic network model of hydrated proteins. <i>Journal of Chemical Physics</i> , 2012, 137, 165101.	1.2	14
330	Long-Ranged Attraction between Disordered Heterogeneous Surfaces. <i>Physical Review Letters</i> , 2012, 109, 168305.	2.9	47
331	Non-enzymatic Polymerization of Nucleic Acids from Monomers: Monomer Self-Condensation and Template-Directed Reactions. <i>Current Organic Synthesis</i> , 2012, 9, 735-763.	0.7	15
332	Spectral pattern of urinary water as a biomarker of estrus in the giant panda. <i>Scientific Reports</i> , 2012, 2, 856.	1.6	57
333	Polarizable Molecular Dynamics Simulations of Aqueous Dipeptides. <i>Journal of Physical Chemistry B</i> , 2012, 116, 8733-8740.	1.2	8
334	Water structural transformation at molecular hydrophobic interfaces. <i>Nature</i> , 2012, 491, 582-585.	13.7	466
335	Liquid Water: From Symmetry Distortions to Diffusive Motion. <i>Accounts of Chemical Research</i> , 2012, 45, 63-73.	7.6	78

#	ARTICLE	IF	CITATIONS
336	Aqueous Solutions at the Interface with Phospholipid Bilayers. <i>Accounts of Chemical Research</i> , 2012, 45, 74-82.	7.6	100
337	Water Dynamics in Water/DMSO Binary Mixtures. <i>Journal of Physical Chemistry B</i> , 2012, 116, 5479-5490.	1.2	155
338	Preferential Formation of the Different Hydrogen Bonds and Their Effects in Tetrahydrofuran and Tetrahydropyran Microhydrated Complexes. <i>Journal of Physical Chemistry A</i> , 2012, 116, 4199-4210.	1.1	13
339	Long-range hydrogen-bond structure in aqueous solutions and the vapor-water interface. <i>Journal of Chemical Physics</i> , 2012, 137, 034508.	1.2	34
340	Quantification of Local Hydration at the Surface of Biomolecules Using Dual-Fluorescence Labels. <i>Journal of Physical Chemistry A</i> , 2012, 116, 3103-3109.	1.1	22
341	Terahertz absorption of dilute aqueous solutions. <i>Journal of Chemical Physics</i> , 2012, 137, 235103.	1.2	51
342	Effect of Water's Water Hydrogen Bonding on the Hydrophobic Hydration of Large-Scale Particles and Its Temperature Dependence. <i>Journal of Physical Chemistry B</i> , 2012, 116, 2820-2830.	1.2	15
344	Artificial Water Channels. <i>Angewandte Chemie - International Edition</i> , 2012, 51, 11674-11676.	7.2	115
345	Ionization-Induced Solvent Migration in Acetanilide-Methanol Clusters Inferred from Isomer-Selective Infrared Spectroscopy. <i>ChemPhysChem</i> , 2012, 13, 3875-3881.	1.0	14
346	Virtual fragment screening: exploration of MM-PBSA re-scoring. <i>Journal of Computer-Aided Molecular Design</i> , 2012, 26, 921-934.	1.3	7
347	Targeted nano analysis of water and ions using cryocorrelative light and scanning transmission electron microscopy. <i>Journal of Structural Biology</i> , 2012, 180, 352-361.	1.3	7
348	Quantifying Protein-Ligand Binding Constants using Electrospray Ionization Mass Spectrometry: A Systematic Binding Affinity Study of a Series of Hydrophobically Modified Trypsin Inhibitors. <i>Journal of the American Society for Mass Spectrometry</i> , 2012, 23, 1768-1777.	1.2	39
350	Water-wire catalysis in photoinduced acid-base reactions. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 8974.	1.3	27
351	Intramolecular vibrational coupling in water molecules revealed by compatible multiple nonlinear vibrational spectroscopic measurements. <i>Analyst</i> , The, 2012, 137, 4981.	1.7	9
352	DNA tetraplex structure formation from human telomeric repeat motif (TTAGGG):(CCCTAA) in nanocavity water pools of reverse micelles. <i>Chemical Communications</i> , 2012, 48, 4815.	2.2	43
353	The importance of the shape of the protein-water interface of a kinesin motor domain for dynamics of the surface atoms of the protein. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 5561.	1.3	15
354	Dielectric spectroscopy in the GHz region on fully hydrated zwitterionic amino acids. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 11352.	1.3	56
355	Does cation dehydration drive the binding of metal ions to polyelectrolytes in water? What we can learn from the behaviour of aluminium(III) and chromium(III). <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 7950.	1.3	19

#	ARTICLE	IF	CITATIONS
356	Oriented Confined Water Induced by Cationic Lipids. <i>Langmuir</i> , 2012, 28, 4712-4722.	1.6	10
357	Quantum-Mechanical Study on the Mechanism of Peptide Bond Formation in the Ribosome. <i>Journal of the American Chemical Society</i> , 2012, 134, 5817-5831.	6.6	31
358	Slow Relaxation Dynamics of Water in Hydroxypropyl Cellulose-Water Mixture Traces Its Phase Transition Pathway: A Spectroscopic Investigation. <i>Journal of Physical Chemistry B</i> , 2012, 116, 1508-1516.	1.2	19
359	Kirkwood's Buff Analysis of Liquid Mixtures in an Open Boundary Simulation. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 375-379.	2.3	39
360	Recent Trends and Applications in 3D Virtual Screening. <i>Combinatorial Chemistry and High Throughput Screening</i> , 2012, 15, 749-769.	0.6	16
361	Comparing the ultraviolet photostability of azole chromophores. <i>Chemical Science</i> , 2012, 3, 1192.	3.7	19
362	Solvated calcium ions in charged silica nanopores. <i>Journal of Chemical Physics</i> , 2012, 137, 064706.	1.2	32
363	Spatial Distribution of Lipid Headgroups and Water Molecules at Membrane/Water Interfaces Visualized by Three-Dimensional Scanning Force Microscopy. <i>ACS Nano</i> , 2012, 6, 9013-9020.	7.3	81
364	Far/Mid-Infrared Signatures of Solvent-Solute Interactions in a Microhydrated Model Peptide Chain. <i>Journal of Physical Chemistry Letters</i> , 2012, 3, 3307-3311.	2.1	23
365	Hydrophobic Drying and Hysteresis at Different Length Scales by Molecular Dynamics Simulations. <i>Langmuir</i> , 2012, 28, 3152-3158.	1.6	14
366	Steering the enzymatic activity of proteins by ionic liquids. A case study of the enzyme kinetics of yeast alcohol dehydrogenase. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 4635.	1.3	27
367	Spectroscopy and Dynamics of the Multiple Free OH Species at an Aqueous/Hydrophobic Interface. <i>Journal of Physical Chemistry C</i> , 2012, 116, 21734-21741.	1.5	15
368	Hydration Force between Mica Surfaces in Aqueous KCl Electrolyte Solution. <i>Langmuir</i> , 2012, 28, 5339-5349.	1.6	90
369	IR Spectroscopy of Protonation in Benzene-Water Nanoclusters: Hydronium, Zundel, and Eigen at a Hydrophobic Interface. <i>Journal of the American Chemical Society</i> , 2012, 134, 13046-13055.	6.6	63
370	Does Solution Viscosity Scale the Rate of Aggregation of Folded Proteins?. <i>Journal of Physical Chemistry Letters</i> , 2012, 3, 1258-1263.	2.1	13
371	Revealing Charge-Transfer Effects in Gas-Phase Water Chemistry. <i>Accounts of Chemical Research</i> , 2012, 45, 1571-1580.	7.6	107
372	Temperature-Enhanced Association of Proteins Due to Electrostatic Interaction: A Coarse-Grained Simulation of Actin-Myosin Binding. <i>Journal of the American Chemical Society</i> , 2012, 134, 8918-8925.	6.6	41
373	Evaporation rate of water in hydrophobic confinement. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2012, 109, 4365-4370.	3.3	150

#	ARTICLE	IF	CITATIONS
374	Hydroxide Ion Can Move Faster Than an Excess Proton through One-Dimensional Water Chains in Hydrophobic Narrow Pores. <i>Journal of Physical Chemistry B</i> , 2012, 116, 9744-9757.	1.2	37
375	Protein Structure. , 2012, , .		2
376	Effect of Nanochannel Dimension on the Transport of Water Molecules. <i>Journal of Physical Chemistry B</i> , 2012, 116, 5925-5932.	1.2	90
377	How ionic liquids can help to stabilize native proteins. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 415-426.	1.3	250
378	Why the Solvation Water around Proteins Is More Dense than Bulk Water. <i>Journal of Physical Chemistry B</i> , 2012, 116, 12113-12124.	1.2	52
379	Thermodynamic Investigations Using Molecular Dynamics Simulations with Potential of Mean Force Calculations for Cardiotoxin Protein Adsorption on Mixed Self-Assembled Monolayers. <i>Journal of Physical Chemistry B</i> , 2012, 116, 12661-12668.	1.2	14
380	Functional and conformational changes in the aspartic protease cardosin A induced by TFE. <i>International Journal of Biological Macromolecules</i> , 2012, 50, 323-330.	3.6	3
381	Dynamics of Water Near Oxidized Polystyrene Films. <i>Macromolecular Theory and Simulations</i> , 2012, 21, 544-552.	0.6	2
383	The effect of pressure on the hydration structure around hydrophobic solute: A molecular dynamics simulation study. <i>Journal of Chemical Physics</i> , 2012, 136, 114510.	1.2	42
384	Dynamic Behavior of Oligomeric Inorganic Pyrophosphatase Explored by Quasielastic Neutron Scattering. <i>Journal of Physical Chemistry B</i> , 2012, 116, 9917-9921.	1.2	9
385	Surface Polarity and Nanoscale Solvation. <i>Journal of Physical Chemistry Letters</i> , 2012, 3, 3685-3689.	2.1	10
386	Dehydration from conserved stem regions is fundamental for ligand-dependent conformational transition of the adenine-specific riboswitch. <i>Chemical Communications</i> , 2012, 48, 9693.	2.2	15
387	Ultrafast Vibrational Dynamics of Water Confined in Phospholipid Reverse Micelles. <i>Journal of Physical Chemistry B</i> , 2012, 116, 5752-5759.	1.2	44
388	On the absolute thermodynamics of water from computer simulations: A comparison of first-principles molecular dynamics, reactive and empirical force fields. <i>Journal of Chemical Physics</i> , 2012, 137, 244507.	1.2	59
389	Application of Adaptive QM/MM Methods to Molecular Dynamics Simulations of Aqueous Systems. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 2868-2877.	2.3	54
390	The Silica-Water Interface: How the Silanols Determine the Surface Acidity and Modulate the Water Properties. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 1037-1047.	2.3	352
391	Molecular dynamics simulation study of the water-mediated interaction between zwitterionic and charged surfaces. <i>Journal of Chemical Physics</i> , 2012, 136, 024501.	1.2	10
392	Dynamical Coupling of Intrinsically Disordered Proteins and Their Hydration Water: Comparison with Folded Soluble and Membrane Proteins. <i>Biophysical Journal</i> , 2012, 103, 129-136.	0.2	79

#	ARTICLE	IF	CITATIONS
393	Structure and electronic properties of a benzene-water solution. <i>Journal of Chemical Physics</i> , 2012, 136, 014507.	1.2	29
394	On the photophysics and photochemistry of the water dimer. <i>Journal of Chemical Physics</i> , 2012, 137, 244309.	1.2	24
395	From Conventional to Phase-Sensitive Vibrational Sum Frequency Generation Spectroscopy: Probing Water Organization at Aqueous Interfaces. <i>Journal of Physical Chemistry Letters</i> , 2012, 3, 3012-3028.	2.1	67
396	Guest-Host Interactions Investigated by Time-Resolved X-ray Spectroscopies and Scattering at MHz Rates: Solvation Dynamics and Photoinduced Spin Transition in Aqueous Fe(bipy) ₃ ²⁺ . <i>Journal of Physical Chemistry A</i> , 2012, 116, 9878-9887.	1.1	112
397	The effects of electronic polarization on water adsorption in metal-organic frameworks: H ₂ O in MIL-53(Cr). <i>Journal of Chemical Physics</i> , 2012, 137, 054704.	1.2	45
398	Bioinspired Nanoscale Water Channel and its Potential Applications. <i>Biological and Medical Physics Series</i> , 2012, , 1-55.	0.3	0
399	Multiscale Molecular Methods in Applied Chemistry. <i>Topics in Current Chemistry</i> , 2012, , .	4.0	39
400	Critical Dipole Length for the Wetting Transition Due to Collective Water-dipoles Interactions. <i>Scientific Reports</i> , 2012, 2, 358.	1.6	64
401	Dipolar response of hydrated proteins. <i>Journal of Chemical Physics</i> , 2012, 136, 085102.	1.2	39
402	Hydrophobic nanoconfinement suppresses fluctuations in supercooled water. <i>Journal of Physics Condensed Matter</i> , 2012, 24, 064111.	0.7	17
403	Fluid dynamics in fascial tissues. , 2012, , 177-181.		1
404	Site-Specific Hydration Dynamics of Globular Proteins and the Role of Constrained Water in Solvent Exchange with Amphiphilic Cosolvents. <i>Journal of Physical Chemistry B</i> , 2012, 116, 5604-5611.	1.2	75
405	Role of Glucose in Enhancing Stability of Aqueous Silica Gels Against Dehydration. <i>Journal of Physical Chemistry C</i> , 2012, 116, 9481-9486.	1.5	6
406	BASIC NANOSCIENCE. , 2012, , 121-147.		0
407	Progress in Modeling of Ion Effects at the Vapor/Water Interface. <i>Annual Review of Physical Chemistry</i> , 2012, 63, 401-418.	4.8	119
408	Sealed Gravitational Capillary Viscometry of Dimethyl Ether and Two Next-Generation Alternative Refrigerants. <i>Journal of Research of the National Institute of Standards and Technology</i> , 2012, 117, 231.	0.4	38
409	<i>Ab Initio</i> Molecular Dynamics Study of Dissociation of Water under an Electric Field. <i>Physical Review Letters</i> , 2012, 108, 207801.	2.9	181
410	The controlled relay of multiple protons required at the active site of nitrogenase. <i>Dalton Transactions</i> , 2012, 41, 7647.	1.6	50

#	ARTICLE	IF	CITATIONS
411	Impact of chemical heterogeneity on protein self-assembly in water. Proceedings of the National Academy of Sciences of the United States of America, 2012, 109, 7636-7641.	3.3	109
412	Protein Crowding Affects Hydration Structure and Dynamics. Journal of the American Chemical Society, 2012, 134, 4842-4849.	6.6	189
413	Molecular dynamics extended for fluctuating networks: Application to water. Journal of Computational Chemistry, 2012, 33, 1364-1373.	1.5	0
414	Molecular Dynamics Simulations of G Protein-Coupled Receptors. Molecular Informatics, 2012, 31, 222-230.	1.4	15
415	Viscosity and diffusion: crowding and salt effects in protein solutions. Soft Matter, 2012, 8, 1404-1419.	1.2	86
416	A Polymer Surfactant Corona Dynamically Replaces Water in Solvent-Free Protein Liquids and Ensures Macromolecular Flexibility and Activity. Journal of the American Chemical Society, 2012, 134, 13168-13171.	6.6	45
419	Molecular Assemblies of Perylene Bisimide Dyes in Water. Angewandte Chemie - International Edition, 2012, 51, 6328-6348.	7.2	417
420	Watching Water Migration around a Peptide Bond. Angewandte Chemie - International Edition, 2012, 51, 6604-6607.	7.2	63
421	Molecular Hydrogels from Bolaform Amino Acid Derivatives: A Structure-Properties Study Based on the Thermodynamics of Gel Solubilization. Chemistry - A European Journal, 2012, 18, 4063-4072.	1.7	80
422	From <i>lin</i> -Benzoguanines to <i>lin</i> -Benzohypoxanthines as Ligands for <i>Zymomonas mobilis</i> tRNA-Guanine Transglycosylase: Replacement of Protein-Ligand Hydrogen Bonding by Importing Water Clusters. Chemistry - A European Journal, 2012, 18, 9246-9257.	1.7	19
423	Nanobubbles are not a Superficial Matter. ChemPhysChem, 2012, 13, 2173-2177.	1.0	33
424	Assessment of density functional theory to calculate the phase transition pressure of ice. Physical Chemistry Chemical Physics, 2012, 14, 11484.	1.3	22
425	Aqueous solutions of nonelectrolytes. Journal of Thermal Analysis and Calorimetry, 2012, 108, 547-558.	2.0	7
426	Peptide Self-Assembly on Mica under Ethanol-Containing Atmospheres: Effects of Ethanol on Epitaxial Growth of Peptide Nanofilaments. Journal of Physical Chemistry B, 2012, 116, 2927-2933.	1.2	15
427	Excited-State Dynamics of Organic Dyes at Liquid/Liquid Interfaces. Langmuir, 2012, 28, 11291-11301.	1.6	16
428	A theoretical study on 2-deoxyguanosine and its mono-hydration: Intermolecular hydrogen bonding weakening induces the fluorescence strengthening. Chemical Physics Letters, 2012, 528, 53-58.	1.2	15
429	An ultrasensitive tool exploiting hydration dynamics to decipher weak lipid membrane-polymer interactions. Journal of Magnetic Resonance, 2012, 215, 115-119.	1.2	32
430	Structural changes in ethanol-water mixtures: Ultrasonics, Brillouin scattering and molecular dynamics studies. Vibrational Spectroscopy, 2012, 60, 102-106.	1.2	34

#	ARTICLE	IF	CITATIONS
432	Molecular Recognition at the Active Site of Factor Xa: Cation-π Interactions, Stacking on Planar Peptide Surfaces, and Replacement of Structural Water. <i>Chemistry - A European Journal</i> , 2012, 18, 213-222.	1.7	51
433	Effect of hydrophobic environments on the hypothesized liquid-liquid critical point of water. <i>Journal of Biological Physics</i> , 2012, 38, 97-111.	0.7	17
434	Semi-quantal molecular dynamics simulations of hydrogen-bond dynamics in liquid water using spherical gaussian wave packets. <i>International Journal of Quantum Chemistry</i> , 2013, 113, 356-365.	1.0	6
435	Changes to cellular water and element content induced by nucleolar stress: investigation by a cryo-correlative nano-imaging approach. <i>Cellular and Molecular Life Sciences</i> , 2013, 70, 2383-2394.	2.4	29
437	A morphometric approach for the accurate solvation thermodynamics of proteins and ligands. <i>Journal of Computational Chemistry</i> , 2013, 34, 1969-1974.	1.5	9
438	On the cooperative formation of non-hydrogen-bonded water at molecular hydrophobic interfaces. <i>Nature Chemistry</i> , 2013, 5, 796-802.	6.6	136
439	Effect of surface hydrophobicity on the dynamics of water at the nanoscale confinement: A molecular dynamics simulation study. <i>Chemical Physics</i> , 2013, 421, 68-76.	0.9	15
440	Water at Biological and Inorganic Interfaces. <i>Food Biophysics</i> , 2013, 8, 153-169.	1.4	28
441	Wetting Reversal at Gelation Transition Freezes Thermodynamically Unstable States. <i>Langmuir</i> , 2013, 29, 9041-9045.	1.6	2
442	Solvated protein-DNA docking using HADDOCK. <i>Journal of Biomolecular NMR</i> , 2013, 56, 51-63.	1.6	23
443	Water and water-like liquids: relationships between structure, entropy and mobility. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 14162.	1.3	66
444	Dynamics of Water Confined in Reversed Micelles: Multidimensional Vibrational Spectroscopy Study. <i>Journal of Physical Chemistry B</i> , 2013, 117, 15545-15558.	1.2	82
445	Properties of water in the region between a tubulin dimer and a single motor head of kinesin. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 4527.	1.3	9
446	Molecular intermittent dynamics of interfacial water: probing adsorption and bulk confinement. <i>Soft Matter</i> , 2013, 9, 8654.	1.2	20
447	Asymmetrical free diffusion with orientation-dependence of molecules in finite timescales. <i>Science China: Physics, Mechanics and Astronomy</i> , 2013, 56, 1047-1052.	2.0	7
448	Correlation of Structural Order, Anomalous Density, and Hydrogen Bonding Network of Liquid Water. <i>Journal of Physical Chemistry B</i> , 2013, 117, 8831-8843.	1.2	46
449	Self-Assembled Supramolecular Channels: Toward Biomimetic Materials for Directional Translocation. <i>Chemical Record</i> , 2013, 13, 524-538.	2.9	18
450	Excess second-order thermodynamic derivatives of the {2-propanol+water} system from 313.15K to 403.15K up to 140MPa. Experimental and Monte Carlo simulation study. <i>Fluid Phase Equilibria</i> , 2013, 358, 7-26.	1.4	13

#	ARTICLE	IF	CITATIONS
451	Dissecting Hydrophobic Hydration and Association. <i>Journal of Physical Chemistry B</i> , 2013, 117, 15479-15491.	1.2	51
452	An Ab Initio Microscope: Molecular Contributions to the Femtosecond Time-Dependent Fluorescence Shift of a Reichardt-Type Dye. <i>Angewandte Chemie - International Edition</i> , 2013, 52, 1813-1816.	7.2	21
453	Hydrophobic force, a Casimir-like effect due to hydrogen-bond fluctuations. <i>Physica A: Statistical Mechanics and Its Applications</i> , 2013, 392, 4804-4823.	1.2	2
454	Radical re-appraisal of water structure in hydrophilic confinement. <i>Chemical Physics Letters</i> , 2013, 590, 1-15.	1.2	40
455	Reaching new levels of realism in modeling biological macromolecules in cellular environments. <i>Journal of Molecular Graphics and Modelling</i> , 2013, 45, 144-156.	1.3	58
456	Biological Water Dynamics and Entropy: A Biophysical Origin of Cancer and Other Diseases. <i>Entropy</i> , 2013, 15, 3822-3876.	1.1	46
457	Combining Solvent Thermodynamic Profiles with Functionality Maps of the Hsp90 Binding Site to Predict the Displacement of Water Molecules. <i>Journal of Chemical Information and Modeling</i> , 2013, 53, 2571-2586.	2.5	39
458	Stability and solid-state polymerization reactivity of imidazolyl- and benzimidazolyl-substituted diacetylenes: pivotal role of lattice water. <i>CrystEngComm</i> , 2013, 15, 4261.	1.3	14
459	Nitrogenase: a general hydrogenator of small molecules. <i>Chemical Communications</i> , 2013, 49, 10893.	2.2	68
460	Ultrafast Energy Transfer to Liquid Water by Sub-Picosecond High-Intensity Terahertz Pulses: An Ab-Initio Molecular Dynamics Study. <i>Angewandte Chemie - International Edition</i> , 2013, 52, 13685-13687.	7.2	18
461	Cucurbit[8]uril and Blue-Box: High-Energy Water Release Overwhelms Electrostatic Interactions. <i>Journal of the American Chemical Society</i> , 2013, 135, 14879-14888.	6.6	174
462	Surface Processes on Interstellar Amorphous Solid Water: Adsorption, Diffusion, Tunneling Reactions, and Nuclear-Spin Conversion. <i>Chemical Reviews</i> , 2013, 113, 8783-8839.	23.0	245
463	Wetting Behavior of Water near Nonpolar Surfaces. <i>Journal of Physical Chemistry C</i> , 2013, 117, 23017-23026.	1.5	48
464	Critical Role of Water in the Binding of Volatile Anesthetics to Proteins. <i>Journal of Physical Chemistry B</i> , 2013, 117, 12007-12012.	1.2	11
465	Surface Corrugation Effects on the Water-Graphene Interfacial and Confinement Behavior. <i>Journal of Physical Chemistry C</i> , 2013, 117, 23875-23886.	1.5	20
466	Real-Time Probing of Hydrogen-Bond Exchange Dynamics in Aqueous NaPF ₆ Solutions by Two-Dimensional Infrared Spectroscopy. <i>Journal of Physical Chemistry B</i> , 2013, 117, 13604-13613.	1.2	13
467	On the Origin of Proton Mobility Suppression in Aqueous Solutions of Amphiphiles. <i>Journal of Physical Chemistry B</i> , 2013, 117, 15426-15435.	1.2	12
468	Revisiting the fundamentals in the design and control of nanoparticulate colloids in the frame of soft chemistry. <i>Review Journal of Chemistry</i> , 2013, 3, 271-303.	1.0	11

#	ARTICLE	IF	CITATIONS
469	Changing hydration level in an internal cavity modulates the proton affinity of a key glutamate in cytochrome <i>c</i> oxidase. Proceedings of the National Academy of Sciences of the United States of America, 2013, 110, 18886-18891.	3.3	58
470	Vibrational Signature of Water Molecules in Asymmetric Hydrogen Bonding Environments. Journal of Physical Chemistry Letters, 2013, 4, 3245-3250.	2.1	46
471	Spatial Dependence of Protein-Water Collective Hydrogen-Bond Dynamics. Physical Review Letters, 2013, 111, 218101.	2.9	111
472	Insights on Hydrogen-Bond Lifetimes in Liquid and Supercooled Water. Journal of Physical Chemistry B, 2013, 117, 16188-16195.	1.2	50
473	Dielectric relaxation of the extended hydration sheathe of DNA in the THz frequency region. Chemical Physics Letters, 2013, 586, 143-147.	1.2	29
474	Modeling the cysteamine catalyzed cysteine proteinases using DFT: mechanistic insights into the hydrolysis of acetyl-p-nitroanilide. New Journal of Chemistry, 2013, 37, 4061.	1.4	3
475	Halogen bonding in complexes of proteins and non-natural amino acids. Computational Biology and Chemistry, 2013, 47, 231-239.	1.1	22
476	Low concentrated hydroxyectoine solutions in presence of DPPC lipid bilayers: A computer simulation study. Biophysical Chemistry, 2013, 180-181, 102-109.	1.5	23
477	Many-Body Convergence of the Electrostatic Properties of Water. Journal of Chemical Theory and Computation, 2013, 9, 4844-4852.	2.3	29
478	Strategic Targeting of Multiple Water-Mediated Interactions: A Concise and Rational Structure-Based Design Approach to Potent and Selective MMP-13 Inhibitors. ChemMedChem, 2013, 8, 1457-1461.	1.6	16
479	Spatial decomposition and assignment of infrared spectra of simple ions in water from mid-infrared to THz frequencies: Li ⁺ (aq) and F ⁻ (aq). Journal of Chemical Physics, 2013, 139, 014506.	1.2	27
480	Microscopic mechanism of protein cryopreservation in an aqueous solution with trehalose. Scientific Reports, 2013, 3, 1218.	1.6	115
481	Anomalous Debye-like dielectric relaxation of water in micro-sized confined polymeric systems. Physical Chemistry Chemical Physics, 2013, 15, 20153.	1.3	14
482	The role of solvent cohesion in nonpolar solvation. Chemical Science, 2013, 4, 2953.	3.7	37
483	Concluding remarks: Cum grano salis. Faraday Discussions, 2013, 160, 405-414.	1.6	9
484	A Paradigm Shift in Drying of Food Materials via Free-Volume Concepts. Drying Technology, 2013, 31, 1817-1825.	1.7	7
485	Water mediated proton hopping empowers proteins. Soft Matter, 2013, 9, 643-646.	1.2	23
486	Water PMF for predicting the properties of water molecules in protein binding site. Journal of Computational Chemistry, 2013, 34, 583-592.	1.5	25

#	ARTICLE	IF	CITATIONS
487	Investigation of organelle-specific intracellular water structures with Raman microspectroscopy. <i>Journal of Raman Spectroscopy</i> , 2013, 44, 167-169.	1.2	8
488	Protein dynamics: Complex by itself. <i>Complexity</i> , 2013, 18, 48-56.	0.9	13
489	Capturing the energetics of water insertion in biological systems: The water flooding approach. <i>Proteins: Structure, Function and Bioinformatics</i> , 2013, 81, 93-106.	1.5	41
490	Solvated protein-protein docking using Kyte-Doolittle-based water preferences. <i>Proteins: Structure, Function and Bioinformatics</i> , 2013, 81, 510-518.	1.5	26
491	Effect of organic molecules on hydrolysis of peptide bond: A DFT study. <i>Chemical Physics</i> , 2013, 415, 282-290.	0.9	7
492	State-Dependent Electron Delocalization Dynamics at the Solute-Solvent Interface: Soft-X-Ray Absorption Spectroscopy and <i>Ab Initio</i> Calculations. <i>Physical Review Letters</i> , 2013, 111, 083002.	2.9	74
493	Modeling cooking of chicken meat in industrial tunnel ovens with the Flory-Rehner theory. <i>Meat Science</i> , 2013, 95, 940-957.	2.7	42
494	Microscopic Origin of the Deviation from Stokes-Einstein Behavior Observed in Dynamics of the KSCN Aqueous Solutions: A MD Simulation Study. <i>Journal of Physical Chemistry B</i> , 2013, 117, 2992-3004.	1.2	24
495	Surface Transformations and Water Uptake on Liquid and Solid Butanol near the Melting Temperature. <i>Journal of Physical Chemistry C</i> , 2013, 117, 6678-6685.	1.5	16
496	The interfacial-organized monolayer water film (MWF) induced two-step aggregation of nanographene: both in stacking and sliding assembly pathways. <i>Nanoscale</i> , 2013, 5, 2765.	2.8	17
497	Nonlinear Scaling of Surface Water Diffusion with Bulk Water Viscosity of Crowded Solutions. <i>Journal of the American Chemical Society</i> , 2013, 135, 4175-4178.	6.6	34
498	Molecular simulations on nanoconfined water molecule behaviors for nanoporous material applications. <i>Microfluidics and Nanofluidics</i> , 2013, 15, 191-205.	1.0	49
499	Further Studies on the Role of Water in R67 Dihydrofolate Reductase. <i>Biochemistry</i> , 2013, 52, 2118-2127.	1.2	10
500	Molecular dynamics simulations and density functional theory studies of NALMA and NAGMA dipeptides. <i>Journal of Biomolecular Structure and Dynamics</i> , 2013, 31, 158-173.	2.0	16
501	The Importance of Water. , 2013, , 169-210.		12
502	Slow dynamics, hydration and heterogeneity in Laponite dispersions. <i>Soft Matter</i> , 2013, 9, 2003.	1.2	22
503	Redox potential (Eh) and pH as drivers of soil/plant/microorganism systems: a transdisciplinary overview pointing to integrative opportunities for agronomy. <i>Plant and Soil</i> , 2013, 362, 389-417.	1.8	461
504	Biomolecular hydration dynamics: a jump model perspective. <i>Chemical Society Reviews</i> , 2013, 42, 5672.	18.7	100

#	ARTICLE	IF	CITATIONS
505	Ethanol promotes dewetting transition at low concentrations. <i>Soft Matter</i> , 2013, 9, 4655.	1.2	20
506	From Natural to Bioassisted and Biomimetic Artificial Water Channel Systems. <i>Accounts of Chemical Research</i> , 2013, 46, 2814-2823.	7.6	155
507	Properties of a water layer on hydrophilic and hydrophobic self-assembled monolayer surfaces: A molecular dynamics study. <i>Science China Chemistry</i> , 2013, 56, 773-781.	4.2	23
508	Microsolvation and hydration enthalpies of $\text{CaC}_2\text{O}_4(\text{H}_2\text{O})_n$ ($n = 0-16$) and $\text{C}_2\text{O}_4^{2-}(\text{H}_2\text{O})_n$ ($n = 0-14$): an ab initio study. <i>Journal of Molecular Modeling</i> , 2013, 19, 1459-1471.	0.8	4
509	Stepwise-Resolved Thermodynamics of Hydrophobic Self-Assembly. <i>Angewandte Chemie - International Edition</i> , 2013, 52, 8358-8362.	7.2	28
510	Partition coefficients of ionizable solutes in aqueous micellar two-phase systems. <i>Chemical Engineering Journal</i> , 2013, 218, 204-213.	6.6	27
511	Water Network Perturbation in Ligand Binding: Adenosine A_{2A} Antagonists as a Case Study. <i>Journal of Chemical Information and Modeling</i> , 2013, 53, 1700-1713.	2.5	114
512	Water Bending Mode at the Water-Vapor Interface Probed by Sum-Frequency Generation Spectroscopy: A Combined Molecular Dynamics Simulation and Experimental Study. <i>Journal of Physical Chemistry Letters</i> , 2013, 4, 1872-1877.	2.1	100
513	Water's Structure around Hydrophobic Solutes and the Iceberg Model. <i>Journal of Physical Chemistry B</i> , 2013, 117, 2153-2159.	1.2	193
514	Quantum Behavior of Water Molecules Confined to Nanocavities in Gemstones. <i>Journal of Physical Chemistry Letters</i> , 2013, 4, 2015-2020.	2.1	54
515	Patchy Supramolecules as Versatile Tools To Probe Hydrophobicity in Nanoglobular Systems. <i>Journal of the American Chemical Society</i> , 2013, 135, 3815-3817.	6.6	15
516	Towards the understanding at the molecular level of the structured-water absorption and fluorescence spectra: a fingerprint of β -stacked water. <i>Molecular Physics</i> , 2013, 111, 1308-1315.	0.8	10
517	Robustness of Frequency, Transition Dipole, and Coupling Maps for Water Vibrational Spectroscopy. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 3109-3117.	2.3	86
518	Microscopic structure of water in a water/oil emulsion. <i>Journal of Chemical Physics</i> , 2013, 138, 204503.	1.2	10
519	Effect of Ion Pairing on the Solution Dynamics Investigated by the Simulations of the Optical Kerr Effect and the Dielectric Relaxation Spectra. <i>Journal of Physical Chemistry B</i> , 2013, 117, 15395-15406.	1.2	15
520	Probabilistic Approach to the Length-Scale Dependence of the Effect of Water Hydrogen Bonding on Hydrophobic Hydration. <i>Journal of Physical Chemistry B</i> , 2013, 117, 7015-7025.	1.2	13
521	Solvation Free Energies of Alanine Peptides: The Effect of Flexibility. <i>Journal of Physical Chemistry B</i> , 2013, 117, 16428-16435.	1.2	27
522	Water-Compatible Hydrogen-Bond Activation: A Scalable and Organocatalytic Model for the Stereoselective Multicomponent Aza-Henry Reaction. <i>Chemistry - A European Journal</i> , 2013, 19, 16550-16554.	1.7	42

#	ARTICLE	IF	CITATIONS
523	SPAM: A Simple Approach for Profiling Bound Water Molecules. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 5539-5549.	2.3	40
524	Tetraedrisch, wenn fl¼ssig. <i>Nachrichten Aus Der Chemie</i> , 2013, 61, 1203-1206.	0.0	2
525	Beyond the Continuum: How Molecular Solvent Structure Affects Electrostatics and Hydrodynamics at Solidâ€“Electrolyte Interfaces. <i>Journal of Physical Chemistry B</i> , 2013, 117, 11397-11413.	1.2	110
526	On the binding affinity of macromolecular interactions: daring to ask why proteins interact. <i>Journal of the Royal Society Interface</i> , 2013, 10, 20120835.	1.5	353
527	Excited-State Dynamics of Charged Dyes at Alkane/Water Interfaces in the Presence of Salts and Ionic Surfactants. <i>Langmuir</i> , 2013, 29, 14865-14872.	1.6	12
528	Water's non-tetrahedral side. <i>Faraday Discussions</i> , 2013, 167, 529.	1.6	40
529	Strong Intermolecular Vibrational Coupling through Cyclic Hydrogen-Bonded Structures Revealed by Ultrafast Continuum Mid-IR Spectroscopy. <i>Journal of Physical Chemistry B</i> , 2013, 117, 15714-15719.	1.2	83
530	The Hydrogen Bond of Water from the Perspective of Soft Xâ€“Ray Spectroscopy. <i>Chemistry - an Asian Journal</i> , 2013, 8, 318-327.	1.7	11
531	Functional supramolecular nanomaterials: robust yet adaptive. <i>Proceedings of SPIE</i> , 2013, , .	0.8	0
532	Vibrational dynamics of a non-degenerate ultrafast rotor: The (C12,C13)-oxalate ion. <i>Journal of Chemical Physics</i> , 2013, 139, 164514.	1.2	12
533	Temperature effect on the small-to-large crossover lengthscale of hydrophobic hydration. <i>Journal of Chemical Physics</i> , 2013, 139, 184709.	1.2	7
534	Cause of the fragile-to-strong transition observed in water confined in C-S-H gel. <i>Journal of Chemical Physics</i> , 2013, 139, 164714.	1.2	23
535	Micro and Extended-Nano Fluidics and Optics for Chemical and Bioanalytical Technology. <i>Nano-optics and Nanophotonics</i> , 2013, , 121-164.	0.2	3
536	Vibrational spectroscopy of water in hydrated lipid multi-bilayers. III. Water clustering and vibrational energy transfer. <i>Journal of Chemical Physics</i> , 2013, 139, 175103.	1.2	12
537	Molecular component distribution imaging of living cells by multivariate curve resolution analysis of space-resolved Raman spectra. <i>Journal of Biomedical Optics</i> , 2013, 19, 011016.	1.4	55
538	Polyethylene glycol binding alters human telomere G-quadruplex structure by conformational selection. <i>Nucleic Acids Research</i> , 2013, 41, 7934-7946.	6.5	122
539	Dâ€™Arcy Thompsonâ€™s Legacy in Contemporary Studies of Patterns and Morphology. <i>Interdisciplinary Science Reviews</i> , 2013, 38, 12-34.	1.0	2
540	Linear relationship between water wetting behavior and microscopic interactions of super-hydrophilic surfaces. <i>Journal of Chemical Physics</i> , 2013, 139, 234703.	1.2	12

#	ARTICLE	IF	CITATIONS
541	Interaction between heterogeneously charged surfaces: Surface patches and charge modulation. <i>Physical Review E</i> , 2013, 87, 022402.	0.8	44
542	Theoretical Study on Hydrogen Bonding of Mono- and Dihydrated Complexes of 7-(3-Pyridyl)indole in Excited States. <i>Journal of the Chinese Chemical Society</i> , 2013, 60, 618-624.	0.8	3
543	Thermodynamic and structural signatures of water-driven methane-methane attraction in coarse-grained mW water. <i>Journal of Chemical Physics</i> , 2013, 139, 054511.	1.2	52
544	Direct observation of self-assembled chain-like water structures in a nanoscopic water meniscus. <i>Journal of Chemical Physics</i> , 2013, 139, 054701.	1.2	14
545	Power-law trapping of water molecules on the lipid-membrane surface induces water retardation. <i>Physical Review E</i> , 2013, 87, 052715.	0.8	23
546	Linking hydrophobicity and hydrodynamics by the hybrid fluctuating hydrodynamics and molecular dynamics methodologies. <i>Physical Review E</i> , 2013, 88, 023305.	0.8	4
547	Probing water micro-solvation in proteins by water catalysed proton-transfer tautomerism. <i>Nature Communications</i> , 2013, 4, 2611.	5.8	63
551	Separation, Immobilization, and Biocatalytic Utilization of Proteins by a Supramolecular Membrane. <i>PLoS ONE</i> , 2013, 8, e63188.	1.1	19
552	Stabilization and Anomalous Hydration of Collagen Fibril under Heating. <i>PLoS ONE</i> , 2013, 8, e78526.	1.1	25
553	Small Molecules and Peptides Inside Carbon Nanotubes: Impact of Nanoscale Confinement. , 0, , .		2
554	Identification of Free OH and its Implication on Structural Changes of Liquid Water. <i>Chinese Journal of Chemical Physics</i> , 2013, 26, 121-127.	0.6	20
555	Hydrophobic hydration of globular proteins studied with 2D-IR spectroscopy. <i>EPJ Web of Conferences</i> , 2013, 41, 06008.	0.1	0
556	Aluminum-Induced Entropy in Biological Systems: Implications for Neurological Disease. <i>Journal of Toxicology</i> , 2014, 2014, 1-27.	1.4	37
557	Quantum behaviour of water molecule in gemstone: terahertz fingerprints. <i>Journal of Physics: Conference Series</i> , 2014, 486, 012019.	0.3	3
558	Structure of complexes of poly- β -benzyl-L-glutamate with water and dioxane molecules studied by IR spectroscopy and quantum chemical calculations. <i>Journal of Structural Chemistry</i> , 2014, 55, 1565-1573.	0.3	0
559	Local water diffusivity as a molecular probe of surface hydrophilicity. <i>MRS Bulletin</i> , 2014, 39, 1082-1088.	1.7	12
560	Hydration and hydrogen bond network of water around hydrophobic surface investigated by terahertz spectroscopy. <i>Journal of Chemical Physics</i> , 2014, 141, 235103.	1.2	33
561	Simulating ion clustering in potassium thiocyanate aqueous solutions with various ion-water models. <i>Science China Chemistry</i> , 2014, 57, 1723-1730.	4.2	2

#	ARTICLE	IF	CITATIONS
562	Comparative study of hydration shell dynamics around a hyperactive antifreeze protein and around ubiquitin. <i>Journal of Chemical Physics</i> , 2014, 141, 22D529.	1.2	50
563	Hydration free energies calculated using the AMBER ff03 charge model for natural and unnatural amino acids and multiple water models. <i>Computers and Chemical Engineering</i> , 2014, 71, 745-752.	2.0	8
564	Interactions between Charged Lamellae in Aqueous Solution. <i>Physical Review Letters</i> , 2014, 113, 268302.	2.9	10
565	Sum frequency spectroscopy of the hydrophobic nanodroplet/water interface: Absence of hydroxyl ion and dangling OH bond signatures. <i>Chemical Physics Letters</i> , 2014, 615, 124-131.	1.2	49
566	Electron Transfers and Holographic Molecules: Why Neuroscientists Should Take Quantum Phenomena into Consideration. <i>NeuroQuantology</i> , 2014, 12, .	0.1	1
567	Possible Further Evidence for the Thixotropic Phenomenon of Water. <i>Entropy</i> , 2014, 16, 2146-2160.	1.1	7
568	Can the Hexagonal Ice-like Model Render the Spectroscopic Fingerprints of Structured Water? Feedback from Quantum-Chemical Computations. <i>Entropy</i> , 2014, 16, 4101-4120.	1.1	12
569	Study of solvation dynamics in the interior of staphylococcal nuclease (SNase) using picosecond-resolved emission spectra of tryptophan. , 2014, , .		0
570	Multibody correlations in the hydrophobic solvation of glycine peptides. <i>Journal of Chemical Physics</i> , 2014, 141, 22D525.	1.2	14
571	Observation of ice-like water layers at an aqueous protein surface. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2014, 111, 17732-17736.	3.3	144
572	Changes in the hydrogen-bonding strength of internal water molecules and cysteine residues in the conductive state of channelrhodopsin-1. <i>Journal of Chemical Physics</i> , 2014, 141, 22D507.	1.2	39
573	Hydration shell effects in the relaxation dynamics of photoexcited Fe-II complexes in water. <i>Journal of Chemical Physics</i> , 2014, 141, 044304.	1.2	9
574	Collective vibrations of water-solvated hydroxide ions investigated with broadband 2DIR spectroscopy. <i>Journal of Chemical Physics</i> , 2014, 140, 204508.	1.2	53
575	Microhydrated aromatic cluster cations: Binding motifs of 4-aminobenzonitrile-(H ₂ O) _n cluster cations with n ≈ 4. <i>Journal of Chemical Physics</i> , 2014, 141, 214301.	1.2	29
576	Hydration shells of proteins probed by depolarized light scattering and dielectric spectroscopy: Orientational structure is significant, positional structure is not. <i>Journal of Chemical Physics</i> , 2014, 141, 22D501.	1.2	26
577	In silico studies of the properties of water hydrating a small protein. <i>Journal of Chemical Physics</i> , 2014, 141, 22D502.	1.2	20
578	An "Ingredients" Approach to Functional Self-Synthesizing Materials: A Metal-Ion-Selective, Multi-Responsive, Self-Assembled Hydrogel. <i>Chemistry - A European Journal</i> , 2014, 20, 15709-15714.	1.7	42
579	Temperature dependence of local solubility of hydrophobic molecules in the liquid-vapor interface of water. <i>Journal of Chemical Physics</i> , 2014, 141, 18C516.	1.2	9

#	ARTICLE	IF	CITATIONS
580	Influence of electric fields on the structure and structure transition of water confined in a carbon nanotube. <i>Journal of Chemical Physics</i> , 2014, 140, 154508.	1.2	26
581	<i>Ab initio</i> calculation of the electronic absorption spectrum of liquid water. <i>Journal of Chemical Physics</i> , 2014, 140, 164511.	1.2	8
583	CHAPTER 21. Partial Molar Volumes of Proteins in Solution. , 2014, , 542-574.		1
584	CHAPTER 1. Volumetric Properties: Introduction, Concepts and Selected Applications. , 2014, , 1-72.		2
585	Water Repellency in Hydrophobic Nanocapsules – Molecular View on Dewetting. <i>Chemistry - A European Journal</i> , 2014, 20, 6659-6664.	1.7	12
586	The role of material flexibility on the drying transition of water between hydrophobic objects: A thermodynamic analysis. <i>Journal of Chemical Physics</i> , 2014, 141, 18C531.	1.2	25
587	Sum frequency and second harmonic generation from the surface of a liquid microjet. <i>Journal of Chemical Physics</i> , 2014, 141, 18C524.	1.2	7
588	Solvation dynamics monitored by combined X-ray spectroscopies and scattering: photoinduced spin transition in aqueous [Fe(bpy) ₃] ²⁺ . <i>Faraday Discussions</i> , 2014, 171, 169-178.	1.6	17
589	Discrete Cuboidal 15- and 16-Membered Water Clusters in Brucine 3.86-Hydrate, Water Release and Its Consequences. <i>Crystal Growth and Design</i> , 2014, 14, 6537-6541.	1.4	4
590	Ab Initio Molecular Dynamics Study of the Mechanism of Proton Recombination with a Weak Base. <i>Journal of Physical Chemistry B</i> , 2014, 118, 13903-13912.	1.2	16
591	An artificial primitive mimic of the Gramicidin-A channel. <i>Nature Communications</i> , 2014, 5, 4142.	5.8	85
593	Structure and dynamics of water in crowded environments slows down peptide conformational changes. <i>Journal of Chemical Physics</i> , 2014, 141, 045101.	1.2	15
594	Water in the presence of inert Lennard-Jones obstacles. <i>Molecular Physics</i> , 2014, 112, 1132-1148.	0.8	8
595	Viscosity measurements of DNA solutions with and without condensing agents. <i>Biorheology</i> , 2014, 51, 15-28.	1.2	12
596	Infrared spectral marker bands characterizing a transient water wire inside a hydrophobic membrane protein. <i>Journal of Chemical Physics</i> , 2014, 141, 22D524.	1.2	40
597	Comparative assessment of the ELBA coarse-grained model for water. <i>Molecular Physics</i> , 2014, 112, 1566-1576.	0.8	82
598	Distribution of internal parameters of the hydration shell structure of proteins. <i>Biophysics (Russian)</i> Tj ETQq0 0 0 rgBT /Overlock 10 Tf 5 0.2 6		
599	Progressive compression of 1,1%-diammonium-alkanes inside a rigid crystalline molecular cage. <i>Chemical Communications</i> , 2014, 50, 14086-14088.	2.2	19

#	ARTICLE	IF	CITATIONS
600	The solvation and ion condensation properties for sulfonated polyelectrolytes in different solvents—a computational study. <i>New Journal of Physics</i> , 2014, 16, 025001.	1.2	40
601	Water science on the molecular scale: new insights into the characteristics of water. <i>National Science Review</i> , 2014, 1, 179-181.	4.6	6
602	Wavefunction methods for the accurate characterization of water clusters. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2014, 4, 199-224.	6.2	43
603	The alteration of lipid bilayer dynamics by phloretin and 6-ketocholestanol. <i>Chemistry and Physics of Lipids</i> , 2014, 178, 38-44.	1.5	8
604	Modulation of hydrogen bonding upon ion binding: Insights into cooperativity. <i>International Journal of Quantum Chemistry</i> , 2014, 114, 145-153.	1.0	11
605	Is it the shape of the cavity, or the shape of the water in the cavity?. <i>European Physical Journal: Special Topics</i> , 2014, 223, 853-891.	1.2	116
606	Enhanced ordering of water at hydrophobic surfaces. <i>Journal of Chemical Physics</i> , 2014, 140, 054711.	1.2	121
607	Crowding Induced Collective Hydration of Biological Macromolecules over Extended Distances. <i>Journal of the American Chemical Society</i> , 2014, 136, 188-194.	6.6	122
608	High performance integrated terahertz sensor for detection of biomolecular processes in solution. <i>IEEE Microwaves, Antennas and Propagation</i> , 2014, 8, 394-400.	0.7	13
609	Study on the transport of water molecules under the geometry confinement of aquaporin-like nanopores. <i>Applied Thermal Engineering</i> , 2014, 72, 120-125.	3.0	19
610	Chemical Thermodynamics: A Journey of Many Vistas. <i>Journal of Solution Chemistry</i> , 2014, 43, 525-576.	0.6	14
611	Improved protein–ligand binding affinity prediction by using a curvature-dependent surface-area model. <i>Bioinformatics</i> , 2014, 30, 1674-1680.	1.8	126
612	Entropy is Key to the Formation of Pentacyclic Terpenoids by Enzyme-Catalyzed Polycyclization. <i>Angewandte Chemie - International Edition</i> , 2014, 53, 4845-4849.	7.2	25
613	Capsules with Highly Active Pores and Interiors: Versatile Platforms at the Nanoscale. <i>Chemistry - A European Journal</i> , 2014, 20, 4862-4873.	1.7	48
614	Interaction with the Surrounding Water Plays a Key Role in Determining the Aggregation Propensity of Proteins. <i>Angewandte Chemie - International Edition</i> , 2014, 53, 3961-3964.	7.2	87
615	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.	1.6	121
616	The Armstrong experiment revisited. <i>European Physical Journal: Special Topics</i> , 2014, 223, 959-977.	1.2	14
617	Pressure-induced amorphization and polyamorphism: Inorganic and biochemical systems. <i>Progress in Materials Science</i> , 2014, 61, 216-282.	16.0	124

#	ARTICLE	IF	CITATIONS
618	Confinement of Water in Hydrophobic Nanopores: Effect of the Geometry on the Energy of Intrusion. <i>Langmuir</i> , 2014, 30, 213-219.	1.6	21
619	Noncanonical Structures and Their Thermodynamics of DNA and RNA Under Molecular Crowding. <i>International Review of Cell and Molecular Biology</i> , 2014, 307, 205-273.	1.6	30
620	Computational Methods in Drug Discovery. <i>Pharmacological Reviews</i> , 2014, 66, 334-395.	7.1	1,370
621	Osmolyte Effects: Impact on the Aqueous Solution around Charged and Neutral Spheres. <i>Journal of Physical Chemistry B</i> , 2014, 118, 771-782.	1.2	65
622	Depolarized light scattering and dielectric response of a peptide dissolved in water. <i>Journal of Chemical Physics</i> , 2014, 140, 035101.	1.2	10
623	The viscosity B and D coefficient (Jones's Dole equation) studies in aqueous solutions of alkyltrimethylammonium bromides at 298.15K. <i>Journal of Molecular Liquids</i> , 2014, 200, 416-424.	2.3	25
624	An introduction to biomolecular simulations and docking. <i>Molecular Simulation</i> , 2014, 40, 732-764.	0.9	33
625	Possible causes of apoptotic volume decrease: an attempt at quantitative review. <i>American Journal of Physiology - Cell Physiology</i> , 2014, 306, C417-C424.	2.1	36
626	Structure and dynamics of TIP3P, TIP4P, and TIP5P water near smooth and atomistic walls of different hydroaffinity. <i>Journal of Chemical Physics</i> , 2014, 140, 174501.	1.2	193
627	Neutron Diffraction of Ice in Hydrogels. <i>Journal of Physical Chemistry B</i> , 2014, 118, 13453-13457.	1.2	3
628	Are hot-spots occluded from water?. <i>Journal of Biomolecular Structure and Dynamics</i> , 2014, 32, 186-197.	2.0	11
629	Non-linear infrared spectroscopy of the water bending mode: direct experimental evidence of hydration shell reorganization?. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 13172-13181.	1.3	42
630	Anomalous water diffusion in salt solutions. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2014, 111, 3310-3315.	3.3	124
631	Insights into water coordination associated with the Cu ^{II} /Cu ^I electron transfer at a biomimetic Cu centre. <i>Dalton Transactions</i> , 2014, 43, 6436-6445.	1.6	16
632	Dependence of structure of polymer side chain on water structure in hydrogels. <i>Polymer</i> , 2014, 55, 6320-6324.	1.8	27
633	Water-mediated inclusion of benzoates and tosylates inside the bambusuril macrocycle. <i>Chemical Communications</i> , 2014, 50, 1372-1374.	2.2	36
634	Ergodic-to-nonergodic phase inversion and reentrant ergodicity transition in DNA's nanoclay dispersions. <i>Soft Matter</i> , 2014, 10, 149-156.	1.2	7
635	Mechanistic understanding of domino cyclization between gem-dialkylthio vinylallenes and benzylamine towards economic synthesis: a computational study. <i>Green Chemistry</i> , 2014, 16, 2653.	4.6	27

#	ARTICLE	IF	CITATIONS
636	Co-nonsolvency of PNIPAM at the transition between solvation mechanisms. <i>Soft Matter</i> , 2014, 10, 8288-8295.	1.2	77
637	Electricity Resonance-Induced Fast Transport of Water through Nanochannels. <i>Nano Letters</i> , 2014, 14, 4931-4936.	4.5	78
638	Terahertz Dynamics in Human Cells and Their Chromatin. <i>Journal of Physical Chemistry Letters</i> , 2014, 5, 2177-2181.	2.1	4
639	Comparison of the Influence of Humidity and D-Mannitol on the Organization of Tetraethylene Glycol-Terminated Self-Assembled Monolayers and Immobilized Antimicrobial Peptides. <i>Langmuir</i> , 2014, 30, 7143-7151.	1.6	5
640	Energetics of Hydrophilic Protein-Protein Association and the Role of Water. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 3512-3524.	2.3	27
641	Molecular Simulation of Water and Hydration Effects in Different Environments: Challenges and Developments for DFTB Based Models. <i>Journal of Physical Chemistry B</i> , 2014, 118, 11007-11027.	1.2	97
642	Incorporation of the TIP4P water model into a continuum solvent for computing solvation free energy. <i>Chemical Physics</i> , 2014, 443, 93-106.	0.9	7
643	Molecular Structures of Water and Its Features. , 2014, , 1-88.		0
644	Mechanism of Stapled Peptide Binding to MDM2: Possible Consequences for Peptide Design. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 1753-1761.	2.3	15
645	Ultraslow Dynamics of Water in Organic Molecular Solids. <i>Journal of Physical Chemistry C</i> , 2014, 118, 4941-4950.	1.5	19
646	Survival kit of <i>Saccharomyces cerevisiae</i> for anhydrobiosis. <i>Applied Microbiology and Biotechnology</i> , 2014, 98, 8821-8834.	1.7	78
647	Ion-Specific Long-Range Correlations on Interfacial Water Driven by Hydrogen Bond Fluctuations. <i>Journal of Physical Chemistry B</i> , 2014, 118, 1861-1866.	1.2	10
648	Solvation Dynamics and Intermittent Oscillation of Cell Membrane: Live Chinese Hamster Ovary Cell. <i>Journal of Physical Chemistry B</i> , 2014, 118, 2949-2956.	1.2	22
649	Protein Folding Thermodynamics: A New Computational Approach. <i>Journal of Physical Chemistry B</i> , 2014, 118, 5017-5025.	1.2	18
650	The protein irreversible denaturation studied by means of the bending vibrational mode. <i>Physica A: Statistical Mechanics and Its Applications</i> , 2014, 412, 39-44.	1.2	10
651	A Delocalized Proton-Binding Site within a Membrane Protein. <i>Biophysical Journal</i> , 2014, 107, 174-184.	0.2	25
652	Direct observation of intermolecular interactions mediated by hydrogen bonding. <i>Journal of Chemical Physics</i> , 2014, 141, 034502.	1.2	50
653	Observing the Hydration Layer of Trehalose with a Linked Molecular Terahertz Probe. <i>Journal of Physical Chemistry Letters</i> , 2014, 5, 1845-1849.	2.1	35

#	ARTICLE	IF	CITATIONS
654	Computational Modeling of Lauric Acid at the Organic–Water Interface. <i>Journal of Physical Chemistry C</i> , 2014, 118, 10024-10032.	1.5	11
655	New Insights into the Role of Water in Biological Function: Studying Solvated Biomolecules Using Terahertz Absorption Spectroscopy in Conjunction with Molecular Dynamics Simulations. <i>Journal of the American Chemical Society</i> , 2014, 136, 12800-12807.	6.6	240
656	Formation of T4(1) water tapes interconnected via centrosymmetric nickel(II) Schiff base complex to produce a 3D architecture. <i>Inorganic Chemistry Communication</i> , 2014, 48, 12-17.	1.8	15
657	Excited-State Dynamics of an Environment-Sensitive Push–Pull Diketopyrrolopyrrole: Major Differences between the Bulk Solution Phase and the Dodecane/Water Interface. <i>Journal of Physical Chemistry B</i> , 2014, 118, 9952-9963.	1.2	37
658	Reversible State Transition in Nanoconfined Aqueous Solutions. <i>Physical Review Letters</i> , 2014, 112, 078301.	2.9	23
660	Effects of geometry and chemistry on hydrophobic solvation. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2014, 111, 14681-14686.	3.3	62
661	Distribution of Topologically Distinct Isomers of Water Clusters and Dipole Moments of Constituent Water Molecules at Finite Atmospheric Temperatures. <i>Journal of Physical Chemistry A</i> , 2014, 118, 7911-7924.	1.1	12
662	Anion Complexation and The Hofmeister Effect. <i>Angewandte Chemie - International Edition</i> , 2014, 53, 11498-11500.	7.2	92
663	Are Waters around RNA More than Just a Solvent? – An Insight from Molecular Dynamics Simulations. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 401-411.	2.3	33
665	Implementing electrostatic polarization cannot fill the gap between experimental and theoretical measurements for the ultrafast fluorescence decay of myoglobin. <i>Journal of Molecular Modeling</i> , 2014, 20, 2189.	0.8	2
666	Characterization of Dielectric Responses of Human Cancer Cells in the Terahertz Region. <i>Journal of Infrared, Millimeter, and Terahertz Waves</i> , 2014, 35, 493-502.	1.2	93
667	Temperature Dependence of Hydrophobic Hydration Dynamics: From Retardation to Acceleration. <i>Journal of Physical Chemistry B</i> , 2014, 118, 1574-1583.	1.2	34
668	Water Dynamics in Protein Hydration Shells: The Molecular Origins of the Dynamical Perturbation. <i>Journal of Physical Chemistry B</i> , 2014, 118, 7715-7729.	1.2	207
669	Pressure-Dependent Properties of Elementary Hydrophobic Interactions: Ramifications for Activation Properties of Protein Folding. <i>Journal of Physical Chemistry B</i> , 2014, 118, 7488-7509.	1.2	49
670	On the Hofmeister Effect: Fluctuations at the Protein–Water Interface and the Surface Tension. <i>Journal of Physical Chemistry B</i> , 2014, 118, 8496-8504.	1.2	22
671	Effect of the Hydrophobic Alcohol Chain Length on the Hydrogen-Bond Network of Water. <i>Journal of Physical Chemistry B</i> , 2014, 118, 8750-8755.	1.2	38
672	Rapid evaluation of the interaction energies for O–H⋯O hydrogen-bonded complexes. <i>Theoretical Chemistry Accounts</i> , 2014, 133, 1.	0.5	9
673	Liquid-liquid phase transition in water. <i>Science China: Physics, Mechanics and Astronomy</i> , 2014, 57, 810-818.	2.0	14

#	ARTICLE	IF	CITATIONS
674	Investigation of conformational mobility of insulin superfamily peptides: Use of SPC/E and TIP4P water models. <i>Molecular Biology</i> , 2014, 48, 432-438.	0.4	1
675	Molecular dynamics study of mixed alkanethiols covering a gold surface at three different arrangements. <i>Chemical Physics Letters</i> , 2014, 600, 79-86.	1.2	13
676	On the Coupling between the Collective Dynamics of Proteins and Their Hydration Water. <i>Journal of Physical Chemistry Letters</i> , 2014, 5, 1181-1186.	2.1	59
677	Exploiting Hydrophobic Interactions at the Nanoscale. <i>Journal of Physical Chemistry Letters</i> , 2014, 5, 2455-2463.	2.1	26
678	Understanding THz Spectra of Aqueous Solutions: Glycine in Light and Heavy Water. <i>Journal of the American Chemical Society</i> , 2014, 136, 5031-5038.	6.6	88
679	Perturbation of Fluid Dynamics Properties of Water Molecules during G Protein-Coupled Receptor-Ligand Recognition: The Human A _{2A} Adenosine Receptor as a Key Study. <i>Journal of Chemical Information and Modeling</i> , 2014, 54, 2846-2855.	2.5	24
680	Wettability of Azobenzene Self-Assembled Monolayers. <i>Langmuir</i> , 2014, 30, 4415-4421.	1.6	5
681	Heterogeneous Preferential Solvation of Water and Trifluoroethanol in Homologous Lysozymes. <i>Journal of Physical Chemistry B</i> , 2014, 118, 8118-8127.	1.2	14
682	Hydration and rotational diffusion of levoglucosan in aqueous solutions. <i>Journal of Chemical Physics</i> , 2014, 140, 184505.	1.2	10
683	Direct Mixing of Atomistic Solutes and Coarse-Grained Water. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 4684-4693.	2.3	43
684	Fabrication of Multiresponsive Bioactive Nanocapsules through Orthogonal Self-Assembly. <i>Angewandte Chemie - International Edition</i> , 2014, 53, n/a-n/a.	7.2	22
685	Reply to "Comment on "Water's Structure around Hydrophobic Solutes and the Iceberg Model". <i>Journal of Physical Chemistry B</i> , 2014, 118, 2600-2603.	1.2	16
686	Water Tetrahedrons, Hydrogen-Bond Dynamics, and the Orientational Mobility of Water around Hydrophobic Solutes. <i>Journal of Physical Chemistry B</i> , 2014, 118, 4169-4176.	1.2	65
687	On the hexagonal ice-like model of structured water: Theoretical analysis of the low-lying excited states. <i>Computational and Theoretical Chemistry</i> , 2014, 1040-1041, 266-273.	1.1	3
688	Water adsorption on etched hydrophobic surfaces of L-, D- and DL-valine crystals. <i>Surface Science</i> , 2014, 621, 191-196.	0.8	1
689	Multiphysics pore-scale model for the rehydration of porous foods. <i>Innovative Food Science and Emerging Technologies</i> , 2014, 24, 69-79.	2.7	20
690	Water-Peptide Site-Specific Interactions: A Structural Study on the Hydration of Glutathione. <i>Biophysical Journal</i> , 2014, 106, 1701-1709.	0.2	40
691	Unifying Family A GPCR Theories of Activation. , 2014, 143, 51-60.		169

#	ARTICLE	IF	CITATIONS
692	A Simple Atomic-Level Hydrophobicity Scale Reveals Protein Interfacial Structure. <i>Journal of Molecular Biology</i> , 2014, 426, 484-498.	2.0	107
693	Encapsulated Water Inside Mo ₁₃₂ Capsules: The Role of Long-Range Correlations of about 1 nm. <i>Journal of Physical Chemistry C</i> , 2014, 118, 5545-5555.	1.5	11
694	Reorientational Dynamics of Water Confined in Zeolites. <i>ChemPhysChem</i> , 2014, 15, 521-529.	1.0	42
695	Phase Diagram of Aging Laponite Dispersions. <i>Springer Theses</i> , 2014, , 37-51.	0.0	0
697	Understanding the Effect of Fluorocarbons in Aqueous Supramolecular Polymerization: Ultrastrong Noncovalent Binding and Cooperativity. <i>Journal of the American Chemical Society</i> , 2014, 136, 9443-9452.	6.6	67
698	High productivity purification of immunoglobulin G monoclonal antibodies on starch-coated magnetic nanoparticles by steric exclusion of polyethylene glycol. <i>Journal of Chromatography A</i> , 2014, 1324, 171-180.	1.8	39
700	Nonfreezing Water Structuration in Heteroprotein Coacervates. <i>Langmuir</i> , 2015, 31, 8661-8666.	1.6	18
701	Structure and Dynamics of Water and Nonaqueous Solvents Confined in Extended Nanospaces Characterized by NMR Spectroscopy. <i>Bunseki Kagaku</i> , 2015, 64, 261-271.	0.1	2
702	Quantifying Density Fluctuations in Water at a Hydrophobic Surface: Evidence for Critical Drying. <i>Physical Review Letters</i> , 2015, 115, 016103.	2.9	49
703	Bulk and interfacial liquid water as a transient network. <i>Physical Review E</i> , 2015, 92, 052130.	0.8	9
704	Water-COOH Composite Structure with Enhanced Hydrophobicity Formed by Water Molecules Embedded into Carboxyl-Terminated Self-Assembled Monolayers. <i>Physical Review Letters</i> , 2015, 115, 186101.	2.9	40
705	Oxidative footprinting in the study of structure and function of membrane proteins: current state and perspectives. <i>Biochemical Society Transactions</i> , 2015, 43, 983-994.	1.6	15
706	Molecular hydrogen solvated in water – A computational study. <i>Journal of Chemical Physics</i> , 2015, 143, 244505.	1.2	7
707	Microscopic origin of temporal heterogeneities in translational dynamics of liquid water. <i>Journal of Chemical Physics</i> , 2015, 143, 054503.	1.2	17
708	Multi-reference approach to the calculation of photoelectron spectra including spin-orbit coupling. <i>Journal of Chemical Physics</i> , 2015, 143, 074104.	1.2	48
709	Dehydration-mediated cluster formation of nanoparticles. <i>Scientific Reports</i> , 2015, 5, 11383.	1.6	3
710	Vibrational dynamics of aqueous hydroxide solutions probed using broadband 2DIR spectroscopy. <i>Journal of Chemical Physics</i> , 2015, 143, 194501.	1.2	26
711	Dynamical changes in hydration water accompanying lysozyme thermal denaturation. <i>Frontiers of Physics</i> , 2015, 10, 1.	2.4	9

#	ARTICLE	IF	CITATIONS
712	A novel hypothesis for atherosclerosis as a cholesterol sulfate deficiency syndrome. <i>Theoretical Biology and Medical Modelling</i> , 2015, 12, 9.	2.1	23
714	Direct Observation of Kinetic Pathways of Biomolecular Recognition. <i>Chemistry - A European Journal</i> , 2015, 21, 16172-16177.	1.7	10
715	On the Origin of Water Flow through Carbon Nanotubes. <i>ChemPhysChem</i> , 2015, 16, 3488-3492.	1.0	13
716	Water response to intense electric fields: A molecular dynamics study. <i>Bioelectromagnetics</i> , 2015, 36, 377-385.	0.9	29
717	A π -Shaped Polyaromatic Amphiphile: Solubilization of Various Nanocarbons in Water and Enhanced Photostability. <i>Chemistry - A European Journal</i> , 2015, 21, 12741-12746.	1.7	39
718	Bright molecules for sensing, computing and imaging: a tale of two once-troubled cities. <i>Beilstein Journal of Organic Chemistry</i> , 2015, 11, 2774-2784.	1.3	8
719	The role of water, ice nucleators, and inoculation in insect cold survival. <i>Open Access Insect Physiology</i> , 0, , 21.	0.8	6
720	Structural and Computational Biology in the Design of Immunogenic Vaccine Antigens. <i>Journal of Immunology Research</i> , 2015, 2015, 1-17.	0.9	66
721	Dynamics of water, methanol, and ethanol in a room temperature ionic liquid. <i>Journal of Chemical Physics</i> , 2015, 142, 212408.	1.2	75
722	Structure and dynamics of POPC bilayers in water solutions of room temperature ionic liquids. <i>Journal of Chemical Physics</i> , 2015, 142, 124706.	1.2	59
723	Hydration water mobility is enhanced around tau amyloid fibers. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2015, 112, 6365-6370.	3.3	79
724	Structure and Nanostructure in Ionic Liquids. <i>Chemical Reviews</i> , 2015, 115, 6357-6426.	23.0	1,793
725	Distribution of Residence Time of Water around DNA Base Pairs: Governing Factors and the Origin of Heterogeneity. <i>Journal of Physical Chemistry B</i> , 2015, 119, 11371-11381.	1.2	36
726	Translational diffusion of hydration water correlates with functional motions in folded and intrinsically disordered proteins. <i>Nature Communications</i> , 2015, 6, 6490.	5.8	199
727	Interactions by the Fungal Flo11 Adhesin Depend on a Fibronectin Type III-like Adhesin Domain Girdled by Aromatic Bands. <i>Structure</i> , 2015, 23, 1005-1017.	1.6	51
728	Pore Hydration States of KcsA Potassium Channels in Membranes. <i>Journal of Biological Chemistry</i> , 2015, 290, 26765-26775.	1.6	11
729	Room temperature freezing and orientational control of surface-immobilized peptides in air. <i>Chemical Communications</i> , 2015, 51, 11015-11018.	2.2	12
730	Self-organization and properties of dilute aqueous solutions of cetyltrimethylammonium bromide in a range of physiologically important temperatures. <i>Russian Chemical Bulletin</i> , 2015, 64, 579-589.	0.4	11

#	ARTICLE	IF	CITATIONS
731	Mixtures of Isobutyric Acid and Water Confined in Cylindrical Silica Nanopores Revisited: A Combined Solid-State NMR and Molecular Dynamics Simulation Study. <i>Journal of Physical Chemistry C</i> , 2015, 119, 28961-28969.	1.5	20
732	Protein electron transfer: is biology (thermo)dynamic?. <i>Journal of Physics Condensed Matter</i> , 2015, 27, 473001.	0.7	49
733	Replacement of Water Molecules in a Phosphate Binding Site by Furanoside-Appended Benzoguanine Ligands of tRNA-Guanine Transglycosylase (TGT). <i>Chemistry - A European Journal</i> , 2015, 21, 126-135.	1.7	8
734	Probing Water Environment of Trp59 in Ribonuclease T1: Insight of the Structure-Water Network Relationship. <i>Journal of Physical Chemistry B</i> , 2015, 119, 2157-2167.	1.2	19
735	Determination of Conformational Entropy of Fully and Partially Folded Conformations of Holo- and Apomyoglobin. <i>Journal of Physical Chemistry B</i> , 2015, 119, 72-82.	1.2	25
736	Electricity from the Silk Cocoon Membrane. <i>Scientific Reports</i> , 2014, 4, 5434.	1.6	63
737	Solvent effects of 1-ethyl-3-methylimidazolium acetate: solvation and dynamic behavior of polar and apolar solutes. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 8480-8490.	1.3	40
738	Effect of the hydroaffinity and topology of pore walls on the structure and dynamics of confined water. <i>Journal of Chemical Physics</i> , 2015, 142, 034703.	1.2	28
739	Solubilities, Fugacities and All That in Solution Chemistry. <i>Journal of Solution Chemistry</i> , 2015, 44, 1004-1061.	0.6	23
740	The role of water in protein's behavior: The two dynamical crossovers studied by NMR and FTIR techniques. <i>Computational and Structural Biotechnology Journal</i> , 2015, 13, 33-37.	1.9	65
741	Formation of Hydrogen-Bonded Self-assembled Structures in Polar Solvents. <i>Lecture Notes in Quantum Chemistry II</i> , 2015, , 187-225.	0.3	0
742	Water-mediated long-range interactions between the internal vibrations of remote proteins. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 6728-6733.	1.3	10
743	Real-Time Measurement of the Vertical Binding Energy during the Birth of a Solvated Electron. <i>Journal of the American Chemical Society</i> , 2015, 137, 3520-3524.	6.6	41
744	Dielectric anomalous response of water at 60°C. <i>Philosophical Magazine</i> , 2015, 95, 683-690.	0.7	18
745	Hydrophobic Hydration in Water-tert-Butyl Alcohol Solutions by Extended Depolarized Light Scattering. <i>Journal of Physical Chemistry B</i> , 2015, 119, 9236-9243.	1.2	15
746	Molecular Dynamics Simulations of Heart-type Fatty Acid Binding Protein in Apo and Holo Forms, and Hydration Structure Analyses in the Binding Cavity. <i>Journal of Physical Chemistry B</i> , 2015, 119, 114-127.	1.2	26
747	Stepwise Microhydration of Aromatic Amide Cations: Formation of Water Solvation Network Revealed by Infrared Spectra of Formanilide ⁺ (H ₂ O) _n Clusters (n = 5). <i>Journal of Physical Chemistry B</i> , 2015, 119, 1388-1406.	1.2	32
748	Molecular Recognition in Chemical and Biological Systems. <i>Angewandte Chemie - International Edition</i> , 2015, 54, 3290-3327.	7.2	491

#	ARTICLE	IF	CITATIONS
749	Driving force of water entry into hydrophobic channels of carbon nanotubes: entropy or energy?. <i>Molecular Simulation</i> , 2015, 41, 504-511.	0.9	20
750	Dipolar Nanodomains in Protein Hydration Shells. <i>Journal of Physical Chemistry Letters</i> , 2015, 6, 407-412.	2.1	46
751	Strategies to create hierarchical self-assembled structures via cooperative non-covalent interactions. <i>Chemical Society Reviews</i> , 2015, 44, 2543-2572.	18.7	371
753	Adaptive resolution simulation of a biomolecule and its hydration shell: Structural and dynamical properties. <i>Journal of Chemical Physics</i> , 2015, 142, 195101.	1.2	47
754	Editorial of the PCCP themed issue on "Solvation Science". <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 8295-8296.	1.3	12
755	Propeller-shaped molecules with a thiazole hub: structural landscape and hydrazone cap mediated tunable host behavior in 4-hyrazino-1,3-thiazoles. <i>CrystEngComm</i> , 2015, 17, 5978-5986.	1.3	3
756	Progress and challenges in simulating and understanding electron transfer in proteins. <i>Archives of Biochemistry and Biophysics</i> , 2015, 582, 28-41.	1.4	19
757	Hydration in Discrete Water (II): From Neutral to Charged Solutes. <i>Journal of Physical Chemistry B</i> , 2015, 119, 5970-5978.	1.2	6
758	Spatial and Orientational Structure of the Hydration Shell of Benzene in Sub- and Supercritical Water. <i>Journal of Physical Chemistry B</i> , 2015, 119, 8600-8612.	1.2	16
759	Illuminating the Interactions between Small Solutes in Liquid Water. <i>Journal of Physical Chemistry Letters</i> , 2015, 6, 1616-1617.	2.1	1
760	Effects of Water on the Single-Chain Elasticity of Poly(U) RNA. <i>Langmuir</i> , 2015, 31, 6107-6113.	1.6	13
761	Structure and Dynamics of the Instantaneous Water/Vapor Interface Revisited by Path-Integral and Ab Initio Molecular Dynamics Simulations. <i>Journal of Physical Chemistry B</i> , 2015, 119, 10079-10086.	1.2	61
762	Structural Order of Water Molecules around Hydrophobic Solutes: Length-Scale Dependence and Solute-Solvent Coupling. <i>Journal of Physical Chemistry B</i> , 2015, 119, 11346-11357.	1.2	33
763	Biological Water or Rather Water in Biology?. <i>Journal of Physical Chemistry Letters</i> , 2015, 6, 2449-2451.	2.1	72
764	Water organization between oppositely charged surfaces: Implications for protein sliding along DNA. <i>Journal of Chemical Physics</i> , 2015, 142, 085102.	1.2	13
765	Polarized Water Wires under Confinement in Chiral Channels. <i>Journal of Physical Chemistry B</i> , 2015, 119, 8707-8717.	1.2	11
766	Molecular machines " a new dimension of biological sciences. <i>Cellular and Molecular Biology Letters</i> , 2015, 20, 248-64.	2.7	0
767	Simplified TiO ₂ force fields for studies of its interaction with biomolecules. <i>Journal of Chemical Physics</i> , 2015, 142, 234102.	1.2	41

#	ARTICLE	IF	CITATIONS
768	Solvation Thermodynamics of Organic Molecules by the Molecular Integral Equation Theory: Approaching Chemical Accuracy. <i>Chemical Reviews</i> , 2015, 115, 6312-6356.	23.0	166
769	Conserved water molecules in bacterial serine hydroxymethyltransferases. <i>Protein Engineering, Design and Selection</i> , 2015, 28, 415-426.	1.0	4
770	Revealing Water Films Structure from Force Reconstruction in Dynamic AFM. <i>Journal of Physical Chemistry C</i> , 2015, 119, 8258-8265.	1.5	29
771	Thermodynamic Profiles of Salt Effects on a Host-Guest System: New Insight into the Hofmeister Effect. <i>Journal of Physical Chemistry B</i> , 2015, 119, 5624-5638.	1.2	50
772	Direct Observation of Coupling between Structural Fluctuation and Ultrafast Hydration Dynamics of Fluorescent Probes in Anionic Micelles. <i>Journal of Physical Chemistry B</i> , 2015, 119, 10849-10857.	1.2	34
773	Ultrafast Vibrational Dynamics of Water Disentangled by Reverse Nonequilibrium <i>Ab Initio</i> Molecular Dynamics Simulations. <i>Physical Review X</i> , 2015, 5, .	2.8	31
774	Low-molecular-weight metabolite systems chemistry. <i>Frontiers in Environmental Science</i> , 2015, 3, .	1.5	26
775	Biomolecular hydration dynamics probed with 2D-IR spectroscopy: From dilute solution to a macromolecular crowd. <i>Chinese Chemical Letters</i> , 2015, 26, 435-438.	4.8	7
776	Subnanoscale hydrophobic modulation of salt bridges in aqueous media. <i>Science</i> , 2015, 348, 555-559.	6.0	51
777	Competing factors on the frequency separation between the OH stretching modes in water. <i>Journal of Molecular Liquids</i> , 2015, 205, 42-45.	2.3	13
778	Dominant Alcohol-Protein Interaction via Hydration-Enabled Enthalpy-Driven Binding Mechanism. <i>Journal of Physical Chemistry B</i> , 2015, 119, 5367-5375.	1.2	11
779	The local compressibility of liquids near non-adsorbing substrates: a useful measure of solvophobicity and hydrophobicity?. <i>Journal of Physics Condensed Matter</i> , 2015, 27, 194111.	0.7	44
780	Water structure and chaotropicity: their uses, abuses and biological implications. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 8297-8305.	1.3	215
781	Ultrafast 2D-IR and Simulation Investigations of Preferential Solvation and Cosolvent Exchange Dynamics. <i>Journal of Physical Chemistry B</i> , 2015, 119, 6271-6279.	1.2	27
782	How does a hydrocarbon staple affect peptide hydrophobicity?. <i>Journal of Computational Chemistry</i> , 2015, 36, 773-784.	1.5	8
783	Hydrogen-bond dynamics of water in presence of an amphiphile, tetramethylurea: signature of confinement-induced effects. <i>Molecular Simulation</i> , 2015, 41, 471-482.	0.9	30
785	Molecular Mechanisms of Hematin Crystallization from Organic Solvent. <i>Crystal Growth and Design</i> , 2015, 15, 5535-5542.	1.4	34
786	Exploring water as building bricks in enzyme engineering. <i>Chemical Communications</i> , 2015, 51, 17221-17224.	2.2	12

#	ARTICLE	IF	CITATIONS
787	Keto-Enol Tautomeric Equilibrium of Acetylacetone Solution Confined in Extended Nanospaces. <i>Journal of Physical Chemistry B</i> , 2015, 119, 14750-14755.	1.2	18
788	The pathway for serial proton supply to the active site of nitrogenase: enhanced density functional modeling of the Grothuss mechanism. <i>Dalton Transactions</i> , 2015, 44, 18167-18186.	1.6	47
789	Weighted protein residue networks based on joint recurrences between residues. <i>BMC Bioinformatics</i> , 2015, 16, 173.	1.2	14
790	Computational Study of Phosphate Vibrations as Reporters of DNA Hydration. <i>Journal of Physical Chemistry Letters</i> , 2015, 6, 4012-4017.	2.1	25
791	Prediction of Water Binding to Protein Hydration Sites with a Discrete, Semiexplicit Solvent Model. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 5961-5972.	2.3	14
792	Water density fluctuations relevant to hydrophobic hydration are unaltered by attractions. <i>Journal of Chemical Physics</i> , 2015, 142, 024502.	1.2	22
793	Ultrafast phosphate hydration dynamics in bulk H ₂ O. <i>Journal of Chemical Physics</i> , 2015, 142, 212406.	1.2	30
794	Water structure and solvation of osmolytes at high hydrostatic pressure: pure water and TMAO solutions at 10 kbar versus 1 bar. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 24224-24237.	1.3	67
795	Membrane Hydration. <i>Sub-Cellular Biochemistry</i> , 2015, , .	1.0	21
796	Long-Range Lipid-Water Interaction as Observed by ATR-FTIR Spectroscopy. <i>Sub-Cellular Biochemistry</i> , 2015, 71, 127-159.	1.0	9
797	The mechanism of water/ion exchange at a protein surface: a weakly bound chloride in <i>Helicobacter pylori</i> apoflavodoxin. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 28635-28646.	1.3	4
798	Broadband dielectric spectroscopy of glucose aqueous solution: Analysis of the hydration state and the hydrogen bond network. <i>Journal of Chemical Physics</i> , 2015, 142, 234504.	1.2	70
799	Thermodynamic and Structural Evidence for Reduced Hydrogen Bonding among Water Molecules near Small Hydrophobic Solutes. <i>Journal of Physical Chemistry B</i> , 2015, 119, 12108-12116.	1.2	35
800	Protein NMR. <i>Biological Magnetic Resonance</i> , 2015, , .	0.4	4
801	Theoretical study on the hydrophobic and hydrophilic hydration on large solutes: The case of phthalocyanines in water. <i>Journal of Chemical Physics</i> , 2015, 143, 044502.	1.2	3
803	Biocomposite Nanomaterials for Electrochemical Biosensors. , 2015, , 1-29.		1
804	Path integral molecular dynamics within the grand canonical-like adaptive resolution technique: Simulation of liquid water. <i>Journal of Chemical Physics</i> , 2015, 143, 094102.	1.2	45
805	Local and global structural drivers for the photoactivation of the orange carotenoid protein. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2015, 112, E5567-74.	3.3	121

#	ARTICLE	IF	CITATIONS
806	Generality of hydrophobic phenomena for aqueous solutions of amphiphiles. <i>Chemical Physics Letters</i> , 2015, 640, 184-187.	1.2	19
807	Chemical basis for the recognition of trimethyllysine by epigenetic reader proteins. <i>Nature Communications</i> , 2015, 6, 8911.	5.8	72
808	Properties of the polarizable MARTINI water model: A comparative study for aqueous electrolyte solutions. <i>Journal of Molecular Liquids</i> , 2015, 212, 103-110.	2.3	25
809	Molecular density functional theory for multiscale modeling of hydration free energy. <i>Chemical Engineering Science</i> , 2015, 126, 370-382.	1.9	19
810	The structure of water; from ambient to deeply supercooled. <i>Journal of Non-Crystalline Solids</i> , 2015, 407, 399-417.	1.5	51
811	Hydration and aggregation of lysozyme by extended frequency range depolarized light scattering. <i>Journal of Non-Crystalline Solids</i> , 2015, 407, 472-477.	1.5	18
812	Hydrogen-bond relaxation dynamics: Resolving mysteries of water ice. <i>Coordination Chemistry Reviews</i> , 2015, 285, 109-165.	9.5	136
813	Reply to the comment on "A simple method for estimating in vitro air-tissue and in vivo blood-tissue partition coefficients". <i>Chemosphere</i> , 2015, 120, 797-798.	4.2	0
814	Water-Water and Water-Solute Interactions in Microsolvated Organic Complexes. <i>Angewandte Chemie - International Edition</i> , 2015, 54, 979-982.	7.2	59
815	Effect of fibrillation on the excited state dynamics of tryptophan in serum protein - A time-resolved fluorescence study. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2015, 299, 73-79.	2.0	0
816	Hydrophobic hydration of poly-N-isopropyl acrylamide: a matter of the mean energetic state of water. <i>Scientific Reports</i> , 2014, 4, 4377.	1.6	139
817	Molecular containers assembled through the hydrophobic effect. <i>Chemical Society Reviews</i> , 2015, 44, 547-585.	18.7	260
818	Biomimetic cavity-based metal complexes. <i>Chemical Society Reviews</i> , 2015, 44, 467-489.	18.7	156
819	Role of Internal Water on Protein Thermal Stability: The Case of Homologous G Domains. <i>Journal of Physical Chemistry B</i> , 2015, 119, 8939-8949.	1.2	21
820	Unraveling Entropic Rate Acceleration Induced by Solvent Dynamics in Membrane Enzymes. <i>Journal of Visualized Experiments</i> , 2016, , e53168.	0.2	0
821	Imaging Water Thin Films in Ambient Conditions Using Atomic Force Microscopy. <i>Materials</i> , 2016, 9, 182.	1.3	24
822	Correlation between the Increasing Conductivity of Aqueous Solutions of Cation Chlorides with Time and the "Salting-Out" Properties of the Cations. <i>Entropy</i> , 2016, 18, 66.	1.1	1
823	Pressure as a Limiting Factor for Life. <i>Life</i> , 2016, 6, 34.	1.1	25

#	ARTICLE	IF	CITATIONS
824	Wide-field medium-repetition-rate multiphoton microscopy reduces photodamage of living cells. <i>Biomedical Optics Express</i> , 2016, 7, 1458.	1.5	26
825	Assessing the accuracy of improved force-matched water models derived from <i>Ab initio</i> molecular dynamics simulations. <i>Journal of Computational Chemistry</i> , 2016, 37, 1828-1838.	1.5	11
826	Exploration of the presence of bulk-like water in AOT reverse micelles and water-in-oil nanodroplets: the role of charged interfaces, confinement size and properties of water. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 21767-21779.	1.3	26
828	Free energies of solvation in the context of protein folding: Implications for implicit and explicit solvent models. <i>Journal of Computational Chemistry</i> , 2016, 37, 629-640.	1.5	24
829	Direct Observation of Self-Organized Water-Containing Structures in the Liquid Phase and Their Influence on 5-(Hydroxymethyl)furfural Formation in Ionic Liquids. <i>Angewandte Chemie</i> , 2016, 128, 2201-2206.	1.6	8
830	Confined Water in Amyloid-Competent Oligomers of the Prion Protein. <i>ChemPhysChem</i> , 2016, 17, 2804-2807.	1.0	11
831	Water: A Tale of Two Liquids. <i>Chemical Reviews</i> , 2016, 116, 7463-7500.	23.0	627
832	Direct Observation of Self-Organized Water-Containing Structures in the Liquid Phase and Their Influence on 5-(Hydroxymethyl)furfural Formation in Ionic Liquids. <i>Angewandte Chemie - International Edition</i> , 2016, 55, 2161-2166.	7.2	82
833	Effect of water polyamorphism on the molecular vibrations of glycerol in its glassy aqueous solutions. <i>Journal of Chemical Physics</i> , 2016, 145, 024501.	1.2	10
834	Mechanisms of Protein Translocation on DNA Are Differentially Responsive to Water Activity. <i>Biochemistry</i> , 2016, 55, 6957-6960.	1.2	1
835	Spatially resolved dielectric constant of confined water and its connection to the non-local nature of bulk water. <i>Journal of Chemical Physics</i> , 2016, 145, 084901.	1.2	32
836	Effect of ethanol concentrations on temperature driven structural changes of chymotrypsin inhibitor 2. <i>Journal of Chemical Physics</i> , 2016, 144, 165101.	1.2	15
837	Direct visualization of both DNA and RNA quadruplexes in human cells via an uncommon spectroscopic method. <i>Scientific Reports</i> , 2016, 6, 32141.	1.6	67
838	Non-monotonic dynamics of water in its binary mixture with 1,2-dimethoxy ethane: A combined THz spectroscopic and MD simulation study. <i>Journal of Chemical Physics</i> , 2016, 145, 164501.	1.2	18
839	Hydrogen Bond Network of Water around Protein Investigated with Terahertz and Infrared Spectroscopy. <i>Biophysical Journal</i> , 2016, 111, 2629-2641.	0.2	56
840	Changes in hydration structure are necessary for collective motions of a multi-domain protein. <i>Scientific Reports</i> , 2016, 6, 26302.	1.6	48
841	Towards a structural biology of the hydrophobic effect in protein folding. <i>Scientific Reports</i> , 2016, 6, 28285.	1.6	91
842	Structure of solvation water around the active and inactive regions of a type III antifreeze protein and its mutants of lowered activity. <i>Journal of Chemical Physics</i> , 2016, 145, 075101.	1.2	12

#	ARTICLE	IF	CITATIONS
843	Combining Surface Plasmon Resonance and Quartz Crystal Microbalance To Determine Hydration of Dendrimer Monolayers. <i>Journal of Physical Chemistry C</i> , 2016, 120, 19678-19685.	1.5	26
844	Tuning the tetrahedrality of the hydrogen-bonded network of water: Comparison of the effects of pressure and added salts. <i>Journal of Chemical Physics</i> , 2016, 144, 234509.	1.2	7
845	Extracting water and ion distributions from solution x-ray scattering experiments. <i>Journal of Chemical Physics</i> , 2016, 144, 214105.	1.2	15
846	A hydrated ion model of [UO ₂] ²⁺ in water: Structure, dynamics, and spectroscopy from classical molecular dynamics. <i>Journal of Chemical Physics</i> , 2016, 145, 224502.	1.2	17
847	Interaction of ice binding proteins with ice, water and ions. <i>Biointerphases</i> , 2016, 11, 018906.	0.6	31
848	Dissecting ion-specific from electrostatic salt effects on amyloid fibrillation: A case study of insulin. <i>Biointerphases</i> , 2016, 11, 019008.	0.6	12
849	Challenges in the Structure Determination of Self-Assembled Metallacages: What Do Cage Cavities Contain, Internal Vapor Bubbles or Solvent and/or Counterions?. <i>Journal of the American Chemical Society</i> , 2016, 138, 6676-6687.	6.6	10
850	Aqueous solvation of amphiphilic molecules by extended depolarized light scattering: the case of trimethylamine-N-oxide. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 8881-8889.	1.3	11
851	Artificial water channels – incipient innovative developments. <i>Chemical Communications</i> , 2016, 52, 5657-5665.	2.2	71
852	Solute-Solvent Interactions in Aqueous Solutions of Sulfobutyl Ether- β -cyclodextrin As Probed by UV-Raman and FTIR-ATR Analysis. <i>Journal of Physical Chemistry B</i> , 2016, 120, 3746-3753.	1.2	6
853	Solvation of arsenate anion: combined quantum mechanics and molecular dynamics based investigation. <i>Molecular Physics</i> , 2016, 114, 2029-2036.	0.8	3
854	Trehalose matrix effects on charge-recombination kinetics in Photosystem I of oxygenic photosynthesis at different dehydration levels. <i>Biochimica Et Biophysica Acta - Bioenergetics</i> , 2016, 1857, 1440-1454.	0.5	31
855	Hydration of proteins and nucleic acids: Advances in experiment and theory. A review. <i>Biochimica Et Biophysica Acta - General Subjects</i> , 2016, 1860, 1821-1835.	1.1	47
856	Structural evidence for solvent-stabilisation by aspartic acid as a mechanism for halophilic protein stability in high salt concentrations. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 18054-18062.	1.3	18
857	Recent developments in the theoretical, simulational, and experimental studies of the role of water hydrogen bonding in hydrophobic phenomena. <i>Advances in Colloid and Interface Science</i> , 2016, 235, 23-45.	7.0	11
858	Water Determines the Structure and Dynamics of Proteins. <i>Chemical Reviews</i> , 2016, 116, 7673-7697.	23.0	645
859	Molecular Shape and the Hydrophobic Effect. <i>Annual Review of Physical Chemistry</i> , 2016, 67, 307-329.	4.8	101
860	Water-Mediated Hydrophobic Interactions. <i>Annual Review of Physical Chemistry</i> , 2016, 67, 617-638.	4.8	155

#	ARTICLE	IF	CITATIONS
861	Role of Local Response in Ion Solvation: Born Theory and Beyond. <i>Journal of Physical Chemistry B</i> , 2016, 120, 6238-6249.	1.2	21
862	Enthalpic Breakdown of Water Structure on Protein Active-Site Surfaces. <i>Journal of Physical Chemistry B</i> , 2016, 120, 8743-8756.	1.2	33
863	Sparse Sampling of Water Density Fluctuations in Interfacial Environments. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 706-713.	2.3	36
864	Probing Solvation Dynamics around Aromatic and Biological Molecules at the Single-Molecular Level. <i>Chemical Reviews</i> , 2016, 116, 5432-5463.	23.0	78
865	Semiempirical Quantum Mechanical Methods for Noncovalent Interactions for Chemical and Biochemical Applications. <i>Chemical Reviews</i> , 2016, 116, 5301-5337.	23.0	312
866	Salt-Excluding Artificial Water Channels Exhibiting Enhanced Dipolar Water and Proton Translocation. <i>Journal of the American Chemical Society</i> , 2016, 138, 5403-5409.	6.6	111
867	Temperature Dependence of Nanoconfined Water Properties: Application to Cementitious Materials. <i>Journal of Physical Chemistry C</i> , 2016, 120, 11465-11480.	1.5	30
868	Fast and slow dynamics and the local structure of liquid and supercooled water next to a hydrophobic amino acid. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 27639-27647.	1.3	12
869	Cord factor as an invisibility cloak? A hypothesis for asymptomatic TB persistence. <i>Tuberculosis</i> , 2016, 101, S2-S8.	0.8	11
870	Anomalous Dynamics of Water Confined in Protein-Protein and Protein-DNA Interfaces. <i>Journal of Physical Chemistry Letters</i> , 2016, 7, 3967-3972.	2.1	35
871	Long-term effects of salinity on extracellular polymeric substances, microbial activity and microbial community from biofilm and suspended sludge in an anoxic-aerobic sequencing batch biofilm reactor. <i>Journal of the Taiwan Institute of Chemical Engineers</i> , 2016, 68, 275-280.	2.7	35
872	Water Rearrangements upon Disorder-to-Order Amyloid Transition. <i>Journal of Physical Chemistry Letters</i> , 2016, 7, 4105-4110.	2.1	26
873	Structure and dynamics of water molecules confined in triglyceride oils. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 29361-29368.	1.3	2
874	Molecular Origin of Ultrafast Water-Protein Coupled Interactions. <i>Journal of Physical Chemistry Letters</i> , 2016, 7, 4171-4177.	2.1	29
875	Surface free energy of organized phospholipid/lauryl gallate monolayers on mica. <i>Colloids and Surfaces A: Physicochemical and Engineering Aspects</i> , 2016, 510, 213-220.	2.3	6
876	Protein dynamics and thermodynamics crossover at 10 Å°C: Different roles of hydration at hydrophilic and hydrophobic groups. <i>Chemical Physics Letters</i> , 2016, 664, 108-113.	1.2	3
877	Picosecond to nanosecond dynamics provide a source of conformational entropy for protein folding. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 21527-21538.	1.3	32
878	Study of Hydrophobic Clustering in Partially Sulfonated Polystyrene Solutions with a Systematic Coarse-Grained Model. <i>Macromolecules</i> , 2016, 49, 7571-7580.	2.2	5

#	ARTICLE	IF	CITATIONS
879	Ultraslow Water-Mediated Transmembrane Interactions Regulate the Activation of A _{2A} Adenosine Receptor. <i>Biophysical Journal</i> , 2016, 111, 1180-1191.	0.2	33
880	Arginine and proline applied as food additives stimulate high freeze tolerance in larvae of <i>Drosophila melanogaster</i> . <i>Journal of Experimental Biology</i> , 2016, 219, 2358-2367.	0.8	76
881	Mechanistic insight on methyl 3-(2-aminophenyl)acrylate cyclization reaction by multicatalysis of solvent and substrate. <i>Journal of Computational Chemistry</i> , 2016, 37, 2386-2394.	1.5	6
882	Environment-sensitive quinolone demonstrating long-lived fluorescence and unusually slow excited-state intramolecular proton transfer kinetics. <i>Methods and Applications in Fluorescence</i> , 2016, 4, 034004.	1.1	14
883	Dielectric spectroscopy of biomolecules at low frequencies: Evidence of proton wires. <i>Journal of Molecular Liquids</i> , 2016, 223, 136-140.	2.3	5
884	Water molecules inside protein structure affect binding of monosaccharides with HIV-1 antibody 2G12. <i>Journal of Computational Chemistry</i> , 2016, 37, 2341-2348.	1.5	3
885	Phospholipids and glycolipids mediate proton containment and circulation along the surface of energy-transducing membranes. <i>Progress in Lipid Research</i> , 2016, 64, 1-15.	5.3	18
886	The Search for Nanobubbles by Using Specular and Off-Specular Neutron Reflectometry. <i>Langmuir</i> , 2016, 32, 9091-9096.	1.6	8
887	The i-TTM model for ab initio-based ion-water interaction potentials. II. Alkali metal ion-water potential energy functions. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 30334-30343.	1.3	43
888	Hydration Dynamics of a Peripheral Membrane Protein. <i>Journal of the American Chemical Society</i> , 2016, 138, 11526-11535.	6.6	57
889	Water-mediated aggregation of 2-butoxyethanol. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 24937-24943.	1.3	15
890	Molecular Effects of Concentrated Solutes on Protein Hydration, Dynamics, and Electrostatics. <i>Biophysical Journal</i> , 2016, 111, 743-755.	0.2	29
891	Terahertz Time-Domain Spectroscopy of Thermoresponsive Polymers in Aqueous Solution. <i>Journal of Physical Chemistry B</i> , 2016, 120, 9778-9787.	1.2	10
892	Preparative scale and convenient synthesis of a water-soluble, deep cavitand. <i>Nature Protocols</i> , 2016, 11, 1371-1387.	5.5	37
893	Modeling somite scaling in small embryos in the framework of Turing patterns. <i>Physical Review E</i> , 2016, 93, 042402.	0.8	9
894	Enthalpic and Entropic Contributions to Hydrophobicity. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 4600-4610.	2.3	68
895	Cation-Induced Hydration Effects Cause Lower Critical Solution Temperature Behavior in Protein Solutions. <i>Journal of Physical Chemistry B</i> , 2016, 120, 7731-7736.	1.2	49
896	Functionalized single walled carbon nanotubes as template for water storage device. <i>Chemical Physics</i> , 2016, 479, 42-52.	0.9	1

#	ARTICLE	IF	CITATIONS
897	Rational Design of Thermodynamic and Kinetic Binding Profiles by Optimizing Surface Water Networks Coating Protein-Bound Ligands. <i>Journal of Medicinal Chemistry</i> , 2016, 59, 10530-10548.	2.9	64
898	Glucose induced variation of water structure from temperature dependent near infrared spectra. <i>RSC Advances</i> , 2016, 6, 105729-105736.	1.7	48
899	Water based on a molecular model behaves like a hard-sphere solvent for a nonpolar solute when the reference interaction site model and related theories are employed. <i>Journal of Physics Condensed Matter</i> , 2016, 28, 344003.	0.7	14
900	Electrolytes induce long-range orientational order and free energy changes in the H-bond network of bulk water. <i>Science Advances</i> , 2016, 2, e1501891.	4.7	151
901	Elastic Scattering Spectroscopy (ESS): an Instrument-Concept for Dynamics of Complex (Bio-) Systems From Elastic Neutron Scattering. <i>Scientific Reports</i> , 2016, 6, 34266.	1.6	13
902	Protein States as Symmetry Transitions in the Correlation Matrices. <i>Journal of Physical Chemistry B</i> , 2016, 120, 11428-11435.	1.2	8
903	Ice-like water supports hydration forces and eases sliding friction. <i>Science Advances</i> , 2016, 2, e1600763.	4.7	52
904	Revealing Single Molecular Solvent Reorientation Dynamics by Complementary Use of Picosecond Time Resolved IR Spectroscopy and MD Simulation. <i>Molecular Science</i> , 2016, 10, A0087.	0.2	0
905	Synchrotron X-ray footprinting as a method to visualize water in proteins. <i>Journal of Synchrotron Radiation</i> , 2016, 23, 1056-1069.	1.0	21
906	Water Dynamics in <i>Shewanella oneidensis</i> at Ambient and High Pressure using Quasi-Elastic Neutron Scattering. <i>Scientific Reports</i> , 2016, 6, 18862.	1.6	18
907	The critical size of hydrogen-bonded alcohol clusters as effective Brønsted bases in solutions. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 24880-24889.	1.3	13
908	When proteins are completely hydrated in crystals. <i>International Journal of Biological Macromolecules</i> , 2016, 89, 137-143.	3.6	12
909	Molecular properties of aqueous solutions: a focus on the collective dynamics of hydration water. <i>Soft Matter</i> , 2016, 12, 5501-5514.	1.2	57
910	Asymmetric self-diffusion with orientation-dependence of water molecule in finite timescale. <i>Science China: Physics, Mechanics and Astronomy</i> , 2016, 59, 1.	2.0	1
911	Difference in the hydration water mobility around F-actin and myosin subfragment-1 studied by quasielastic neutron scattering. <i>Biochemistry and Biophysics Reports</i> , 2016, 6, 220-225.	0.7	11
912	Colloidal crystals and water: Perspectives on liquid–solid nanoscale phenomena in wet particulate media. <i>Advances in Colloid and Interface Science</i> , 2016, 234, 142-160.	7.0	14
913	Confinement, entropic effects and hydrogen bond network fluctuations of water in Nafion membrane. <i>Journal of Molecular Liquids</i> , 2016, 219, 1161-1164.	2.3	3
914	Tuning water transport through nanochannels by changing the direction of an external electric field. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 17991-17996.	1.3	23

#	ARTICLE	IF	CITATIONS
915	A highly efficient hybrid method for calculating the hydration free energy of a protein. <i>Journal of Computational Chemistry</i> , 2016, 37, 712-723.	1.5	6
916	Amide III SFG Signals as a Sensitive Probe of Protein Folding at Cell Membrane Surface. <i>Journal of Physical Chemistry C</i> , 2016, 120, 15322-15328.	1.5	23
917	Dynamics and mechanism of ultrafast water-protein interactions. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2016, 113, 8424-8429.	3.3	118
918	Effect of Lauryl Gallate on Wetting Properties of Organized Thin Phospholipid Films on Mica. <i>Journal of Physical Chemistry B</i> , 2016, 120, 6657-6666.	1.2	4
919	Toward high-throughput predictions of the hydration free energies of small organic molecules from first principles. <i>Fluid Phase Equilibria</i> , 2016, 407, 304-313.	1.4	11
920	Implications of hydrogen/halogen-bond in the stabilization of confined water and anion-water clusters by a cationic receptor. <i>Journal of Molecular Structure</i> , 2016, 1108, 298-306.	1.8	5
921	Noninvasive Experimental Evidence of the Linear Pore Size Dependence of Water Diffusion in Nanoconfinement. <i>Journal of Physical Chemistry Letters</i> , 2016, 7, 393-398.	2.1	18
922	Hydration Layer-Mediated Pairwise Interaction of Nanoparticles. <i>Nano Letters</i> , 2016, 16, 786-790.	4.5	103
923	i-TTM Model for Ab Initio-Based Ion-Water Interaction Potentials. 1. Halide-Water Potential Energy Functions. <i>Journal of Physical Chemistry B</i> , 2016, 120, 1822-1832.	1.2	61
924	Influence of Inorganic Salts on the Phase Equilibrium of Triton X-114 Aqueous Two-Phase Systems. <i>Journal of Chemical & Engineering Data</i> , 2016, 61, 1496-1501.	1.0	38
925	Low-Density Water Structure Observed in a Nanosegregated Cryoprotectant Solution at Low Temperatures from 285 to 238 K. <i>Journal of Physical Chemistry B</i> , 2016, 120, 4439-4448.	1.2	26
926	Interplay of Electrostatic Interactions and Hydrophobic Hydration at the Surface of Tetra- <i>n</i> -alkylammonium Bromide Solutions. <i>Journal of Physical Chemistry C</i> , 2016, 120, 17290-17295.	1.5	2
927	Correlation Between Chain Architecture and Hydration Water Structure in Polysaccharides. <i>Biomacromolecules</i> , 2016, 17, 1198-1204.	2.6	62
928	What did Erwin mean? The physics of information from the materials genomics of aperiodic crystals and water to molecular information catalysts and life. <i>Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences</i> , 2016, 374, 20150067.	1.6	15
929	Wonders of Water. <i>Springer Series in Chemical Physics</i> , 2016, , 1-24.	0.2	1
930	The problems of biological information. <i>Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences</i> , 2016, 374, 20150072.	1.6	9
931	A proactive role of water molecules in acceptor recognition by protein O-fucosyltransferase 2. <i>Nature Chemical Biology</i> , 2016, 12, 240-246.	3.9	58
932	Dual emissive analogue of deoxyuridine as a sensitive hydration-reporting probe for discriminating mismatched from matched DNA and DNA/DNA from DNA/RNA duplexes. <i>Journal of Materials Chemistry C</i> , 2016, 4, 3010-3017.	2.7	20

#	ARTICLE	IF	CITATIONS
933	Reconciling the understanding of "hydrophobicity"™ with physics-based models of proteins. <i>Journal of Physics Condensed Matter</i> , 2016, 28, 083003.	0.7	17
934	Cooperativity in Noncovalent Interactions. <i>Chemical Reviews</i> , 2016, 116, 2775-2825.	23.0	680
935	Impact of Surface Water Layers on Protein" Ligand Binding: How Well Are Experimental Data Reproduced by Molecular Dynamics Simulations in a Thermolysin Test Case?. <i>Journal of Chemical Information and Modeling</i> , 2016, 56, 223-233.	2.5	29
936	Water-mediated influence of a crowded environment on internal vibrations of a protein molecule. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 4881-4890.	1.3	3
937	Anion"water interactions of weakly hydrated anions: molecular dynamics simulations of aqueous NaBF ₄ and NaPF ₆ . <i>Molecular Physics</i> , 2016, 114, 1831-1846.	0.8	14
938	Fast transport of water molecules across carbon nanotubes induced by static electric fields. <i>Chemical Physics Letters</i> , 2016, 644, 201-204.	1.2	12
939	Anisotropic structure and dynamics of the solvation shell of a benzene solute in liquid water from ab initio molecular dynamics simulations. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 6132-6145.	1.3	20
940	Supramolecular Polymers in Aqueous Media. <i>Chemical Reviews</i> , 2016, 116, 2414-2477.	23.0	625
941	Effect of Short Chain Poly(ethylene glycol)s on the Hydration Structure and Dynamics around Human Serum Albumin. <i>Langmuir</i> , 2016, 32, 831-837.	1.6	30
942	Astrobiology and the Possibility of Life on Earth and Elsewhere". <i>Space Science Reviews</i> , 2017, 209, 1-42.	3.7	66
943	Real-time and quantitative fluorescent live-cell imaging with quadruplex-specific red-edge probe (G4-REP). <i>Biochimica Et Biophysica Acta - General Subjects</i> , 2017, 1861, 1312-1320.	1.1	18
944	Watching Proteins Wiggle: Mapping Structures with Two-Dimensional Infrared Spectroscopy. <i>Chemical Reviews</i> , 2017, 117, 10726-10759.	23.0	195
945	The Multiple Roles of Waters in Protein Solvation. <i>Journal of Physical Chemistry B</i> , 2017, 121, 3636-3643.	1.2	17
946	Origin of hydrophobicity and enhanced water hydrogen bond strength near purely hydrophobic solutes. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2017, 114, 322-327.	3.3	169
947	Solvation Shell Structure of Small Molecules and Proteins by IR-MCR Spectroscopy. <i>Journal of Physical Chemistry Letters</i> , 2017, 8, 611-614.	2.1	24
948	Biological Activity of Ionic Liquids and Their Application in Pharmaceuticals and Medicine. <i>Chemical Reviews</i> , 2017, 117, 7132-7189.	23.0	1,201
949	On the use of ultracentrifugal devices for routine sample preparation in biomolecular magic-angle-spinning NMR. <i>Journal of Biomolecular NMR</i> , 2017, 67, 165-178.	1.6	38
950	Observation of the Global Dynamic Collectivity of a Hydration Shell around Apomyoglobin. <i>Journal of Physical Chemistry Letters</i> , 2017, 8, 1124-1131.	2.1	16

#	ARTICLE	IF	CITATIONS
951	Humidity-induced formation of water channels in supramolecular assemblies of wedge-shaped amphiphiles: the effect of the molecular architecture on the channel topology. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 7714-7720.	1.3	7
952	Local and Global Effects of Dissolved Sodium Chloride on the Structure of Water. <i>Journal of Physical Chemistry Letters</i> , 2017, 8, 1496-1502.	2.1	87
953	Hydration-Shell Transformation of Thermosensitive Aqueous Polymers. <i>Journal of Physical Chemistry Letters</i> , 2017, 8, 1360-1364.	2.1	33
954	New Information on the Hydrophobic Interaction Revealed by Frequency Modulation AFM. <i>Langmuir</i> , 2017, 33, 2485-2496.	1.6	30
955	Water Dynamics in the Hydration Shells of Biomolecules. <i>Chemical Reviews</i> , 2017, 117, 10694-10725.	23.0	574
956	Protonic Surface Conductivity and Proton Space-Charge Relaxation in Hydrated Fullerol. <i>Journal of Physical Chemistry C</i> , 2017, 121, 4873-4881.	1.5	6
957	On the coupling between the dynamics of protein and water. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 8243-8257.	1.3	33
958	How water mediates the long-range interactions between remote protein molecules. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 5441-5448.	1.3	7
959	The adaptive nature of protein residue networks. <i>Proteins: Structure, Function and Bioinformatics</i> , 2017, 85, 917-923.	1.5	6
960	A refined polarizable water model for the coarse-grained MARTINI force field with long-range electrostatic interactions. <i>Journal of Chemical Physics</i> , 2017, 146, 054501.	1.2	69
961	Structural motifs of water on metal oxide surfaces. <i>Chemical Society Reviews</i> , 2017, 46, 1785-1806.	18.7	170
962	Bis-15-crown-5-ether-pillar[5]arene K ⁺ -Responsive Channels. <i>Organic Letters</i> , 2017, 19, 1438-1441.	2.4	44
963	Structure of liquid water â€“ a dynamical mixture of tetrahedral and â€“ring-and-chainâ€™™ like structures. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 11931-11936.	1.3	50
964	A balanced view of casein interactions. <i>Current Opinion in Colloid and Interface Science</i> , 2017, 28, 74-86.	3.4	53
965	Solvent fluctuations around solvophobic, solvophilic, and patchy nanostructures and the accompanying solvent mediated interactions. <i>Journal of Chemical Physics</i> , 2017, 146, 124703.	1.2	21
966	Enhancement of the Hydrogen-Bonding Network of Water Confined in a Polyelectrolyte Brush. <i>Langmuir</i> , 2017, 33, 3954-3959.	1.6	44
967	Characterization of the hydrogen-bond network of water around sucrose and trehalose: Microwave and terahertz spectroscopic study. <i>Journal of Chemical Physics</i> , 2017, 146, 105102.	1.2	66
968	Liquid Water Restricts Habitability in Extreme Deserts. <i>Astrobiology</i> , 2017, 17, 309-318.	1.5	8

#	ARTICLE	IF	CITATIONS
969	Aqueous ionic liquids and their effects on protein structures: an overview on recent theoretical and experimental results. <i>Journal of Physics Condensed Matter</i> , 2017, 29, 233001.	0.7	81
970	Better Than the Best Polar Solvent: Tuning the Polarity of 1,2,4-Triazolium-Based Ionic Liquids. <i>ChemistrySelect</i> , 2017, 2, 3943-3947.	0.7	9
971	Redesign of water networks for efficient biocatalysis. <i>Current Opinion in Chemical Biology</i> , 2017, 37, 107-114.	2.8	10
972	Novel Hydrogen-Bonding Pattern of Water in Polycarbonate. <i>Bulletin of the Chemical Society of Japan</i> , 2017, 90, 527-536.	2.0	2
973	Intracellular water – an overlooked drug target? Cisplatin impact in cancer cells probed by neutrons. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 2702-2713.	1.3	36
974	Water structure around hydrophobic amino acid side chain analogs using different water models. <i>Journal of Chemical Physics</i> , 2017, 146, 225104.	1.2	18
975	Modeling of Polarization Transfer Kinetics in Protein Hydration Using Hyperpolarized Water. <i>Journal of Physical Chemistry B</i> , 2017, 121, 6492-6498.	1.2	26
976	Hydrophobic Effect of Alkyl Groups Stabilizing Self-Assembled Colloids in Water. <i>Journal of Physical Chemistry B</i> , 2017, 121, 6280-6285.	1.2	7
977	Water Dynamics from the Surface to the Interior of a Supramolecular Nanostructure. <i>Journal of the American Chemical Society</i> , 2017, 139, 8915-8921.	6.6	53
978	Water is an active matrix of life for cell and molecular biology. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2017, 114, 13327-13335.	3.3	296
979	Energetic Analysis of Adsorption and Absorption of Small Molecule to Nanodroplet of Water. <i>Journal of Physical Chemistry B</i> , 2017, 121, 5995-6001.	1.2	6
980	Unifying the microscopic picture of His-containing turns: from gas phase model peptides to crystallized proteins. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 17128-17142.	1.3	11
981	A Simple Approach to Achieve Self-Buffering Protic Ionic Liquid-Water Mixtures. <i>ChemistrySelect</i> , 2017, 2, 4294-4299.	0.7	13
982	The interfacial structure of water droplets in a hydrophobic liquid. <i>Nature Communications</i> , 2017, 8, 15548.	5.8	56
983	Explicit Solvent Hydration Benchmark for Proteins with Application to the PBSA Method. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 2762-2776.	2.3	1
984	Nuclear Quantum Effects in Water Reorientation and Hydrogen-Bond Dynamics. <i>Journal of Physical Chemistry Letters</i> , 2017, 8, 2602-2607.	2.1	51
985	WatAA: Atlas of Protein Hydration. Exploring synergies between data mining and ab initio calculations. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 17094-17102.	1.3	8
986	Estimation of kinetic and thermodynamic ligand-binding parameters using computational strategies. <i>Future Medicinal Chemistry</i> , 2017, 9, 507-523.	1.1	30

#	ARTICLE	IF	CITATIONS
987	The Deeply Understanding of the Self-Healing Mechanism for Self-Healing Behavior of Supramolecular Materials Based on Cyclodextrin-Guest Interactions. <i>Macromolecular Chemistry and Physics</i> , 2017, 218, 1600593.	1.1	12
988	A controllable water signal transistor. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 9625-9629.	1.3	2
989	Dynamics of hydration water and coupled protein sidechains around a polymerase protein surface. <i>Chemical Physics Letters</i> , 2017, 683, 658-665.	1.2	5
990	Exploring Fluorescent Dyes at Biomimetic Interfaces with Second Harmonic Generation and Molecular Dynamics. <i>Langmuir</i> , 2017, 33, 3373-3383.	1.6	9
991	The aqueous supramolecular chemistry of cucurbit[n]urils, pillar[n]arenes and deep-cavity cavitands. <i>Chemical Society Reviews</i> , 2017, 46, 2479-2496.	18.7	473
992	Role of the hydrophobic and hydrophilic sites in the dynamic crossover of the protein-hydration water. <i>Physica A: Statistical Mechanics and Its Applications</i> , 2017, 468, 733-739.	1.2	20
993	Short-Range π - π Stacking Assembly on P25 TiO ₂ Nanoparticles for Enhanced Visible-Light Photocatalysis. <i>ACS Catalysis</i> , 2017, 7, 652-663.	5.5	98
994	On the micro-heterogeneous structure of neat and aqueous propylamine mixtures: A computer simulation study. <i>Journal of Molecular Liquids</i> , 2017, 227, 210-217.	2.3	7
995	Modified Poisson equations for calculating solvation free energy. <i>Biophysical Chemistry</i> , 2017, 221, 26-40.	1.5	1
996	Mesoscopic Solute-Rich Clusters in Olanzapine Solutions. <i>Crystal Growth and Design</i> , 2017, 17, 6668-6676.	1.4	26
997	A solution-based single-molecule study of surface-bound PBIs: solvent-mediated environmental effects on molecular flexibility. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 29255-29262.	1.3	1
998	The behavior of hydroxide and hydronium ions at the hexadecane-water interface studied with second harmonic generation and zeta potential measurements. <i>Soft Matter</i> , 2017, 13, 7962-7968.	1.2	27
999	Ion-induced alterations of the local hydration environment elucidate Hofmeister effect in a simple classical model of Trp-cage miniprotein. <i>Journal of Molecular Modeling</i> , 2017, 23, 298.	0.8	2
1000	Validating the Water Flooding Approach by Comparing It to Grand Canonical Monte Carlo Simulations. <i>Journal of Physical Chemistry B</i> , 2017, 121, 9358-9365.	1.2	13
1001	Unraveling protein folding mechanism by analyzing the hierarchy of models with increasing level of detail. <i>Journal of Chemical Physics</i> , 2017, 147, 125102.	1.2	21
1002	Protein Hydration Dynamics: Much Ado about Nothing?. <i>Journal of Physical Chemistry Letters</i> , 2017, 8, 4878-4882.	2.1	47
1003	Spatially Heterogeneous Surface Water Diffusivity around Structured Protein Surfaces at Equilibrium. <i>Journal of the American Chemical Society</i> , 2017, 139, 17890-17901.	6.6	60
1004	Ab initio theory and modeling of water. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2017, 114, 10846-10851.	3.3	340

#	ARTICLE	IF	CITATIONS
1005	X-ray absorption of liquid water by advanced <i>ab initio</i> methods. <i>Physical Review B</i> , 2017, 96, .	1.1	11
1006	Effect of a Tertiary Butyl Group on Polar Solvation Dynamics in Aqueous Solution: Femtosecond Fluorescence Spectroscopy. <i>Journal of Physical Chemistry B</i> , 2017, 121, 9631-9638.	1.2	13
1007	Low-Temperature Decoupling of Water and Protein Dynamics Measured by Neutron Scattering. <i>Journal of Physical Chemistry Letters</i> , 2017, 8, 4883-4886.	2.1	18
1008	Cell volume change through water efflux impacts cell stiffness and stem cell fate. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2017, 114, E8618-E8627.	3.3	362
1009	Dynamics of Water Monolayers Confined by Chemically Heterogeneous Surfaces: Observation of Surface-Induced Anisotropic Diffusion. <i>Journal of Physical Chemistry B</i> , 2017, 121, 9666-9675.	1.2	9
1010	Proton Network Flexibility Enables Robustness and Large Electric Fields in the Ketosteroid Isomerase Active Site. <i>Journal of Physical Chemistry B</i> , 2017, 121, 9807-9815.	1.2	34
1011	Picosecond orientational dynamics of water in living cells. <i>Nature Communications</i> , 2017, 8, 904.	5.8	57
1012	Highly compressed water structure observed in a perchlorate aqueous solution. <i>Nature Communications</i> , 2017, 8, 919.	5.8	39
1013	Sucrose modulates insulin amyloid-like fibril formation: effect on the aggregation mechanism and fibril morphology. <i>RSC Advances</i> , 2017, 7, 10487-10493.	1.7	18
1014	A First-Principles Molecular Dynamics Study of the Solvation Shell Structure, Vibrational Spectra, Polarity, and Dynamics around a Nitrate Ion in Aqueous Solution. <i>Journal of Physical Chemistry B</i> , 2017, 121, 9032-9044.	1.2	32
1015	The Hydrophobic Effect and the Role of Cosolvents. <i>Journal of Physical Chemistry B</i> , 2017, 121, 9986-9998.	1.2	87
1016	Dynamics of Hydration Water Plays a Key Role in Determining the Binding Thermodynamics of Protein Complexes. <i>Scientific Reports</i> , 2017, 7, 8744.	1.6	52
1017	Thermodynamics of Hydration Water around an Antifreeze Protein: A Molecular Simulation Study. <i>Journal of Physical Chemistry B</i> , 2017, 121, 9498-9507.	1.2	20
1018	Gliding and trudging. <i>Nature Chemistry</i> , 2017, 9, 934-936.	6.6	5
1019	Unified elucidation of the entropy-driven and -opposed hydrophobic effects. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 25891-25904.	1.3	16
1020	Addressing a Common Misconception: Ammonium Acetate as Neutral pH "Buffer" for Native Electrospray Mass Spectrometry. <i>Journal of the American Society for Mass Spectrometry</i> , 2017, 28, 1827-1835.	1.2	155
1021	Structural study of the Fox-1 RRM protein hydration reveals a role for key water molecules in RRM-RNA recognition. <i>Nucleic Acids Research</i> , 2017, 45, 8046-8063.	6.5	28
1022	Defect-Induced Wetting Behavior on Solid Polar Surfaces with Small Charge Dipole Length. <i>Journal of Physical Chemistry C</i> , 2017, 121, 17365-17370.	1.5	5

#	ARTICLE	IF	CITATIONS
1023	Toward chemical accuracy in the description of ion-water interactions through many-body representations. Alkali-water dimer potential energy surfaces. <i>Journal of Chemical Physics</i> , 2017, 147, 161715.	1.2	57
1024	Pairwise Hydrophobicity at Low Temperature: Appearance of a Stable Second Solvent-Separated Minimum with Possible Implication in Cold Denaturation. <i>Journal of Physical Chemistry B</i> , 2017, 121, 7016-7026.	1.2	18
1025	Elevation of the Energy Threshold for Isomerization of 5-Hydroxyindole-(<i>tert</i> -butyl) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 662 Td (1.1	2
1026	Electron-transfer chain in respiratory complex I. <i>Scientific Reports</i> , 2017, 7, 5495.	1.6	36
1027	Mechanism of translational jump of a hydrophobic solute in supercooled water: Importance of presolvation. <i>Chemical Physics Letters</i> , 2017, 685, 322-327.	1.2	12
1028	Signatures of Solvation Thermodynamics in Spectra of Intermolecular Vibrations. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 4467-4481.	2.3	52
1029	General Principles and Strategies for Salting-Out Informed by the Hofmeister Series. <i>Organic Process Research and Development</i> , 2017, 21, 1355-1370.	1.3	307
1030	Coarse-Grained Model of the Dynamics of Electrolyte Solutions. <i>Journal of Physical Chemistry B</i> , 2017, 121, 8195-8202.	1.2	49
1031	Crowders and Cosolvents Major Contributors to the Cellular Milieu and Efficient Means to Counteract Environmental Stresses. <i>ChemPhysChem</i> , 2017, 18, 2951-2972.	1.0	82
1032	Genuine antiplasticizing effect of water on a glass-former drug. <i>Scientific Reports</i> , 2017, 7, 7470.	1.6	17
1033	Deciphering environment effects in peptide bond solvation dynamics by experiment and theory. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 22564-22572.	1.3	11
1034	Homology Modeling and Molecular Dynamics Simulation Combined with X-ray Solution Scattering Defining Protein Structures of Thromboxane and Prostacyclin Synthases. <i>Journal of Physical Chemistry B</i> , 2017, 121, 11229-11240.	1.2	7
1035	Structural water as an essential comonomer in supramolecular polymerization. <i>Science Advances</i> , 2017, 3, eaao0900.	4.7	139
1036	Improved Solution-State Properties of Monoclonal Antibodies by Targeted Mutations. <i>Journal of Physical Chemistry B</i> , 2017, 121, 10818-10827.	1.2	25
1037	Influences of lone-pair electrons on directionality of hydrogen bonds formed by hydrophilic amino acid side chains in molecular dynamics simulation. <i>Scientific Reports</i> , 2017, 7, 15859.	1.6	18
1038	Soft X-ray Absorption Spectroscopy of Liquids and Solutions. <i>Chemical Reviews</i> , 2017, 117, 13909-13934.	23.0	103
1039	Orientational order and dynamics of interfacial water near a hexagonal boron-nitride sheet: An <i>ab initio</i> molecular dynamics study. <i>Journal of Chemical Physics</i> , 2017, 147, 164704.	1.2	13
1040	An Ålceberg Coating Preserves Bulk Hydration Dynamics in Aqueous PEG Solutions. <i>Journal of Physical Chemistry B</i> , 2017, 121, 10574-10582.	1.2	27

#	ARTICLE	IF	CITATIONS
1041	Asymmetric nanoparticle may go "active" at room temperature. <i>Science China: Physics, Mechanics and Astronomy</i> , 2017, 60, 1.	2.0	1
1042	Distinct Protein Hydration Water Species Defined by Spatially Resolved Spectra of Intermolecular Vibrations. <i>Journal of Physical Chemistry B</i> , 2017, 121, 7431-7442.	1.2	30
1043	Preservation of nucleic acids by freeze-drying for next generation sequencing analyses of soil microbial communities. <i>Journal of Plant Ecology</i> , 2017, 10, 81-90.	1.2	36
1044	Controlling supramolecular polymerization through multicomponent self-assembly. <i>Journal of Polymer Science Part A</i> , 2017, 55, 34-78.	2.5	117
1045	The opposite effects of sodium and potassium cations on water dynamics. <i>Chemical Science</i> , 2017, 8, 1429-1435.	3.7	39
1046	A combined treatment of hydration and dynamical effects for the modeling of host-guest binding thermodynamics: the SAMPL5 blinded challenge. <i>Journal of Computer-Aided Molecular Design</i> , 2017, 31, 29-44.	1.3	18
1047	Description of Hydration Water in Protein (Green Fluorescent Protein) Solution. <i>Journal of the American Chemical Society</i> , 2017, 139, 1098-1105.	6.6	68
1048	Cell biothermodynamics. <i>Journal of Thermal Analysis and Calorimetry</i> , 2017, 127, 525-534.	2.0	0
1049	Supramolecular Aggregation of Tetrameric and Homododecameric Water Clusters in a 1D Cobalt(II) Coordination Polymer Containing 1,2,4,5-Benzenetetracarboxylate. <i>Journal of Inorganic and Organometallic Polymers and Materials</i> , 2017, 27, 105-113.	1.9	11
1050	Is fast relaxation water really a free water?. , 2017, , .		1
1051	Nanoconfined water can orient and cause long-range dipolar interactions with biomolecules. <i>Scientific Reports</i> , 2017, 7, 17852.	1.6	15
1052	Temperature-dependent vibrational spectra and structure of liquid water from classical and quantum simulations with the MB-pol potential energy function. <i>Journal of Chemical Physics</i> , 2017, 147, 244504.	1.2	87
1053	Origin of the blueshift of water molecules at interfaces of hydrophilic cyclic compounds. <i>Science Advances</i> , 2017, 3, e1701400.	4.7	22
1054	Direct Vibrational Energy Transfer in Monomeric Water Probed with Ultrafast Two Dimensional Infrared Spectroscopy. <i>Chinese Journal of Chemical Physics</i> , 2017, 30, 619-625.	0.6	8
1055	Distal Proton Shuttle Mechanism of Ribosome Catalysed Peptide Bond Formation – A Theoretical Study. <i>Molecules</i> , 2017, 22, 571.	1.7	5
1056	In Silico Studies of Small Molecule Interactions with Enzymes Reveal Aspects of Catalytic Function. <i>Catalysts</i> , 2017, 7, 212.	1.6	21
1057	Modulating Nucleation by Kosmotropes and Chaotropes: Testing the Waters. <i>Crystals</i> , 2017, 7, 302.	1.0	5
1058	Effect of Antioxidant Water on the Bioactivities of Cells. <i>International Journal of Cell Biology</i> , 2017, 2017, 1-12.	1.0	8

#	ARTICLE	IF	CITATIONS
1059	Water permeation through the internal water pathway in activated GPCR rhodopsin. PLoS ONE, 2017, 12, e0176876.	1.1	14
1060	Computational simulations of solvation force of water under different hydrophobic interactions. , 2017, , .		0
1061	Solvation Effects in Supramolecular Chemistry. , 2017, , 11-60.		10
1062	Water desorption from a confined biopolymer. Soft Matter, 2018, 14, 2163-2169.	1.2	10
1063	The Molecular Origin of Enthalpy/Entropy Compensation in Biomolecular Recognition. Annual Review of Biophysics, 2018, 47, 223-250.	4.5	130
1064	Interstitial Water Enhances Sliding Friction. Langmuir, 2018, 34, 4084-4094.	1.6	13
1065	Selective Binding of Folic Acid and Derivatives by Imprinted Nanoparticle Receptors in Water. Bioconjugate Chemistry, 2018, 29, 1438-1445.	1.8	14
1066	Unusual Influence of Fluorinated Anions on the Stretching Vibrations of Liquid Water. Journal of Physical Chemistry B, 2018, 122, 3141-3152.	1.2	8
1067	Thermal analysis of ice and glass transitions in insects that do and do not survive freezing. Journal of Experimental Biology, 2018, 221, .	0.8	22
1068	Mechanism of ionic-liquid-based acidic aqueous biphasic system formation. Physical Chemistry Chemical Physics, 2018, 20, 9838-9846.	1.3	26
1069	The Important Roles of Water in Protein Folding: an Approach by Single Molecule Force Spectroscopy. Chinese Journal of Polymer Science (English Edition), 2018, 36, 379-384.	2.0	8
1070	Evaluation of Proteinâ€™Ligand Docking by Cyscore. Methods in Molecular Biology, 2018, 1762, 233-243.	0.4	3
1071	Real-space analysis of radiation-induced specific changes with independent component analysis. Journal of Synchrotron Radiation, 2018, 25, 451-467.	1.0	8
1072	Evidence for the Role of Intracellular Water Lifetime as a Tumour Biomarker Obtained by Inâ€™Vivo Fieldâ€™Cycling Relaxometry. Angewandte Chemie - International Edition, 2018, 57, 7468-7472.	7.2	44
1073	Comparison of permutationally invariant polynomials, neural networks, and Gaussian approximation potentials in representing water interactions through many-body expansions. Journal of Chemical Physics, 2018, 148, 241725.	1.2	142
1074	Heterogeneous structure and solvation dynamics of DME/water binary mixtures: A combined spectroscopic and simulation investigation. Chemical Physics Letters, 2018, 700, 50-56.	1.2	9
1075	Water mediated dielectric polarizability and electron charge transport properties of high resistance natural fibers. Scientific Reports, 2018, 8, 2726.	1.6	6
1076	Water Lone Pair Delocalization in Classical and Quantum Descriptions of the Hydration of Model Ions. Journal of Physical Chemistry B, 2018, 122, 3519-3527.	1.2	27

#	ARTICLE	IF	CITATIONS
1077	Learning about Biomolecular Solvation from Water in Protein Crystals. <i>Journal of Physical Chemistry B</i> , 2018, 122, 2475-2486.	1.2	15
1078	Substrate Channeling of Prostaglandin H ₂ on the Stereochemical Control of a Cascade Cyclization Route. <i>ACS Catalysis</i> , 2018, 8, 2534-2545.	5.5	5
1079	Water at surfaces with tunable surface chemistries. <i>Journal of Physics Condensed Matter</i> , 2018, 30, 113001.	0.7	18
1080	Evolution of Vesicular Self-Assemblies of the Salts of a Natural Triterpenoid Arjunolic Acid into Superstructured Ambidextrous Gels and Study of Their Entrapment Properties. <i>ChemistrySelect</i> , 2018, 3, 951-957.	0.7	7
1081	Nuclear quantum effects on the vibrational dynamics of liquid water. <i>Journal of Chemical Physics</i> , 2018, 148, 102328.	1.2	27
1082	Detection of Anomalous Dynamics for a Single Water Molecule. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 1177-1185.	2.3	0
1083	Microhydration of PAH ⁺ cations: evolution of hydration network in naphthalene ⁺ -(H ₂ O) _n clusters (<i>n</i> = 5). <i>Chemical Science</i> , 2018, 9, 2301-2318.	3.7	35
1084	Gas solubilities in liquid water near the temperature of the density maximum, T _{max} (H ₂ O) = 277.13 K. <i>Monatshefte für Chemie</i> , 2018, 149, 219-230.	0.9	5
1085	Hydrophilic Solvation Dominates the Terahertz Fingerprint of Amino Acids in Water. <i>Journal of Physical Chemistry B</i> , 2018, 122, 1453-1459.	1.2	20
1086	Charge-tunable water transport through boron nitride nanotubes. <i>Journal of Molecular Liquids</i> , 2018, 258, 98-105.	2.3	16
1087	Ion Selectivity in Nonpolymeric Thermosensitive Systems Induced by Water-Attenuated Supramolecular Recognition. <i>Chemistry - A European Journal</i> , 2018, 24, 3854-3861.	1.7	28
1088	² H NMR Studies on Water Dynamics in Functionalized Mesoporous Silica. <i>Zeitschrift für Physikalische Chemie</i> , 2018, 232, 1041-1058.	1.4	14
1089	Lighting-up protein-ligand interactions with fluorescent PET (photoinduced electron transfer) sensor designs. <i>Chemical Communications</i> , 2018, 54, 1319-1322.	2.2	19
1090	Molecular Dynamics Investigation of the Influence of the Hydrogen Bond Networks in Ethanol/Water Mixtures on Dielectric Spectra. <i>Journal of Physical Chemistry B</i> , 2018, 122, 1505-1515.	1.2	41
1091	<i>In Aqua Veritas</i> : The Indispensable yet Mostly Ignored Role of Water in Phase Separation and Membrane-less Organelles. <i>Biochemistry</i> , 2018, 57, 2437-2451.	1.2	59
1092	Structural and Dynamical Nature of Hydration Shells of the Carbonate Ion in Water: An Ab Initio Molecular Dynamics Study. <i>Journal of Physical Chemistry B</i> , 2018, 122, 1495-1504.	1.2	34
1093	The Bend+Libration Combination Band Is an Intrinsic, Collective, and Strongly Solute-Dependent Reporter on the Hydrogen Bonding Network of Liquid Water. <i>Journal of Physical Chemistry B</i> , 2018, 122, 2587-2599.	1.2	76
1094	Exoplanet Biosignatures: A Review of Remotely Detectable Signs of Life. <i>Astrobiology</i> , 2018, 18, 663-708.	1.5	328

#	ARTICLE	IF	CITATIONS
1095	Evidence for the Role of Intracellular Water Lifetime as a Tumour Biomarker Obtained by In Vivo Field-Cycling Relaxometry. <i>Angewandte Chemie</i> , 2018, 130, 7590-7594.	1.6	4
1096	Solvent Composition Drives the Rebinding Kinetics of Nitric Oxide to Microperoxidase. <i>Scientific Reports</i> , 2018, 8, 5281.	1.6	4
1097	Structural, electronic, and dynamical properties of liquid water by <i>ab initio</i> molecular dynamics based on SCAN functional within the canonical ensemble. <i>Journal of Chemical Physics</i> , 2018, 148, 164505.	1.2	58
1098	Bio-Agency and the Possibility of Artificial Agents. <i>European Studies in Philosophy of Science</i> , 2018, , 65-93.	0.4	5
1099	Hierarchical Self-Assembly Induced by Dilution-Enhanced Hydrophobic Hydration. <i>Chemistry - A European Journal</i> , 2018, 24, 6737-6741.	1.7	3
1101	Exclusion zone water is associated with material that exhibits proton diffusion but not birefringent properties. <i>Fluid Phase Equilibria</i> , 2018, 466, 103-109.	1.4	13
1102	Properties of Hydrogen-Bonded Liquids at Interfaces. <i>Zeitschrift Fur Physikalische Chemie</i> , 2018, 232, 937-972.	1.4	16
1103	Oriented chiral water wires in artificial transmembrane channels. <i>Science Advances</i> , 2018, 4, eaao5603.	4.7	69
1104	Hydration Water Distribution around Intrinsically Disordered Proteins. <i>Journal of Physical Chemistry B</i> , 2018, 122, 4206-4218.	1.2	17
1105	Role of structural water for prediction of cation binding sites in apoproteins. <i>Journal of Biomolecular Structure and Dynamics</i> , 2018, 36, 221-232.	2.0	2
1106	Physical constraints on the likelihood of life on exoplanets. <i>International Journal of Astrobiology</i> , 2018, 17, 116-126.	0.9	40
1107	Desiccation: An environmental and food industry stress that bacteria commonly face. <i>Food Microbiology</i> , 2018, 69, 82-88.	2.1	152
1108	Effect of heavy water on the conformational stability of globular proteins. <i>Biopolymers</i> , 2018, 109, e23076.	1.2	8
1109	Patterns produced by dried droplets of protein binary mixtures suspended in water. <i>Colloids and Surfaces B: Biointerfaces</i> , 2018, 161, 103-110.	2.5	31
1110	Hydrogen bonded complexes of oxazole family: electronic structure, stability, and reactivity aspects. <i>Structural Chemistry</i> , 2018, 29, 341-357.	1.0	7
1111	Polymer hydration and stiffness at biointerfaces and related cellular processes. <i>Nanomedicine: Nanotechnology, Biology, and Medicine</i> , 2018, 14, 13-25.	1.7	21
1112	Solvation Structure and Thermodynamic Mapping (SSTMap): An Open-Source, Flexible Package for the Analysis of Water in Molecular Dynamics Trajectories. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 418-425.	2.3	40
1113	Fluorescence quenching of the <i>N</i> -methylquinolinium cation by pairs of water or alcohol molecules. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 307-316.	1.3	11

#	ARTICLE	IF	CITATIONS
1114	Signature of the hydrogen-bonded environment of liquid water in X-ray emission spectra from first-principles calculations. <i>Frontiers of Physics</i> , 2018, 13, 1.	2.4	3
1115	Methodologies for the Examination of Water in GPCRs. <i>Methods in Molecular Biology</i> , 2018, 1705, 207-232.	0.4	7
1116	Dynamical properties of water in living cells. <i>Frontiers of Physics</i> , 2018, 13, 1.	2.4	7
1117	Dynamics of Water and Ions Near DNA: Perspective from Time-Resolved Fluorescence Stokes Shift Experiments and Molecular Dynamics Simulation. <i>Reviews in Fluorescence</i> , 2018, , 231-279.	0.5	2
1118	Reviews in Fluorescence 2017. <i>Reviews in Fluorescence</i> , 2018, , .	0.5	7
1119	Impact of surface wettability on dynamics of supercooled water confined in nitrogen-doped ordered mesoporous carbon. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 28019-28025.	1.3	12
1120	Molecular features of hydration layers probed by atomic force microscopy. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 30492-30501.	1.3	14
1121	Arsenite renal apoptotic effects in chickens co-aggravated by oxidative stress and inflammatory response. <i>Metallomics</i> , 2018, 10, 1805-1813.	1.0	76
1123	Effects of nanobubbles on peptide self-assembly. <i>Nanoscale</i> , 2018, 10, 20007-20012.	2.8	11
1124	Evaluation of xylooligosaccharide production from residual hemicelluloses of dissolving pulp by acid and enzymatic hydrolysis. <i>RSC Advances</i> , 2018, 8, 35211-35217.	1.7	36
1125	Neat Waterâ€™Vapor Interface: Proton Continuum and the Nonresonant Background. <i>Journal of Physical Chemistry Letters</i> , 2018, 9, 6744-6749.	2.1	25
1126	Atomic- and Molecular-Resolution Mapping of Solidâ€™Liquid Interfaces by 3D Atomic Force Microscopy. <i>ACS Nano</i> , 2018, 12, 11785-11797.	7.3	122
1127	Wetting of the Protein Active Site Leads to Non-Marcusian Reaction Kinetics. <i>Journal of Physical Chemistry B</i> , 2018, 122, 10490-10495.	1.2	11
1128	Methane Hydrationâ€™Shell Structure and Fragility. <i>Angewandte Chemie - International Edition</i> , 2018, 57, 15133-15137.	7.2	41
1130	Dynamical disparity between hydration shell water and RNA in a hydrated RNA system. <i>Physical Review E</i> , 2018, 98, .	0.8	7
1131	Collective hydrogen-bond rearrangement dynamics in liquid water. <i>Journal of Chemical Physics</i> , 2018, 149, 244504.	1.2	22
1132	Properties of Ion Complexes and Their Impact on Charge Transport in Organic Solvent-Based Electrolyte Solutions for Lithium Batteries: Insights from a Theoretical Perspective. <i>Batteries</i> , 2018, 4, 62.	2.1	36
1133	The Role of Hydrogen Bonding in the Folding/Unfolding Process of Hydrated Lysozyme: A Review of Recent NMR and FTIR Results. <i>International Journal of Molecular Sciences</i> , 2018, 19, 3825.	1.8	49

#	ARTICLE	IF	CITATIONS
1134	Long distance electron transfer through the aqueous solution between redox partner proteins. Nature Communications, 2018, 9, 5157.	5.8	30
1135	High and low density patches in simulated liquid water. Journal of Chemical Physics, 2018, 149, 204507.	1.2	33
1136	Molecular Insights into the Unusual Structure of an Antifreeze Protein with a Hydrated Core. Journal of Physical Chemistry B, 2018, 122, 9827-9839.	1.2	15
1137	Methane on Mars and Habitability: Challenges and Responses. Astrobiology, 2018, 18, 1221-1242.	1.5	50
1138	Electron-Hole Theory of the Effect of Quantum Nuclei on the X-Ray Absorption Spectra of Liquid Water. Physical Review Letters, 2018, 121, 137401.	2.9	35
1139	Born-Oppenheimer molecular dynamics, hydrogen bond interactions and magnetic properties of liquid hydrogen cyanide. Journal of Molecular Liquids, 2018, 272, 778-786.	2.3	6
1140	Heterogeneous Solvation in Distinctive Protein-Protein Interfaces Revealed by Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2018, 122, 11695-11701.	1.2	7
1141	Dynamics of partially folded and unfolded proteins investigated with quasielastic neutron spectroscopy. AIP Conference Proceedings, 2018, , .	0.3	0
1142	Supercooling and freezing as eco-physiological alternatives rather than mutually exclusive strategies: A case study in <i>Pyrrhocoris apterus</i> . Journal of Insect Physiology, 2018, 111, 53-62.	0.9	35
1143	Cationic Hofmeister Series of Wettability Alteration in Mica-Water-Alkane Systems. Langmuir, 2018, 34, 13574-13583.	1.6	10
1144	How Molecular Crowding Differs from Macromolecular Crowding: A Femtosecond Mid-Infrared Pump-Probe Study. Journal of Physical Chemistry Letters, 2018, 9, 6584-6592.	2.1	13
1145	Communication: Inside the water wheel: Intrinsic differences between hydrated tetraphenylphosphonium and tetraphenylborate ions. Journal of Chemical Physics, 2018, 149, 171101.	1.2	11
1146	Scaling of submicrometric Turing patterns in concentrated growing systems. Physical Review E, 2018, 98, .	0.8	5
1147	Encapsulation versus Self-Aggregation toward Highly Selective Artificial K ⁺ Channels. Accounts of Chemical Research, 2018, 51, 2711-2718.	7.6	56
1148	Methane Hydration-Shell Structure and Fragility. Angewandte Chemie, 2018, 130, 15353-15357.	1.6	0
1149	Disorder in Aqueous Solutions and Peak Broadening in X-ray Photoelectron Spectroscopy. Journal of Physical Chemistry B, 2018, 122, 10600-10606.	1.2	7
1150	Response Mechanisms to Chemical and Physical Stresses in Yeast and Filamentous Fungi. , 2018, , 35-85.		3
1151	Affinity, kinetics, and pathways of anisotropic ligands binding to hydrophobic model pockets. Journal of Chemical Physics, 2018, 149, 094902.	1.2	1

#	ARTICLE	IF	CITATIONS
1152	Green Rust: The Simple Organizing "Seed" of All Life?. <i>Life</i> , 2018, 8, 35.	1.1	65
1153	Role of Polar and Nonpolar Groups in the Activity of Antifreeze Proteins: A Molecular Dynamics Simulation Study. <i>Journal of Physical Chemistry B</i> , 2018, 122, 9389-9398.	1.2	11
1154	Water: Many-Body Potential from First Principles (From the Gas to the Liquid Phase). , 2018, , 1-25.		2
1155	Intermolecular Interactions in Selected Polymer-Water Systems as Seen by Raman Spectroscopy. , 2018, , .		0
1156	Gating the electron transfer at a monocopper centre through the supramolecular coordination of water molecules within a protein chamber mimic. <i>Chemical Science</i> , 2018, 9, 8282-8290.	3.7	8
1157	FT-IR/NIR Spectroscopic Study of the Hydrogen-Bonding of CH to Water in 1-Fluoroheptane. <i>Bulletin of the Chemical Society of Japan</i> , 2018, 91, 1267-1274.	2.0	4
1158	Effect of layered water structures on the anomalous transport through nanoscale graphene channels. <i>Journal of Physics Communications</i> , 2018, 2, 085015.	0.5	12
1159	What is the role of the isolated small water pool near FeMo ω , the active site of nitrogenase?. <i>FEBS Journal</i> , 2018, 285, 2972-2986.	2.2	5
1160	Hydrophobic Collapse of Ubiquitin Generates Rapid Protein "Water Motions. <i>Biochemistry</i> , 2018, 57, 3650-3657.	1.2	14
1161	High-Precision Megahertz-to-Terahertz Dielectric Spectroscopy of Protein Collective Motions and Hydration Dynamics. <i>Journal of Physical Chemistry B</i> , 2018, 122, 6341-6350.	1.2	58
1162	Effects of Water Content of the Mixed Solvent on the Single-Molecule Mechanics of Amylose. <i>ACS Macro Letters</i> , 2018, 7, 672-676.	2.3	15
1163	Volumetric, isentropic compressibility and viscosity coefficient studies of binary solutions involving amides as a solute in aqueous and CCl ₄ solvent systems at 298.15 K. <i>Journal of Molecular Liquids</i> , 2018, 264, 223-232.	2.3	13
1164	Structure and the dynamics of nano-confined water in the vicinity of functionalized graphene. <i>Fluid Phase Equilibria</i> , 2018, 472, 160-171.	1.4	7
1165	Dynamics of water and ions around DNA: What is so special about them?. <i>Journal of Biosciences</i> , 2018, 43, 499-518.	0.5	14
1166	New Nanostructure in a Metastable Ice Phase. <i>Journal of Physical Chemistry C</i> , 2018, 122, 15729-15732.	1.5	2
1167	Water Tetramer Confinement and Photosensitive Schottky Behavior of a 2D Coordination Polymer. <i>ChemistrySelect</i> , 2018, 3, 6985-6991.	0.7	17
1168	Self-assembled phosphate-polyamine networks as biocompatible supramolecular platforms to modulate cell adhesion. <i>Biomaterials Science</i> , 2018, 6, 2230-2247.	2.6	19
1169	Water in the hydration shell of cryoprotectants and their non-cryoprotecting structural analogues as observed by Raman-MCR spectroscopy. <i>Journal of Molecular Liquids</i> , 2018, 266, 118-121.	2.3	13

#	ARTICLE	IF	CITATIONS
1170	Hierarchical lattice models of hydrogen-bond networks in water. <i>Physical Review E</i> , 2018, 97, 062113.	0.8	6
1171	Tetraalkylammonium bromide-water mixtures revisited: Isothermal compressibility and internal pressure variation in limiting concentration range at 298.15 K. <i>Journal of Chemical Thermodynamics</i> , 2018, 126, 119-125.	1.0	10
1172	Hydrophobic Hydration and the Effect of NaCl Salt in the Adsorption of Hydrocarbons and Surfactants on Clathrate Hydrates. <i>ACS Central Science</i> , 2018, 4, 820-831.	5.3	89
1173	Pillar[<i>n</i>]arenes for Construction of Artificial Transmembrane Channels. <i>Israel Journal of Chemistry</i> , 2018, 58, 1209-1218.	1.0	26
1174	Mixtures of Alcohols and Water confined in Mesoporous Silica: A Combined Solid-State NMR and Molecular Dynamics Simulation Study. <i>Journal of Physical Chemistry C</i> , 2018, 122, 19540-19550.	1.5	20
1175	Pressure increases the ice-like order of water at hydrophobic interfaces. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 21257-21261.	1.3	12
1176	A Data Science Approach to Understanding Water Networks Around Biomolecules: The Case of Tri-Alanine in Liquid Water. <i>Journal of Physical Chemistry B</i> , 2018, 122, 7895-7906.	1.2	13
1177	Computational discovery of chemically patterned surfaces that effect unique hydration water dynamics. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2018, 115, 8093-8098.	3.3	43
1178	A polarizable MARTINI model for monovalent ions in aqueous solution. <i>Journal of Chemical Physics</i> , 2018, 149, 163319.	1.2	32
1179	Tailoring the Variational Implicit Solvent Method for New Challenges: Biomolecular Recognition and Assembly. <i>Frontiers in Molecular Biosciences</i> , 2018, 5, 13.	1.6	6
1180	Water Dynamics in Polyacrylamide Hydrogels. <i>Journal of the American Chemical Society</i> , 2018, 140, 9466-9477.	6.6	53
1181	The significance of the properties of water for the working cycle of the kinesin molecular motor. <i>Journal of Chemical Physics</i> , 2018, 148, 235101.	1.2	2
1182	DL_ANALYSER Notation for Atomic Interactions (DANA): A Natural Annotation System for Molecular Interactions, Using Ethanoic Acid Liquid as a Test Case. <i>Molecules</i> , 2018, 23, 36.	1.7	12
1183	Water-Soluble Squaramide Dihydrates: N-Methylation Modulates the Occurrence of One- and Two-Dimensional Water Clusters through Hydrogen Bonding and Dipolar Interactions. <i>Crystal Growth and Design</i> , 2018, 18, 4420-4427.	1.4	7
1184	Effects of ethanol on the secondary structure specific hydration properties of Chymotrypsin Inhibitor 2 in its folded and unfolded forms. <i>Molecular Simulation</i> , 2018, 44, 1278-1290.	0.9	2
1185	Human Topopoisons From Weeds : A Review. <i>Current Traditional Medicine</i> , 2018, 4, 4-15.	0.1	2
1186	Microsolvated complexes of ibuprofen as revealed by high-resolution rotational spectroscopy. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 15635-15640.	1.3	9
1187	Quantum mechanical effects in zwitterionic amino acids: The case of proline, hydroxyproline, and alanine in water. <i>Journal of Chemical Physics</i> , 2018, 148, 222826.	1.2	9

#	ARTICLE	IF	CITATIONS
1188	Polypentagonal ice-like water networks emerge solely in an activity-improved variant of ice-binding protein. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2018, 115, 5456-5461.	3.3	32
1189	Unveiling the structure of a novel artificial heme enzyme with peroxidase-like activity: A theoretical investigation. <i>Biopolymers</i> , 2018, 109, e23225.	1.2	14
1190	Interfacial Water Dynamics. , 2018, , 443-461.		1
1191	Structuring of Organic Solvents at Solid Interfaces and Ramifications for Antimalarial Adsorption on β -Hematin Crystals. <i>ACS Applied Materials & Interfaces</i> , 2018, 10, 29288-29298.	4.0	6
1192	Understanding the microscopic origin behind heterogeneous properties of water confined in and around α -tubulin protofilaments. <i>Journal of Chemical Physics</i> , 2018, 149, 065101.	1.2	7
1193	Universal effects of solvent species on the stabilized structure of a protein. <i>Journal of Chemical Physics</i> , 2018, 149, 045105.	1.2	22
1194	Nature of Lone-Pair Surface Bonds and Their Scaling Relations. <i>Inorganic Chemistry</i> , 2018, 57, 7222-7238.	1.9	43
1195	Unravelling the Composition-Dependent Anomalies of Pair Hydrophobicity in Water-Ethanol Binary Mixtures. <i>Journal of Physical Chemistry B</i> , 2018, 122, 6801-6809.	1.2	19
1196	Molecular Dynamics Simulations of Water, Silica, and Aqueous Mixtures in Bulk and Confinement. <i>Zeitschrift Fur Physikalische Chemie</i> , 2018, 232, 1187-1225.	1.4	28
1197	Temperature dependence of water-water and ion-water correlations in bulk water and electrolyte solutions probed by femtosecond elastic second harmonic scattering. <i>Journal of Chemical Physics</i> , 2018, 148, 222835.	1.2	16
1198	Signature of Pareto optimization in the Escherichia coli proteome. <i>Scientific Reports</i> , 2018, 8, 9141.	1.6	8
1199	Femtosecond Hydration Map of Intrinsically Disordered α -Synuclein. <i>Biophysical Journal</i> , 2018, 114, 2540-2551.	0.2	32
1200	Mimic catechins to develop selective MMP-2 inhibitors. <i>Monatshefte Für Chemie</i> , 2018, 149, 1293-1300.	0.9	3
1201	Effect of Hydrotropic Compounds on the Self-Organization and Solubilization Properties of Cationic Surfactants. <i>Russian Journal of Physical Chemistry A</i> , 2018, 92, 1400-1405.	0.1	6
1202	Dynamic features of water molecules in superconcentrated aqueous electrolytes. <i>Scientific Reports</i> , 2018, 8, 9347.	1.6	20
1203	Self-Assembly of Functional Discrete Three-Dimensional Architectures in Water. <i>Angewandte Chemie - International Edition</i> , 2019, 58, 1280-1307.	7.2	48
1204	Protein-Water Ice Contact Angle. <i>Langmuir</i> , 2019, 35, 7383-7387.	1.6	15
1205	Role of hydration water in the onset of protein structural dynamics. <i>Journal of Physics Condensed Matter</i> , 2019, 31, 463002.	0.7	32

#	ARTICLE	IF	CITATIONS
1206	Temperature dependent anomalous fluctuations in water: shift of $\rho^{\text{H}_2\text{O}}$ between experiment and classical force field simulations. <i>Molecular Physics</i> , 2019, 117, 3232-3240.	0.8	7
1207	Microhydration Structures of Protonated Oxazole. <i>Journal of Physical Chemistry A</i> , 2019, 123, 7637-7650.	1.1	10
1208	Phase, Structure, and Dynamics of the Hydration Layer Probed by Atomic Force Microscopy. <i>Journal of Physical Chemistry C</i> , 2019, 123, 21528-21537.	1.5	8
1209	Ion-Specific Effects on Hydrogen Bond Network at a Submicropore Confined Liquid-Vacuum Interface: An <i>in Situ</i> Liquid ToF-SIMS Study. <i>Journal of Physical Chemistry Letters</i> , 2019, 10, 4935-4941.	2.1	11
1210	The Role of Water Homeostasis in Muscle Function and Frailty: A Review. <i>Nutrients</i> , 2019, 11, 1857.	1.7	87
1211	Role of Water for Life. <i>Molecular Frontiers Journal</i> , 2019, 03, 3-19.	0.9	1
1212	Mixture Composition Effect on Hydrocarbon-Water Transport in Shale Organic Nanochannels. <i>Journal of Physical Chemistry Letters</i> , 2019, 10, 4291-4296.	2.1	50
1213	Hierarchical self-assembly, spongy architecture, liquid crystalline behaviour and phase diagram of Laponite nanoplatelets in alcohol-water binary solvents. <i>Journal of Colloid and Interface Science</i> , 2019, 554, 731-742.	5.0	5
1214	Imaging an isolated water molecule using a single electron wave packet. <i>Journal of Chemical Physics</i> , 2019, 151, 024306.	1.2	16
1215	Does hydrated glycine act as solidification nucleus at multi-kilobar conditions?. <i>Biophysical Chemistry</i> , 2019, 253, 106215.	1.5	3
1216	Glassy dynamics of water at interface with biomolecules: A Mode Coupling Theory test. <i>Science China: Physics, Mechanics and Astronomy</i> , 2019, 62, 1.	2.0	10
1217	Structure and wettability of heterogeneous monomolecular films of phospholipids with cholesterol or lauryl gallate. <i>Applied Surface Science</i> , 2019, 493, 1021-1031.	3.1	4
1218	Adenosine Triphosphate Templated Self-Assembly of Cationic Porphyrin into Chiral Double Superhelices and Enzyme-Mediated Disassembly. <i>Journal of the American Chemical Society</i> , 2019, 141, 12610-12618.	6.6	64
1219	Solid-State Biology and Seed Longevity: A Mechanical Analysis of Classes in Pea and Soybean Embryonic Axes. <i>Frontiers in Plant Science</i> , 2019, 10, 920.	1.7	26
1220	Aquaphotomics—From Innovative Knowledge to Integrative Platform in Science and Technology. <i>Molecules</i> , 2019, 24, 2742.	1.7	87
1221	Analysis of hydration water around human serum albumin using near-infrared spectroscopy. <i>International Journal of Biological Macromolecules</i> , 2019, 138, 927-932.	3.6	16
1222	Odd-even effects on hydration of natural polyelectrolyte multilayers: An <i>in situ</i> synchrotron FTIR microspectroscopy study. <i>Journal of Colloid and Interface Science</i> , 2019, 553, 720-733.	5.0	14
1223	On the coupling of protein and water dynamics in confinement: Spatially resolved molecular dynamics simulation studies. <i>Journal of Chemical Physics</i> , 2019, 150, 245101.	1.2	7

#	ARTICLE	IF	CITATIONS
1224	Chemokine Receptor Crystal Structures: What Can Be Learned from Them?. <i>Molecular Pharmacology</i> , 2019, 96, 765-777.	1.0	25
1225	Structural and dynamical heterogeneities at glutamine-water interfaces. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 16083-16094.	1.3	4
1226	Deep Molecular Orbital Driven High-Temperature Hydrogen Tautomerization Switching. <i>Journal of Physical Chemistry Letters</i> , 2019, 10, 6755-6761.	2.1	12
1227	Unconventional Complex Coacervation between Neutral Polymer and Inorganic Polyoxometalate in Aqueous Solution via Direct Water Mediation. <i>Macromolecules</i> , 2019, 52, 8275-8284.	2.2	18
1228	Optical mapping of biological water in single live cells by stimulated Raman excited fluorescence microscopy. <i>Nature Communications</i> , 2019, 10, 4764.	5.8	35
1229	Confined Dynamics of Water in Transmembrane Pore of TRPV1 Ion Channel. <i>International Journal of Molecular Sciences</i> , 2019, 20, 4285.	1.8	4
1230	Collective Transformation of Water between Hyperactive Antifreeze Proteins: RiAFPs. <i>Crystals</i> , 2019, 9, 188.	1.0	5
1231	Origin of Slow Solvation Dynamics in DNA: DAPI in Minor Groove of Dickerson-Drew DNA. <i>Journal of Physical Chemistry B</i> , 2019, 123, 10202-10216.	1.2	15
1232	Interaction of H ₂ + molecular beam with thin layer graphene foils*. <i>Chinese Physics B</i> , 2019, 28, 093401.	0.7	2
1233	Crystallization of Anhydrous Proton from Acidic Aqueous Solution with Diamide Building Block. <i>Crystal Growth and Design</i> , 2019, 19, 6048-6052.	1.4	6
1234	Mixtures of m-fluoroaniline with apolar aromatic molecules: Phase behaviour, suppression of H-bonded clusters, and local H-bond relaxation dynamics. <i>Journal of Molecular Liquids</i> , 2019, 296, 111998.	2.3	7
1235	Modification of Enzyme Activity by Vibrational Strong Coupling of Water. <i>Angewandte Chemie</i> , 2019, 131, 15468-15472.	1.6	21
1236	Isotope and Hydrogen-Bond Effects on the Self-Assembly of Macroions in Dilute Solution. <i>Chemistry - A European Journal</i> , 2019, 25, 16288-16293.	1.7	7
1237	Catalytic-Type Excited-State N-H Proton-Transfer Reaction in 7-Aminoquinoline and Its Derivatives. <i>Chemistry - A European Journal</i> , 2019, 25, 14972-14982.	1.7	13
1238	Biotechnological Processes. , 2019, , 511-549.		0
1239	Spontaneously Forming Dendritic Voids in Liquid Water Can Host Small Polymers. <i>Journal of Physical Chemistry Letters</i> , 2019, 10, 5585-5591.	2.1	21
1241	Modification of Enzyme Activity by Vibrational Strong Coupling of Water. <i>Angewandte Chemie - International Edition</i> , 2019, 58, 15324-15328.	7.2	126
1242	Ab Initio Molecular Dynamics Investigation of the Electronic and Structural Stability of Anionic O ₂ ⁻ (H ₂ O) _n , $n = 1-16$ Clusters. <i>Journal of Physical Chemistry A</i> , 2019, 123, 7528-7535.	1.1	3

#	ARTICLE	IF	CITATIONS
1243	Hydrogenic Stretch Spectroscopy of Glycineâ€“Water Complexes: Anharmonic Ab Initio Classical Separable Potential Calculations. <i>Journal of Physical Chemistry A</i> , 2019, 123, 8377-8384.	1.1	0
1244	DMSO hydration redefined: Unraveling the hydrophobic hydration of solutes with a mixed hydrophilicâ€“hydrophobic characteristic. <i>Journal of Molecular Liquids</i> , 2019, 294, 111661.	2.3	17
1245	Noncovalent Aqua Materials Based on Perylene Diimides. <i>Accounts of Chemical Research</i> , 2019, 52, 2634-2646.	7.6	53
1246	Ultrafast photoelectron spectroscopy of aqueous solutions. <i>Journal of Chemical Physics</i> , 2019, 151, 090901.	1.2	28
1247	Hierarchically oriented organization in supramolecular peptide crystals. <i>Nature Reviews Chemistry</i> , 2019, 3, 567-588.	13.8	326
1248	Role of Displacing Confined Solvent in the Conformational Equilibrium of β -Cyclodextrin. <i>Journal of Physical Chemistry B</i> , 2019, 123, 8378-8386.	1.2	6
1249	Polymorphism with Conformational Isomerism and Incomplete Crystallization in Solid Ethanolamine. <i>Crystal Growth and Design</i> , 2019, 19, 6360-6369.	1.4	2
1250	Inclusion of enclosed hydration effects in the binding free energy estimation of dopamine D3 receptor complexes. <i>PLoS ONE</i> , 2019, 14, e0222902.	1.1	9
1251	Enzyme-Inspired Synthetic Proton Relays Generate Fast and Acid-Stable Cobalt-Based H_2 Production Electrocatalysts. <i>ACS Catalysis</i> , 2019, 9, 10115-10125.	5.5	41
1252	Decoding signatures of structure, bulk thermodynamics, and solvation in three-body angle distributions of rigid water models. <i>Journal of Chemical Physics</i> , 2019, 151, 094501.	1.2	16
1253	Water follows polar and nonpolar protein surface domains. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2019, 116, 19274-19281.	3.3	66
1254	Supramolecular membranes: A robust platform to develop separation strategies towards water-based applications. <i>Separation and Purification Technology</i> , 2019, 215, 441-453.	3.9	20
1255	The complete conformational panorama of formamideâ€“water complexes: the role of water as a conformational switch. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 2177-2185.	1.3	18
1256	Anionic effects on the structure and dynamics of water in superconcentrated aqueous electrolytes. <i>RSC Advances</i> , 2019, 9, 609-619.	1.7	28
1257	Functional Hydration Behavior: Interrelation between Hydration and Molecular Properties at Lipid Membrane Interfaces. <i>Journal of Chemistry</i> , 2019, 2019, 1-15.	0.9	20
1258	Toward theoretical terahertz spectroscopy of glassy aqueous solutions: partially frozen soluteâ€“solvent couplings of glycine in water. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 4975-4987.	1.3	8
1259	Hydration-Shell Vibrational Spectroscopy. <i>Journal of the American Chemical Society</i> , 2019, 141, 10569-10580.	6.6	60
1260	Pressure Effects on Protein Hydration Water Thermodynamics. <i>Journal of Physical Chemistry B</i> , 2019, 123, 6014-6022.	1.2	8

#	ARTICLE	IF	CITATIONS
1261	Single-Molecule Studies Reveal That Water Is a Special Solvent for Amylose and Natural Cellulose. <i>Macromolecules</i> , 2019, 52, 5006-5013.	2.2	18
1262	In Vivo Water Dynamics in <i>Shewanella oneidensis</i> Bacteria at High Pressure. <i>Scientific Reports</i> , 2019, 9, 8716.	1.6	13
1263	Hydration dynamics of proteins in reverse micelles probed by ¹ H-NOESY/ ¹ H-ROESY NMR and ¹⁷ O-nuclear quadrupole resonance (NQR). <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 14571-14582.	1.3	4
1264	Heterodyne-detected sum frequency generation of water at surfaces with varying hydrophobicity. <i>Journal of Chemical Physics</i> , 2019, 150, 204708.	1.2	23
1265	A beetle antifreeze protein protects lactate dehydrogenase under freeze-thawing. <i>International Journal of Biological Macromolecules</i> , 2019, 136, 1153-1160.	3.6	6
1266	Acyclic Janus-AT Nucleoside Host Channels Precisely Lock Water into Single-File Wires with Local Rotational Flexibility. <i>Angewandte Chemie</i> , 2019, 131, 9703-9712.	1.6	0
1267	The purported square ice in bilayer graphene is a nanoscale, monolayer object. <i>Journal of Chemical Physics</i> , 2019, 150, 231101.	1.2	7
1268	The structure and hydrogen-bond behaviours of binary systems containing ionic liquid 1-butyl-3-methylimidazolium tetrafluoroborate and methanol/ethanol. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2019, 223, 117312.	2.0	16
1269	A study of the hydrogen bonds effect on the water density and the liquid-liquid transition. <i>Science China: Physics, Mechanics and Astronomy</i> , 2019, 62, 1.	2.0	5
1270	How do ribozymes accommodate additional water molecules upon hydrostatic compression deep into the kilobar pressure regime?. <i>Biophysical Chemistry</i> , 2019, 252, 106192.	1.5	6
1271	The onset of the tetrabonded structure in liquid water. <i>Science China: Physics, Mechanics and Astronomy</i> , 2019, 62, 1.	2.0	12
1272	Characterization of Hydration Properties in Structural Ensembles of Biomolecules. <i>Journal of Chemical Information and Modeling</i> , 2019, 59, 3316-3329.	2.5	4
1273	Alcohols as Latent Hydrophobes: Entropically Driven Uptake of 1,2-Diol Functionalized Ligands by a Porous Capsule in Water. <i>Journal of the American Chemical Society</i> , 2019, 141, 9170-9174.	6.6	12
1274	<i>Colloquium</i> : Physical constraints for the evolution of life on exoplanets. <i>Reviews of Modern Physics</i> , 2019, 91, .	16.4	39
1275	Dynamics of proteins in solution. <i>Quarterly Reviews of Biophysics</i> , 2019, 52, .	2.4	78
1276	Formation of a Supramolecular Polymeric Adhesive via Water-Participant Hydrogen Bond Formation. <i>Journal of the American Chemical Society</i> , 2019, 141, 8058-8063.	6.6	101
1277	A general study of actinyl hydration by molecular dynamics simulations using <i>ab initio</i> force fields. <i>Journal of Chemical Physics</i> , 2019, 150, 104504.	1.2	13
1278	Acyclic Janus-AT Nucleoside Host Channels Precisely Lock Water into Single-File Wires with Local Rotational Flexibility. <i>Angewandte Chemie - International Edition</i> , 2019, 58, 9601-9610.	7.2	4

#	ARTICLE	IF	CITATIONS
1279	Enthalpic contributions to solvent-solute and solvent-ion interactions: Electronic perturbation as key to the understanding of molecular attraction. <i>Journal of Chemical Physics</i> , 2019, 150, 174112.	1.2	23
1280	Spatially resolved structure and dynamics of the hydration shell of pyridine in sub- and supercritical water. <i>Journal of Molecular Liquids</i> , 2019, 287, 110881.	2.3	3
1281	Hydration and ion association of aqueous choline chloride and chlorocholine chloride. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 10970-10980.	1.3	24
1282	Why Proteins are Big: Length Scale Effects on Equilibria and Kinetics. <i>Protein Journal</i> , 2019, 38, 95-119.	0.7	7
1283	Oxidative stress resistance during dehydration of three non-Saccharomyces wine yeast strains. <i>Food Research International</i> , 2019, 123, 364-372.	2.9	15
1284	Atomic-Level Viscosity Distribution in the Hydration Layer. <i>Physical Review Letters</i> , 2019, 122, 116001.	2.9	23
1285	Protein Solvent Shell Structure Provides Rapid Analysis of Hydration Dynamics. <i>Journal of Chemical Information and Modeling</i> , 2019, 59, 2407-2422.	2.5	14
1286	A hypothesis concerning callose. <i>Plant Signaling and Behavior</i> , 2019, 14, 1548878.	1.2	4
1287	Slow dynamics of hydration water and the trehalose dynamical transition. <i>Journal of Molecular Liquids</i> , 2019, 282, 617-625.	2.3	17
1288	Heterogeneity of water structure and dynamics at the protein-water interface. <i>Journal of Chemical Physics</i> , 2019, 150, 094701.	1.2	36
1289	Label-free, quantitative and sensitive detection of nanoparticle/membrane interactions through the optical response of water. <i>Sensors and Actuators B: Chemical</i> , 2019, 289, 169-174.	4.0	5
1290	Assembly of peptides in mica-graphene nanocapillaries controlled by confined water. <i>Nanoscale</i> , 2019, 11, 8210-8218.	2.8	6
1291	Water molecular structure underpins extreme desiccation tolerance of the resurrection plant <i>Haberlea rhodopensis</i> . <i>Scientific Reports</i> , 2019, 9, 3049.	1.6	56
1292	Water Dynamics in the Hydration Shell of Amphiphilic Macromolecules. <i>Journal of Physical Chemistry B</i> , 2019, 123, 2971-2977.	1.2	10
1293	Mechanisms of phase separation in temperature-responsive acidic aqueous biphasic systems. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 7462-7473.	1.3	23
1294	Probing the Solute-Solvent Interaction of an Azo-Bonded Prodrug in Neat and Binary Media: Combined Experimental and Computational Study. <i>Scientific Reports</i> , 2019, 9, 3023.	1.6	8
1295	Correlation between the hydration of acyl chains and phosphate groups in lipid bilayers: Effect of phase state, head group, chain length, double bonds and carbonyl groups. <i>Biochimica Et Biophysica Acta - Biomembranes</i> , 2019, 1861, 1197-1203.	1.4	12
1296	The Kohn-Sham electronic density of states of liquid HCN: Tuning a long-range corrected exchange-correlation functional for predicting electron binding energies. <i>Chemical Physics Letters</i> , 2019, 724, 96-102.	1.2	6

#	ARTICLE	IF	CITATIONS
1297	Characterization of Intra/Extracellular Water States Probed by Ultrabroadband Multiplex Coherent Anti-Stokes Raman Scattering (CARS) Spectroscopic Imaging. <i>Journal of Physical Chemistry A</i> , 2019, 123, 3928-3934.	1.1	19
1298	Elastic compliance as a tool to understand Hofmeister ion specific effect in DMPC liposomes. <i>Biophysical Chemistry</i> , 2019, 249, 106148.	1.5	1
1299	Studies of the Effect of Urea on PEG-4000 Polymerâ€™Water Interactions at 298.15 K. <i>Journal of Chemical & Engineering Data</i> , 2019, 64, 2341-2349.	1.0	3
1300	Selbstorganisation von funktionellen diskreten dreidimensionalen Architekturen in Wasser. <i>Angewandte Chemie</i> , 2019, 131, 1292-1320.	1.6	12
1301	Thick Two-Dimensional Water Film Confined between the Atomically Thin Mica Nanosheet and Hydrophilic Substrate. <i>Langmuir</i> , 2019, 35, 5130-5139.	1.6	4
1302	Water models for interfacial water simulations. <i>Science China Technological Sciences</i> , 2019, 62, 729-735.	2.0	2
1303	Water Trapping of Metalâ€™Organic Cages with Endohedral Variation. <i>Crystal Growth and Design</i> , 2019, 19, 2862-2868.	1.4	6
1304	Exploring the enhancement of electron tunneling induced by intermolecular interactions on surface of self-assembled monolayer. <i>Journal of Electroanalytical Chemistry</i> , 2019, 837, 143-150.	1.9	6
1305	<i>N</i> -Methylacetamide Aqueous Solutions: A Neutron Diffraction Study. <i>Journal of Physical Chemistry B</i> , 2019, 123, 1808-1814.	1.2	11
1306	Hyperosmotic stress induces cell-dependent aggregation of Î±-synuclein. <i>Scientific Reports</i> , 2019, 9, 2288.	1.6	10
1307	Mechanism of Solvent Control of Protein Dynamics. <i>Physical Review Letters</i> , 2019, 122, 058101.	2.9	35
1308	Ab initio molecular dynamics investigation on NaCl solution at diluted concentration. <i>Computational and Theoretical Chemistry</i> , 2019, 1153, 25-33.	1.1	3
1309	Encoding biological recognition in a bicomponent cell-membrane mimic. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2019, 116, 5376-5382.	3.3	51
1310	Reorientation of Deeply Cooled Water in Mesoporous Silica: NMR Studies of the Pore-Size Dependence. <i>Journal of Physical Chemistry B</i> , 2019, 123, 2123-2134.	1.2	40
1311	Water in Confinement between Nanowalls: Results for Hexagonal Boron Nitride versus Graphene Sheets from Ab Initio Molecular Dynamics. <i>Journal of Physical Chemistry C</i> , 2019, 123, 6130-6140.	1.5	15
1312	Thermophoresis of biological and biocompatible compounds in aqueous solution. <i>Journal of Physics Condensed Matter</i> , 2019, 31, 503003.	0.7	46
1313	Ordered-to-Disordered Transformation of Enhanced Water Structure on Hydrophobic Surfaces in Concentrated Alcoholâ€™Water Solutions. <i>Journal of Physical Chemistry Letters</i> , 2019, 10, 7922-7928.	2.1	21
1314	Intracluster proton transfer in protonated benzonitrileâ€™(H ₂ O) ₆ nanoclusters: hydrated hydronium core for <i>n</i> â‰¥ 2. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 25226-25246.	1.3	14

#	ARTICLE	IF	CITATIONS
1315	Proof of concept web application for understanding the energetic basis of oligonucleotide unfolding. <i>RSC Advances</i> , 2019, 9, 41453-41461.	1.7	0
1316	Counterion Effect on Vibrational Relaxation and the Rotational Dynamics of Interfacial Water and an Anionic Vibrational Probe in the Confined Reverse Micelles Environment. <i>Journal of Physical Chemistry Letters</i> , 2019, 10, 176-182.	2.1	18
1317	Structural Relaxation Processes and Collective Dynamics of Water in Biomolecular Environments. <i>Journal of Physical Chemistry B</i> , 2019, 123, 480-486.	1.2	14
1318	Effect of truncating electrostatic interactions on predicting thermodynamic properties of water-methanol systems. <i>Molecular Simulation</i> , 2019, 45, 336-350.	0.9	17
1319	Theoretical Insights on Nonlinear Response Theory of Fluorescence Spectroscopy in Liquids. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 471-476.	2.3	2
1320	Bidirectional water transport through non-straight carbon nanotubes. <i>Journal of Molecular Liquids</i> , 2019, 276, 39-46.	2.3	21
1321	Encyclopedia of Food Chemistry: Water. , 2019, , 297-304.		1
1322	An Apparent Binary Choice in Biochemistry: Mutual Reactivity Implies Life Chooses Thiols or Nitrogen-Sulfur Bonds, but Not Both. <i>Astrobiology</i> , 2019, 19, 579-613.	1.5	9
1323	Affinity Improvement of a Cancer-Targeted Antibody through Alanine-Induced Adjustment of Antigen-Antibody Interface. <i>Structure</i> , 2019, 27, 519-527.e5.	1.6	31
1324	Factors Promoting the Formation of Clathrate-Like Ordering of Water in Biomolecular Structure at Ambient Temperature and Pressure. <i>Journal of Physical Chemistry B</i> , 2019, 123, 811-824.	1.2	18
1325	Volumetric properties of the water-tetramethylurea mixture over the temperature range from 274.15 to 333.15 K at atmospheric pressure. <i>Journal of Molecular Liquids</i> , 2019, 278, 279-289.	2.3	13
1326	Unveiling the Hydrogen Bonding Network of Intracellular Water by Fluorescence Lifetime Imaging Microscopy. <i>Journal of Physical Chemistry C</i> , 2019, 123, 2673-2677.	1.5	16
1327	Dissecting water binding sites at protein-protein interfaces: a lesson from the atomic structures in the Protein Data Bank. <i>Journal of Biomolecular Structure and Dynamics</i> , 2019, 37, 1204-1219.	2.0	6
1328	Subsurface exolife. <i>International Journal of Astrobiology</i> , 2019, 18, 112-141.	0.9	33
1329	Synthesis, molecular modeling, and pharmacological evaluation of new 2-substituted benzoxazole derivatives as potent anti-inflammatory agents. <i>Structural Chemistry</i> , 2020, 31, 263-273.	1.0	15
1330	ReaxFF molecular dynamics simulations on the structure and dynamics of electrolyte water systems at ambient temperature. <i>Computational Materials Science</i> , 2020, 172, 109349.	1.4	21
1331	Kinetically controlled morphology in copolymer-based hydrogels crosslinked by crystalline nanodomains determines efficacy of ice inhibition. <i>Molecular Systems Design and Engineering</i> , 2020, 5, 645-655.	1.7	6
1332	Oxygen-oxygen distances in protein-bound crystallographic water suggest the presence of protonated clusters. <i>Biochimica Et Biophysica Acta - General Subjects</i> , 2020, 1864, 129480.	1.1	3

#	ARTICLE	IF	CITATIONS
1333	Characterizing biotransformation products and pathways of the flame retardant triphenyl phosphate in <i>Daphnia magna</i> using non-target screening. <i>Science of the Total Environment</i> , 2020, 708, 135106.	3.9	18
1334	Molecular dynamics in cells: A neutron view. <i>Biochimica Et Biophysica Acta - General Subjects</i> , 2020, 1864, 129475.	1.1	14
1335	The proteinâ€™s water nuclear Overhauser effect (NOE) as an indirect microscope for molecular surface mapping of interaction patterns. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 212-222.	1.3	6
1336	A crucial incorrect understanding in the traditional solution theory. <i>Journal of Molecular Liquids</i> , 2020, 301, 112379.	2.3	3
1337	Computational Investigations of the Chemical Mechanism of the Enzyme Nitrogenase. <i>ChemBioChem</i> , 2020, 21, 1671-1709.	1.3	36
1338	Water-Mediated Heterogeneously Catalyzed Reactions. <i>ACS Catalysis</i> , 2020, 10, 1294-1309.	5.5	156
1340	Negligible Effect on the Structure and Vibrational Spectral Dynamics of Water Molecules Near Hydrophobic Solutes. <i>ChemistrySelect</i> , 2020, 5, 11549-11559.	0.7	0
1341	Confinement Effects on Glass-Forming Aqueous Dimethyl Sulfoxide Solutions. <i>Molecules</i> , 2020, 25, 4127.	1.7	6
1342	Hydration Water Structure, Hydration Forces, and Mechanical Properties of Polysaccharide Films. <i>Biomacromolecules</i> , 2020, 21, 4871-4877.	2.6	10
1343	Dynamic behaviors of interfacial water on the self-assembly monolayer (SAM) heterogeneous surface. <i>Journal of Chemical Physics</i> , 2020, 153, 124705.	1.2	3
1344	The hydrophobic effect: is water afraid, or just not that interested?. <i>ChemTexts</i> , 2020, 6, 1.	1.0	9
1345	Transition-state theory-based analysis of diffusion of water in yeast cells. <i>FEMS Microbiology Letters</i> , 2020, 367, .	0.7	0
1346	First principles molecular dynamics investigation on the water-ion interaction: A case of diluted CsI solution. <i>Chemical Physics Letters</i> , 2020, 760, 137996.	1.2	2
1347	Spatial localization of charged molecules by salt ions in oil-confined water microdroplets. <i>Science Advances</i> , 2020, 6, .	4.7	29
1348	Fast increase of nanofluidic slip in supercooled water: the key role of dynamics. <i>Nanoscale</i> , 2020, 12, 20396-20403.	2.8	20
1349	Hydrophobic dewetting in gating and regulation of transmembrane protein ion channels. <i>Journal of Chemical Physics</i> , 2020, 153, 110901.	1.2	22
1350	A minimum quantum chemistry CCSD(T)/CBS dataset of dimeric interaction energies for small organic functional groups. <i>Journal of Chemical Physics</i> , 2020, 153, 154301.	1.2	6
1351	Quantifying how step-wise fluorination tunes local solute hydrophobicity, hydration shell thermodynamics and the quantum mechanical contributions of soluteâ€™s water interactions. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 22997-23008.	1.3	4

#	ARTICLE	IF	CITATIONS
1352	Decoupling between the translation and rotation of water in the proximity of a protein molecule. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 18132-18140.	1.3	16
1353	Influence of surface hydrophilicity and hydration on the rotational relaxation of supercooled water on graphene oxide surfaces. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 16080-16095.	1.3	6
1354	Cycloaddition reactions in water. , 2020, , 61-114.		1
1355	Chemical Synthesis of an Erythropoietin Glycoform Having a Triantennary <i>N</i> -Glycan: Significant Change of Biological Activity of Glycoprotein by Addition of a Small Molecular Weight Trisaccharide. <i>Journal of the American Chemical Society</i> , 2020, 142, 20671-20679.	6.6	33
1356	Three-Dimensional Molecular Mapping of Ionic Liquids at Electrified Interfaces. <i>ACS Nano</i> , 2020, 14, 17515-17523.	7.3	47
1357	Anomalous dynamics of water at the octopeptide lanreotide surface. <i>RSC Advances</i> , 2020, 10, 33903-33910.	1.7	0
1358	Long-Range Ordered Water Correlations between A/T/C/G Nucleotides. <i>Matter</i> , 2020, 3, 794-804.	5.0	8
1359	Solute-Solvent Interactions in Modern Physical Organic Chemistry: Supramolecular Polymers as a Muse. <i>Journal of the American Chemical Society</i> , 2020, 142, 19781-19798.	6.6	101
1360	Natural-abundance ¹⁷ O NMR spectroscopy of magnetically aligned lipid nanodiscs. <i>Chemical Communications</i> , 2020, 56, 9998-10001.	2.2	10
1361	Application of Synchrotron Radiation X-ray Scattering and Spectroscopy to Soft Matter. <i>Polymers</i> , 2020, 12, 1624.	2.0	14
1362	Exclusion Zone Phenomena in Water—A Critical Review of Experimental Findings and Theories. <i>International Journal of Molecular Sciences</i> , 2020, 21, 5041.	1.8	27
1363	Self-Assembly at Water Nanodroplet Interfaces Quantified with Nonlinear Light Scattering. <i>Langmuir</i> , 2020, 36, 9317-9322.	1.6	13
1364	Dielectric ordering of water molecules arranged in a dipolar lattice. <i>Nature Communications</i> , 2020, 11, 3927.	5.8	33
1365	How the presence of ATP affect caffeine hydration and self-aggregation?. <i>Journal of Molecular Liquids</i> , 2020, 318, 113885.	2.3	10
1366	Infrared signatures of isomer selectivity and symmetry breaking in the Cs+(H ₂ O) ₃ complex using many-body potential energy functions. <i>Journal of Chemical Physics</i> , 2020, 153, 044306.	1.2	15
1367	Experimental tests for a liquid-liquid critical point in water. <i>Science China: Physics, Mechanics and Astronomy</i> , 2020, 63, 1.	2.0	11
1368	Anomalous sub-diffusion of water in biosystems: From hydrated protein powders to concentrated protein solution to living cells. <i>Structural Dynamics</i> , 2020, 7, 054703.	0.9	8
1369	Study of self-interaction errors in density functional predictions of dipole polarizabilities and ionization energies of water clusters using Perdew-Zunger and locally scaled self-interaction corrected methods. <i>Journal of Chemical Physics</i> , 2020, 153, 164304.	1.2	21

#	ARTICLE	IF	CITATIONS
1370	The Dynamism of Intrinsically Disordered Proteins: Binding-Induced Folding, Amyloid Formation, and Phase Separation. <i>Journal of Physical Chemistry B</i> , 2020, 124, 11541-11560.	1.2	31
1371	An organic monolithic capillary column functionalized with human serum albumin and its application for the nano μ chromatography study of its binding with universal cancer peptides and its impact on immunogenicity. <i>Journal of Liquid Chromatography and Related Technologies</i> , 2020, 43, 777-783.	0.5	5
1372	The Effects of Dissolved Hydrophobic and Hydrophilic Groups on Water Structure. <i>Journal of Solution Chemistry</i> , 2020, 49, 1473-1484.	0.6	14
1373	Reorientation-induced relaxation of free OH at the air/water interface revealed by ultrafast heterodyne-detected nonlinear spectroscopy. <i>Nature Communications</i> , 2020, 11, 5344.	5.8	27
1374	Attraction between Permanent Dipoles and London Dispersion Forces Dominate the Thermodynamics of Organic Crystallization. <i>Crystal Growth and Design</i> , 2020, 20, 7429-7438.	1.4	7
1375	Isotope effects in x-ray absorption spectra of liquid water. <i>Physical Review B</i> , 2020, 102, .	1.1	6
1376	Towards molecular movies with X-ray photon correlation spectroscopy. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 19443-19453.	1.3	26
1377	Soft Dynamic Confinement of Membrane Proteins by Dehydrated Trehalose Matrices: High-Field EPR and Fast-Laser Studies. <i>Applied Magnetic Resonance</i> , 2020, 51, 773-850.	0.6	15
1378	On the Correlation between Pair Hydrophobicity and Mixing Enthalpies in Water-Alcohol Binary Mixtures. <i>Journal of Physical Chemistry B</i> , 2020, 124, 8023-8031.	1.2	7
1379	What Came First: The Helix or the H ₂ O?. <i>Matter</i> , 2020, 3, 608-610.	5.0	0
1380	Nuclear Magnetic Resonance and Broadband Dielectric Spectroscopy Studies on the Dynamics of Ethylene Glycol in Mesoporous Silica. <i>Journal of Physical Chemistry C</i> , 2020, 124, 20998-21012.	1.5	12
1381	The Bending Mode of Water: A Powerful Probe for Hydrogen Bond Structure of Aqueous Systems. <i>Journal of Physical Chemistry Letters</i> , 2020, 11, 8459-8469.	2.1	175
1382	Intrinsic Contributions of $2\text{-}\mu\text{-Hydroxyl}$ to the Hydration of Nucleosides at the Monomeric Level. <i>Chemistry - A European Journal</i> , 2020, 26, 17046-17055.	1.7	2
1383	Hydration Shell Changes in Surfactant Aggregate Transitions Revealed by Raman-MCR Spectroscopy. <i>Journal of Physical Chemistry Letters</i> , 2020, 11, 7429-7437.	2.1	9
1384	Molecular Mechanism of Acceleration and Retardation of Collective Orientation Relaxation of Water Molecules in Aqueous Solutions. <i>Journal of Physical Chemistry B</i> , 2020, 124, 11730-11737.	1.2	3
1385	Glucose-water interactions at increasing concentrations and temperatures as revealed by Near-Infrared Spectroscopy. <i>IOP Conference Series: Materials Science and Engineering</i> , 2020, 959, 012003.	0.3	1
1386	Hidden Isolated OH at the Charged Hydrophobic Interface Revealed by Two-Dimensional Heterodyne-Detected VSFG Spectroscopy. <i>Angewandte Chemie</i> , 2020, 132, 9585-9592.	1.6	1
1387	An Ice-Binding Protein from an Antarctic Ascomycete Is Fine-Tuned to Bind to Specific Water Molecules Located in the Ice Prism Planes. <i>Biomolecules</i> , 2020, 10, 759.	1.8	8

#	ARTICLE	IF	CITATIONS
1388	Occurrence and stability of lone pair- π and OH- π interactions between water and nucleobases in functional RNAs. <i>Nucleic Acids Research</i> , 2020, 48, 5825-5838.	6.5	27
1389	Oil-in-water transport in clay-hosted nanopores: Effects of electrostatic forces. <i>AIChE Journal</i> , 2020, 66, e16276.	1.8	18
1390	Interaction of Water at the Hydrophobic Interface of Alkyl Group of Alcohol with p-Nitro-Aniline Charge Transfer State. <i>ChemistrySelect</i> , 2020, 5, 3655-3660.	0.7	2
1391	First-passage fingerprints of water diffusion near glutamine surfaces. <i>Soft Matter</i> , 2020, 16, 9202-9216.	1.2	8
1392	A Novel Tool for Visualization of Water Molecular Structure and Its Changes, Expressed on the Scale of Temperature Influence. <i>Molecules</i> , 2020, 25, 2234.	1.7	8
1393	Does the degree of substitution on the cyclodextrin hosts impact their affinity towards guest binding?. <i>Photochemical and Photobiological Sciences</i> , 2020, 19, 956-965.	1.6	11
1394	Influence of crowding on hydrophobic hydration-shell structure. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 11724-11730.	1.3	13
1396	Mapping solvation heterogeneity in live cells by hyperspectral stimulated Raman scattering microscopy. <i>Journal of Chemical Physics</i> , 2020, 152, 174201.	1.2	14
1397	Origin of Ubiquitous Stripes at the Graphite-Water Interface. <i>Langmuir</i> , 2020, 36, 7789-7794.	1.6	14
1398	Microhydration of protonated biomolecular building blocks: protonated pyrimidine. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 13092-13107.	1.3	7
1399	Oxygen K-shell spectroscopy of isolated progressively solvated peptide. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 12909-12917.	1.3	9
1400	Hydrogen bond-induced responses in mid- and far-infrared spectra of interfacial water at phospholipid bilayers. <i>Fluid Phase Equilibria</i> , 2020, 518, 112626.	1.4	4
1401	BioSentinel: Long-Term <i>Saccharomyces cerevisiae</i> Preservation for a Deep Space Biosensor Mission. <i>Astrobiology</i> , 2023, 23, 617-630.	1.5	23
1402	Complexation of a cationic pyrene derivative with sulfobutylether substituted β -cyclodextrin: Towards a stimulus-responsive supramolecular material. <i>Journal of Molecular Liquids</i> , 2020, 305, 112840.	2.3	12
1403	Water envelope has a critical impact on the design of protein-protein interaction inhibitors. <i>Chemical Communications</i> , 2020, 56, 4360-4363.	2.2	7
1404	Hidden Isolated OH at the Charged Hydrophobic Interface Revealed by Two-Dimensional Heterodyne-Detected VSFG Spectroscopy. <i>Angewandte Chemie - International Edition</i> , 2020, 59, 9498-9505.	7.2	11
1405	Solvent dynamics play a decisive role in the complex formation of biologically relevant redox proteins. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 7451-7459.	1.3	10
1406	On the stability and necessary electrophoretic mobility of bare oil nanodroplets in water. <i>Journal of Chemical Physics</i> , 2020, 152, 241104.	1.2	18

#	ARTICLE	IF	CITATIONS
1407	Volume and compressibility changes on mixing solutions of alkali halides/sodium acetate with sodium salt of butyric acid at 298.15ÅK: Understanding like charge ionic (anionâ€“anion) interactions in water. Journal of Molecular Liquids, 2020, 315, 113654.	2.3	5
1408	Lipid Bilayer-Modified Nanofluidic Channels of Sizes with Hundreds of Nanometers for Characterization of Confined Water and Molecular/Ion Transport. Journal of Physical Chemistry Letters, 2020, 11, 5756-5762.	2.1	10
1409	On the microscopic origins of relaxation processes in aqueous peptide solutions undergoing a glass transition. Journal of Chemical Physics, 2020, 152, 234503.	1.2	9
1410	Mobility of water and of protein atoms at the protein-water interface, monitored by anisotropic atomic displacement parameters, are largely uncorrelated. Amino Acids, 2020, 52, 435-443.	1.2	2
1411	Hydrogen Bond Dynamics in the Solvation Shell on Proton Transfer in Aqueous Solution. Journal of Physical Chemistry B, 2020, 124, 1817-1823.	1.2	9
1412	Insight into the Liquid Structure of Water and Sodium Chloride Solutions Using Stimulated Raman Scattering. Physical Review Applied, 2020, 13, .	1.5	2
1413	Distinctive behavior and two-dimensional vibrational dynamics of water molecules inside glycine solvation shell. RSC Advances, 2020, 10, 6658-6670.	1.7	12
1414	Response Theory for Static and Dynamic Solvation of Ionic and Dipolar Solutes in Water. Journal of Statistical Physics, 2020, 180, 721-738.	0.5	6
1415	Changes in cellular structure of heatâ€“treated Salmonella in lowâ€“moisture environments. Journal of Applied Microbiology, 2020, 129, 434-442.	1.4	8
1416	Volumetric studies of solvation of carboxylic acids in aqueous, carbon tetrachloride, methanolic and methanolic-urea binary solutions at 298.15ÅK. Journal of Molecular Liquids, 2020, 304, 112658.	2.3	0
1417	Slow dynamics of supercooled hydration water in contact with lysozyme: examining the cage effect at different length scales. Philosophical Magazine, 2020, 100, 2582-2595.	0.7	6
1418	Hydrogenâ€“Bond Free Energy of Local Biological Water. Angewandte Chemie, 2020, 132, 7155-7162.	1.6	3
1419	Hydrogenâ€“Bond Free Energy of Local Biological Water. Angewandte Chemie - International Edition, 2020, 59, 7089-7096.	7.2	4
1420	Protonation of Naphthaleneâ€“ (Water) Nanoclusters: Intracuster Proton Transfer to Hydration Shell Revealed by Infrared Photodissociation Spectroscopy. Journal of Physical Chemistry A, 2020, 124, 1134-1151.	1.1	20
1421	Mechanical Unfolding of Spectrin Repeats Induces Water-Molecule Ordering. Biophysical Journal, 2020, 118, 1076-1089.	0.2	3
1422	Why do water molecules around small hydrophobic solutes form stronger hydrogen bonds than in the bulk?. Biochimica Et Biophysica Acta - General Subjects, 2020, 1864, 129537.	1.1	13
1423	The nuclear Overhauser Effect (NOE) as a tool to study macromolecular confinement: Elucidation and disentangling of crowding and encapsulation effects. Journal of Chemical Physics, 2020, 152, 024120.	1.2	1
1424	Underwater adhesion of mussel foot protein on a graphite surface. Applied Surface Science, 2020, 511, 145589.	3.1	7

#	ARTICLE	IF	CITATIONS
1425	Characterizing the Physical Properties and Cell Compatibility of Phytoglycogen Extracted from Different Sweet Corn Varieties. <i>Molecules</i> , 2020, 25, 637.	1.7	9
1426	Eu ³⁺ luminescent ions detect water density anomaly. <i>Journal of Luminescence</i> , 2020, 223, 117263.	1.5	2
1427	Microbial lag phase can be indicative of, or independent from, cellular stress. <i>Scientific Reports</i> , 2020, 10, 5948.	1.6	59
1428	Tumbling with a limp: local asymmetry in water's hydrogen bond network and its consequences. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 10397-10411.	1.3	5
1429	Computational Insights into Molecular Activation and Positive Cooperative Mechanisms of FFAR1 Modulators. <i>Journal of Chemical Information and Modeling</i> , 2020, 60, 3214-3230.	2.5	9
1430	Mass Spectrometry-Based Protein Footprinting for Higher-Order Structure Analysis: Fundamentals and Applications. <i>Chemical Reviews</i> , 2020, 120, 4355-4454.	23.0	149
1431	Dimension-Controlled Dewetting in Hydrophobic Porous Nanocapsules. <i>Journal of Physical Chemistry C</i> , 2020, 124, 10201-10208.	1.5	3
1432	Effect of Cholesterol on the Structure of Networked Water at the Surface of a Model Lipid Membrane. <i>Journal of Physical Chemistry B</i> , 2020, 124, 3686-3694.	1.2	8
1433	Silicon Forms a Rich Diversity of Aliphatic Polyol Complexes in Aqueous Solution. <i>Journal of the American Chemical Society</i> , 2020, 142, 9188-9202.	6.6	5
1434	An introduction to cryo-FIB/SEM cross-sectioning of frozen, hydrated Life Science samples. <i>Journal of Microscopy</i> , 2021, 281, 138-156.	0.8	30
1435	The role of water in ligand binding. <i>Current Opinion in Structural Biology</i> , 2021, 67, 1-8.	2.6	30
1436	Supramolecular Depolymerization in the Mixture of Two Poor Solvents: Mechanistic Insights and Modulation of Supramolecular Polymerization of Ionic π - π Systems. <i>Angewandte Chemie</i> , 2021, 133, 5519-5526.	1.6	8
1437	Supramolecular Depolymerization in the Mixture of Two Poor Solvents: Mechanistic Insights and Modulation of Supramolecular Polymerization of Ionic π - π Systems. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 5459-5466.	7.2	19
1438	Moisture Content of Bacterial Cells Determines Thermal Resistance of <i>Salmonella enterica</i> Serotype Enteritidis PT 30. <i>Applied and Environmental Microbiology</i> , 2021, 87, .	1.4	22
1439	Hydration and dynamics of γ -glutamate ion in aqueous solution. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 1590-1600.	1.3	14
1440	Volumetric properties (water+1,3-dimethylurea) mixture over the temperature range from 274.15 to 333.15 K at the ambient pressure – comparison with other methyl substituted analogues. <i>Journal of Molecular Liquids</i> , 2021, 323, 114637.	2.3	3
1441	Self-Assembly of Photoresponsive Molecular Amphiphiles in Aqueous Media. <i>Angewandte Chemie</i> , 2021, 133, 11708-11731.	1.6	18
1442	Enhancing water sampling of buried binding sites using nonequilibrium candidate Monte Carlo. <i>Journal of Computer-Aided Molecular Design</i> , 2021, 35, 167-177.	1.3	22

#	ARTICLE	IF	CITATIONS
1443	Artificial Water Channels: Towards Biomimetic Membranes for Desalination. <i>Chemistry - A European Journal</i> , 2021, 27, 2224-2239.	1.7	39
1444	Self-Assembly of Photoresponsive Molecular Amphiphiles in Aqueous Media. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 11604-11627.	7.2	81
1445	Breakdown of the Stokes-Einstein relation in supercooled water: the jump-diffusion perspective. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 19964-19986.	1.3	16
1446	Study on the relationship between hydrogen bond network dynamics of water and its terahertz spectrum. <i>Wuli Xuebao/Acta Physica Sinica</i> , 2021, .	0.2	7
1447	Water-Mediated Interactions Determine Helix Formation of Peptides in Open Nanotubes. <i>Journal of Physical Chemistry B</i> , 2021, 125, 817-824.	1.2	1
1448	Water in Livestock – Biological Role and Global Perspective on Water Demand and Supply Chains. <i>Biologically-inspired Systems</i> , 2021, , 315-331.	0.4	0
1449	The transition from salt-in-water to water-in-salt nanostructures in water solutions of organic ionic liquids relevant for biological applications. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 944-959.	1.3	19
1450	Dynamics in supramolecular nanomaterials. <i>Soft Matter</i> , 2021, 17, 5850-5863.	1.2	9
1451	The important role of non-covalent interactions for the vibrational circular dichroism of lactic acid in aqueous solution. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 17232-17241.	1.3	15
1452	Deciphering the evolution of supramolecular nanofibers in solution and solid-state: a combined microscopic and spectroscopic approach. <i>Chemical Science</i> , 2021, 12, 5874-5882.	3.7	25
1453	Development of Time-Resolved Heterodyne-Detected Vibrational Sum Frequency Generation Spectroscopy and Its Application to Interfacial Dynamics. <i>Molecular Science</i> , 2021, 15, A0116.	0.2	1
1454	Characterizing Hydropathy of Amino Acid Side Chain in a Protein Environment by Investigating the Structural Changes of Water Molecules Network. <i>Frontiers in Molecular Biosciences</i> , 2021, 8, 626837.	1.6	25
1455	Structural and dynamical fingerprints of the anomalous dielectric properties of water under confinement. <i>Physical Review Materials</i> , 2021, 5, .	0.9	10
1456	The melibiose-derived glycation product mimics a unique epitope present in human and animal tissues. <i>Scientific Reports</i> , 2021, 11, 2940.	1.6	15
1457	Microhydration of ionized building blocks of DNA/RNA: infrared spectra of pyrimidine ⁺ clusters. <i>European Physical Journal D</i> , 2021, 75, 1.	0.6	1
1458	² H NMR study on temperature-dependent water dynamics in amino-acid functionalized silica nanopores. <i>Journal of Chemical Physics</i> , 2021, 154, 114702.	1.2	4
1459	Thermal inactivation scaling applied for SARS-CoV-2. <i>Biophysical Journal</i> , 2021, 120, 1054-1059.	0.2	5
1460	Rotational dynamics of proteins in nanochannels: role of solvent's local viscosity. <i>Nanotechnology</i> , 2021, 32, 225102.	1.3	1

#	ARTICLE	IF	CITATIONS
1461	Insignificant Effect of Temperature on the Structure and Angular Jumps of Water near a Hydrophobic Cation. ACS Omega, 2021, 6, 8356-8364.	1.6	2
1462	Evaluation of biological activities, structural and conformational properties of bovine beta- and alpha-trypsin isoforms in aqueous-organic media. International Journal of Biological Macromolecules, 2021, 176, 291-303.	3.6	1
1463	Adenosine triphosphate energy independently controls protein homeostasis with unique structure and diverse mechanisms. Protein Science, 2021, 30, 1277-1293.	3.1	38
1464	Characterization of the Features of Water Inside the SecY Translocon. Journal of Membrane Biology, 2021, 254, 133-139.	1.0	2
1466	Confined hydration in nanometer-graded plasma polymer films: Insights from surface-enhanced infrared absorption spectroscopy. Surfaces and Interfaces, 2021, 23, 100922.	1.5	10
1467	Probing Biological Water Using Terahertz Absorption Spectroscopy. , 0, , .		0
1468	Ion effects on the extraction of cesium (I) by 1,3-Diisopropoxycalix [4] arene-crown-6(BPC6) and the highly efficient extraction under neutral conditions. Solvent Extraction and Ion Exchange, 2022, 40, 333-348.	0.8	2
1469	Effects of the Wettability of a Probing Tip on the Hydration Layer Imaged in Atomic Force Microscopy. Journal of Physical Chemistry C, 2021, 125, 11197-11205.	1.5	2
1470	Stepwise Microhydration of Isoxazole: Infrared Spectroscopy of Isoxazole-(Water) _n Clusters in Helium Nanodroplets. Journal of Physical Chemistry A, 2021, 125, 4766-4774.	1.1	3
1471	Ab initio molecular dynamics study on energy relaxation path of hydrogen-bonded OH vibration in bulk water. Journal of Chemical Physics, 2021, 154, 204502.	1.2	5
1472	Two Liquid-Liquid Phase Transitions in Confined Water Nanofilms. Journal of Physical Chemistry Letters, 2021, 12, 4786-4792.	2.1	4
1473	Detection of Water Molecules on the Radical Transfer Pathway of Ribonucleotide Reductase by ¹⁷ O Electron Nuclear Double Resonance Spectroscopy. Journal of the American Chemical Society, 2021, 143, 7237-7241.	6.6	18
1474	The influence of cations on the dipole moments of neighboring polar molecules. International Journal of Quantum Chemistry, 2022, 122, e26758.	1.0	5
1475	Abnormal Properties of Low-Dimensional Confined Water. Small, 2021, 17, e2100788.	5.2	28
1476	Structural and dynamical heterogeneity of water trapped inside Na ⁺ -pumping KR2 rhodopsin in the dark state. Journal of Chemical Physics, 2021, 154, 215101.	1.2	2
1477	Community evolution and frequent subgraph patterns affect the thermostability of B. subtilis lipase A. Food Bioscience, 2021, 41, 100984.	2.0	0
1478	Nonspecific Binding—Fundamental Concepts and Consequences for Biosensing Applications. Chemical Reviews, 2021, 121, 8095-8160.	23.0	113
1480	Local Mutations Can Serve as a Game Changer for Global Protein Solvent Interaction. JACS, 2021, 1, 1076-1085.	3.6	14

#	ARTICLE	IF	CITATIONS
1481	Soil and plant health in relation to dynamic sustainment of Eh and pH homeostasis: A review. <i>Plant and Soil</i> , 2021, 466, 391-447.	1.8	22
1482	Does the release of hydration water come with a Gibbs energy contribution?. <i>Journal of Chemical Thermodynamics</i> , 2021, 158, 106409.	1.0	7
1483	Solvent Relaxation NMR: A Tool for Real-Time Monitoring Water Dynamics in Protein Aggregation Landscape. <i>ACS Chemical Neuroscience</i> , 2021, 12, 2903-2916.	1.7	8
1484	Understanding the Effects of Water Molecules on Cyclohexanol Dehydration over Zeolitic Acid Sites. <i>Journal of Physical Chemistry C</i> , 2021, 125, 15283-15291.	1.5	5
1485	Directional nature of hydrophobic interactions: Implications for the mechanism of molecular recognition. <i>Chemical Physics</i> , 2021, 547, 111200.	0.9	8
1486	Temperature, Pressure, and Length-Scale Dependence of Solvation in Water-like Solvents. II. Large Solvophobic Solute. <i>Journal of Physical Chemistry B</i> , 2021, 125, 8175-8184.	1.2	2
1487	Hydrophilic and Hydrophobic Effects on the Structure and Thermodynamic Properties of Confined Water: Water in Solutions. <i>International Journal of Molecular Sciences</i> , 2021, 22, 7547.	1.8	7
1488	“Whole Organism”™, Systems Biology, and Top-Down Criteria for Evaluating Scenarios for the Origin of Life. <i>Life</i> , 2021, 11, 690.	1.1	13
1489	Effect of an electric field on dewetting transition of nitrogen-water system. <i>Chinese Physics B</i> , 2022, 31, 036801.	0.7	2
1490	Vibrational Spectroscopy of Benzonitrile“(Water) ₁₋₂ Clusters in Helium Droplets. <i>Journal of Physical Chemistry A</i> , 2021, 125, 6954-6963.	1.1	4
1491	Machine learning implicit solvation for molecular dynamics. <i>Journal of Chemical Physics</i> , 2021, 155, 084101.	1.2	35
1492	The Water Polymorphism and the Liquid“Liquid Transition from Transport Data. <i>Physchem</i> , 2021, 1, 202-214.	0.5	4
1493	Toward the understanding of water-in-salt electrolytes: Individual ion activities and liquid junction potentials in highly concentrated aqueous solutions. <i>Journal of Chemical Physics</i> , 2021, 155, 064701.	1.2	15
1494	How polar hydroxyl groups affect surface hydrophobicity on model talc surfaces. <i>Communications in Theoretical Physics</i> , 2021, 73, 115501.	1.1	4
1495	The Structural and Dynamical Properties of the Hydration of SNase Based on a Molecular Dynamics Simulation. <i>Molecules</i> , 2021, 26, 5403.	1.7	6
1496	Influence of drying conditions, food composition, and water activity on the thermal resistance of <i>Salmonella enterica</i> . <i>Food Research International</i> , 2021, 147, 110548.	2.9	18
1497	Rapid changes of miRNAs-20, -30, 410, 515, 134, and 183 and telomerase with psychological activity: A one year study on the relaxation response and epistemological considerations. <i>Journal of Traditional and Complementary Medicine</i> , 2021, 11, 409-418.	1.5	6
1498	Solvent effects on catalytic reactions and related phenomena at liquid-solid interfaces. <i>Surface Science Reports</i> , 2021, 76, 100541.	3.8	31

#	ARTICLE	IF	CITATIONS
1499	Energy relaxation dynamics of hydrogen-bonded OH vibration conjugated with free OH bond at an air/water interface. <i>Journal of Chemical Physics</i> , 2021, 155, 154703.	1.2	4
1500	The shape of water in zeolites and its impact on epoxidation catalysis. <i>Nature Catalysis</i> , 2021, 4, 797-808.	16.1	66
1501	Solute-induced changes in the water H-bond network of different alcohol-aqueous systems. <i>Journal of Molecular Liquids</i> , 2021, 341, 117349.	2.3	7
1502	The role of S and Mo doping on the dissociation of water molecule on FeOCl surface: Experimental and theoretical analysis. <i>Chemical Engineering Journal</i> , 2021, 426, 131353.	6.6	16
1503	Water mapping: Analysis of binding site spaces to enhance binding. , 2021, , 179-201.		0
1504	Investigating states of gas in water encapsulated between graphene layers. <i>Chemical Science</i> , 2021, 12, 2635-2645.	3.7	7
1505	Unravelling the microhydration frameworks of prototype PAH by infrared spectroscopy: naphthalene ³ . <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 14016-14026.	1.3	8
1506	Effective Debye relaxation models for binary solutions of polar liquids at terahertz frequencies. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 4426-4436.	1.3	6
1507	Formation of unexpected S-H covalent bonds in H ₂ S dimers under confinement. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 5963-5968.	1.3	4
1508	Modifying conformational distribution of chiral tetrahydro-2-furoic acid through its interaction with water: a rotational spectroscopic and theoretical investigation. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 3820-3825.	1.3	8
1511	Mapping Out Protein Hydration Dynamics by Overhauser Dynamic Nuclear Polarization. <i>Biological Magnetic Resonance</i> , 2015, , 43-74.	0.4	1
1512	Targeted Nano Analysis of Water and Ions in the Nucleus Using Cryo-Correlative Microscopy. <i>Methods in Molecular Biology</i> , 2015, 1228, 145-158.	0.4	4
1513	Accounting for Solvent in Structure-Based Drug Design. <i>Methods in Molecular Biology</i> , 2012, 841, 251-266.	0.4	1
1514	Water: Many-Body Potential from First Principles (From the Gas to the Liquid Phase). , 2020, , 635-660.		10
1515	Metastable Water Under Pressure. <i>NATO Science for Peace and Security Series A: Chemistry and Biology</i> , 2010, , 197-216.	0.5	4
1516	Conformational Motions of Disordered Proteins. , 2018, , 381-399.		1
1517	Explicit and Implicit Water Models for Biomolecular Simulations. , 2019, , .		1
1519	Critical Review on Gas Hydrate Formation at Solid Surfaces and in Confined Spaces—Why and How Does Interfacial Regime Matter?. <i>Energy & Fuels</i> , 2020, 34, 6751-6760.	2.5	95

#	ARTICLE	IF	CITATIONS
1520	Temperature, Pressure, and Length-Scale Dependence of Solvation in Water-like Solvents. I. Small Solvophobic Solutes. <i>Journal of Physical Chemistry B</i> , 2021, 125, 297-306.	1.2	4
1521	Dynamical Properties of <i>N</i> -Isopropylacrylamide Molecule in Water Revealed by ¹ H NMR Studies. <i>Journal of Physical Chemistry B</i> , 2016, 120, 184-192.	1.2	2
1522	Vibrational Sum Frequency Scattering in Absorptive Media: A Theoretical Case Study of Nano-objects in Water. <i>Journal of Physical Chemistry C</i> , 2020, 124, 23078-23085.	1.5	10
1523	The H ₂ O Helix: The Chiral Water Superstructure Surrounding DNA. <i>ACS Central Science</i> , 2017, 3, 683-685.	5.3	16
1524	Solvent effects on ligand binding to a serine protease. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 10753-10766.	1.3	30
1525	Effect of trehalose on protein cryoprotection: Insights into the mechanism of slowing down of hydration water. <i>Journal of Chemical Physics</i> , 2020, 153, 224503.	1.2	13
1527	Isotope effects in molecular structures and electronic properties of liquid water via deep potential molecular dynamics based on the SCAN functional. <i>Physical Review B</i> , 2020, 102, .	1.1	22
1528	Ambient conditions disordered-ordered phase transition of two-dimensional interfacial water molecules dependent on charge dipole moment. <i>Physical Review Materials</i> , 2019, 3, .	0.9	8
1529	Designing Ligands to Bind Tightly to Proteins. , 2008, , 189-215.		8
1530	Dynamics of a globular protein and its hydration water studied by neutron scattering and MD simulations. <i>Spectroscopy</i> , 2010, 24, 1-24.	0.8	23
1531	Water Reorientation and Ultrafast Infrared Spectroscopy. , 2013, , 73-98.		3
1532	FT-IR/NIR Spectroscopic Study of Interactions between Water and Alkylamines. <i>Bulletin of the Chemical Society of Japan</i> , 2019, 92, 1117-1126.	2.0	2
1533	Why do proteins aggregate? "Intrinsically insoluble proteins" and "dark mediators" revealed by studies on "insoluble proteins" solubilized in pure water. <i>F1000Research</i> , 2013, 2, 94.	0.8	40
1534	Myths in Modern Science: The Hydrogen Bond and its Surroundings Part 2. The Hydrophobic-Bond-Myth. <i>Chem-Bio Informatics Journal</i> , 2018, 18, 10-20.	0.1	2
1535	Sterilization by Cooling in Isochoric Conditions: The Case of <i>Escherichia coli</i> . <i>PLoS ONE</i> , 2015, 10, e0140882.	1.1	4
1538	Recent Advances and Applications in Synchrotron X-Ray Protein Footprinting for Protein Structure and Dynamics Elucidation. <i>Protein and Peptide Letters</i> , 2016, 23, 309-322.	0.4	6
1539	Correct Protonation States and Relevant Waters = Better Computational Simulations?. <i>Current Pharmaceutical Design</i> , 2013, 19, 4291-4309.	0.9	7
1540	Application of Computational Techniques to Unravel Structure-Function Relationship and their Role in Therapeutic Development. <i>Current Topics in Medicinal Chemistry</i> , 2018, 18, 1769-1791.	1.0	5

#	ARTICLE	IF	CITATIONS
1541	Label-free biomedical imaging of hydrodynamics in single human cells. <i>Biomedical Research</i> , 2010, 31, 177-181.	0.3	4
1542	Estimating Hydrogen Bond Energy in Integral Membrane Chromoproteins by High Hydrostatic Pressure Optical Spectroscopy. , 0, , .		2
1543	Quantitative insights into tightly and loosely bound water in hydration shells of amino acids. <i>Soft Matter</i> , 2021, 17, 10080-10089.	1.2	4
1544	Theoretical characterization of zeolite encapsulated platinum clusters in the presence of water molecules. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 23360-23371.	1.3	5
1546	Supercooled nano-droplets of water confined in hydrophobic rubber. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 25347-25355.	1.3	3
1547	Hydration of Cells and Tissues. <i>Soft and Biological Matter</i> , 2021, , 439-479.	0.3	0
1548	Physics-Based Coarse-Grained Modeling in Bio- and Nanochemistry. , 2022, , 31-69.		1
1549	Porous Matrices and Specific Features of Water in Nanostructures. <i>Physics of Wave Phenomena</i> , 2021, 29, 249-277.	0.3	8
1550	Thermally Driven Transformation of Water Clustering Structures at Self-Assembled Monolayers. <i>Langmuir</i> , 2021, 37, 11493-11498.	1.6	2
1551	Water Thermodynamics and Its Effects on the Protein Stability and Activity. <i>Biophysica</i> , 2021, 1, 413-428.	0.6	1
1552	Water in Membranes, Water in Cells. , 2010, , 165-177.		0
1553	Observation of Slow Relaxation on Nano-Confined Water in Nanoporous MCM-41 by Terahertz Spectroscopy. , 2011, , .		0
1554	Science of Water at Nanoscale. , 2012, , 301-311.		0
1555	The Possible Roles of Water in the Prebiotic Chemical Evolution of DNA: An Approach by Single Molecule Studies. , 2013, , 109-123.		0
1556	Reactive Dynamics in Confined Water by Reversed Micelles. <i>Lecture Notes in Nanoscale Science and Technology</i> , 2013, , 265-288.	0.4	3
1557	The Selective Alkylarenes Oxidations with Dioxygen in the Presence of Catalytical Systems. , 2013, , 1-54.		0
1560	Water on Ideal Solid Surfaces. , 2014, , 101-168.		0
1561	Interaction between Disordered Heterogeneous Charged Surfaces. , 2014, , 413-432.		0

#	ARTICLE	IF	CITATIONS
1562	Interaction between Disordered Heterogeneous Charged Surfaces. , 2014, , 393-412.		0
1563	Topology and Geometry of Protein Water Shell by Computer Modeling. , 2014, , 13-33.		0
1565	Advanced Instrumentation of Frequency Modulation AFM for Subnanometer-Scale 2D/3D Measurements at Solid-Liquid Interfaces. Nanoscience and Technology, 2015, , 435-460.	1.5	1
1566	Water, Solvent of Life. , 2015, , 2644-2647.		0
1567	Predictive and Explanatory Power of the Hybrid Model: Analysis of Various Problems. , 2015, , 247-282.		0
1568	Diversity of Hydration Water Around Proteins. Hamon, 2016, 26, 135-138.	0.0	0
1569	Interfacial water at microscopic level: from quasi-one-dimensional, two-dimensional confined space, to biomolecules surfaces and material surfaces. Wuli Xuebao/Acta Physica Sinica, 2016, 65, 186101.	0.2	4
1570	Chapter 7. Computational Characterization of Molecular Mechanisms of Membrane Transporter Function. RSC Theoretical and Computational Chemistry Series, 2016, , 197-236.	0.7	0
1572	Critical Reflections on the Hydrophobic Effect, its Origins and Manifestation: Water Structure, Chemical Reactivity, Micelles and Gels.. Journal of the Turkish Chemical Society, Section A: Chemistry, 0, , 899-914.	0.4	1
1574	Understanding of Water Molecule Dynamics in Terahertz Region and Development of Near-field Array Sensor. Oleoscience, 2018, 18, 447-453.	0.0	0
1576	The Effects of Water on Solid State Fermentation Performance. , 2019, , 151-166.		0
1577	Interactions of Heavy Ions with DNA and Radiative Aspects in Physics of Liquid Matter. Springer Proceedings in Physics, 2019, , 275-299.	0.1	0
1578	Research progress of molecular structure and dynamics of biological water. Wuli Xuebao/Acta Physica Sinica, 2019, 68, 013101.	0.2	3
1579	Using X-ray Footprinting and Mass Spectrometry to Study the Structure and Function of Membrane Proteins. Protein and Peptide Letters, 2019, 26, 44-54.	0.4	3
1581	Surface Reaction Simulation based on Divide-and-Conquer Type Density Functional Tight-Binding Molecular Dynamics (DC-DFTB-MD) Method: Case for Proton Diffusion on Pt(111) Surface. Vacuum and Surface Science, 2019, 62, 486-491.	0.0	0
1582	Hydration interactions beyond the first solvation shell in aqueous phenolate solution. Physical Chemistry Chemical Physics, 2020, 22, 19940-19947.	1.3	1
1584	What Does Time-Dependent Fluorescence Shift (TDFS) in Biomembranes (and Proteins) Report on?. Frontiers in Chemistry, 2021, 9, 738350.	1.8	11
1585	Can water molecules bind by the oxygen oxygen covalent bond? A confinement induced bonding. Computational and Theoretical Chemistry, 2021, 1206, 113493.	1.1	2

#	ARTICLE	IF	CITATIONS
1586	Protein-Protein Interaction Interfaces and their Functional Implications. RSC Drug Discovery Series, 2020, , 1-24.	0.2	17
1587	Unexpected hydrophobicity on self-assembled monolayers terminated with two hydrophilic hydroxyl groups. Nanoscale, 2021, 13, 19604-19609.	2.8	6
1588	Synergistic Effects of Hydration Sites in Protein Stability: A Theoretical Water Thermodynamics Approach. , 2020, , 187-212.		1
1589	Using Computer Simulations and Virtual Reality to Understand, Design and Optimize Artificial Water Channels. Lecture Notes in Bioengineering, 2020, , 78-99.	0.3	2
1591	Advanced craniosacral therapy a combination of Quantum theories and Einstein's relativities. Archive of Biomedical Science and Engineering, 2020, 6, 016-020.	0.3	0
1592	Less-Ordered Hydration Shell around Poly(<i>N,N</i> -diethylacrylamide) Is Insensitive to the Clouding Transition. Journal of Physical Chemistry B, 2021, 125, 12104-12109.	1.2	2
1593	Elevating density functional theory to chemical accuracy for water simulations through a density-corrected many-body formalism. Nature Communications, 2021, 12, 6359.	5.8	45
1595	Investigating hydration dynamics and protein collective motions by high-precision dielectric spectroscopy. , 2020, , .		0
1597	Electromagnetic information delivery as a new tool in translational medicine. International Journal of Clinical and Experimental Medicine, 2014, 7, 2550-6.	1.3	2
1598	Behavior of supramolecular cross-links formed by host-guest interactions in hydrogels responding to water contents. , 2022, 1, 100001.		10
1599	Structure and dynamics of nanoconfined water and aqueous solutions. European Physical Journal E, 2021, 44, 136.	0.7	38
1600	Solutions, in Particular Dilute Solutions of Nonelectrolytes: A Review. Journal of Solution Chemistry, 2022, 51, 626-710.	0.6	2
1601	Understanding Hydrophobic Effects: Insights from Water Density Fluctuations. Annual Review of Condensed Matter Physics, 2022, 13, 303-324.	5.2	28
1602	<i>Ab initio</i> molecular dynamics simulation of liquid water with fragment-based quantum mechanical approach under periodic boundary conditions. Chinese Journal of Chemical Physics, 2021, 34, 761-768.	0.6	1
1603	Structural order of water molecules around polyrotaxane including PEG, β -cyclodextrin, and β -lipoic acid linker on gold surface by molecular dynamics simulations. Physical Chemistry Chemical Physics, 2022, 24, 2176-2184.	1.3	2
1604	Behaviour of water at hydrophobic interfaces. Journal of Molecular Liquids, 2022, 348, 118433.	2.3	4
1605	Supramolecular Membranes for Liquid Separation. Chemistry in the Environment, 2021, , 232-255.	0.2	0
1606	The Current Understanding of the Properties of Liquid Water: A Possible Alternative Solution. Biophysics (Russian Federation), 2021, 66, 709-715.	0.2	1

#	ARTICLE	IF	CITATIONS
1607	Chemometrics: An Excavator in Temperature-Dependent Near-Infrared Spectroscopy. <i>Molecules</i> , 2022, 27, 452.	1.7	11
1608	Cold and freezing injury in insects: An overview of molecular mechanisms. <i>European Journal of Entomology</i> , 0, 119, 43-57.	1.2	8
1609	Advances in liquid-state NMR spectroscopy to study the structure, function, and dynamics of biomacromolecules. , 2022, , 237-266.		2
1610	Size-Dependent Order–Disorder Crossover in Hydrophobic Hydration: Comparison between Spherical Solutes and Linear Alcohols. <i>ACS Omega</i> , 2022, 7, 2671-2678.	1.6	9
1611	Human \hat{I}^3S -Crystallin Resists Unfolding Despite Extensive Chemical Modification from Exposure to Ionizing Radiation. <i>Journal of Physical Chemistry B</i> , 2022, 126, 679-690.	1.2	3
1612	Explicit solvation thermodynamics in ionic solution: extending grid inhomogeneous solvation theory to solvation free energy of salt–water mixtures. <i>Journal of Computer-Aided Molecular Design</i> , 2022, 36, 101-116.	1.3	8
1613	Effect of Humid Air Exposed to IR Radiation on Enzyme Activity. <i>International Journal of Molecular Sciences</i> , 2022, 23, 601.	1.8	1
1614	Conformational and Solvation Dynamics of an Amyloidogenic Intrinsically Disordered Domain of a Melanosomal Protein. <i>Journal of Physical Chemistry B</i> , 2022, 126, 443-452.	1.2	3
1615	Expanding dynamic framework materials into COFs through HOF approach. <i>CheM</i> , 2022, 8, 7-9.	5.8	2
1616	The Seed and the Metabolism Regulation. <i>Biology</i> , 2022, 11, 168.	1.3	26
1617	Confinement effects on glass-forming mixtures: Insights from a combined experimental approach to aqueous ethylene glycol solutions in silica pores. <i>Journal of Chemical Physics</i> , 2022, 156, 084506.	1.2	6
1618	How Far Is “Bulk Water” from Interfaces? Depends on the Nature of the Surface and What We Measure. <i>Journal of Physical Chemistry B</i> , 2022, 126, 1125-1135.	1.2	9
1619	Atomic Insight into the Interfacial Effect on the Molecular Solvation. <i>Journal of Physical Chemistry C</i> , 0, , .	1.5	1
1620	Structure of Water at Hydrophilic and Hydrophobic Interfaces: Raman Spectroscopy of Water Confined in Periodic Mesoporous (Organo)Silicas. <i>Journal of Physical Chemistry C</i> , 2022, 126, 3520-3531.	1.5	11
1621	Aqueous Self-Assembly of Hydrophobic Molecules Influenced by the Molecular Geometry. <i>Journal of Physical Chemistry B</i> , 2022, , .	1.2	1
1622	Enhancing Sampling of Water Rehydration on Ligand Binding: A Comparison of Techniques. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 1359-1381.	2.3	22
1623	Hydration Lubrication in Biomedical Applications: From Cartilage to Hydrogels. <i>Accounts of Materials Research</i> , 2022, 3, 213-223.	5.9	33
1624	Influence of Aqueous Arginine Solution on Regulating Conformational Stability and Hydration Properties of the Secondary Structural Segments of a Protein at Elevated Temperatures: A Molecular Dynamics Study. <i>Journal of Physical Chemistry B</i> , 2022, 126, 1462-1476.	1.2	3

#	ARTICLE	IF	CITATIONS
1625	Charge transfer across H ₂ O hydrogen bonds stabilizes oil droplets in water. <i>Science</i> , 2021, 374, 1366-1370.	6.0	88
1626	Dynamics of water and ions around DNA: What is so special about them?. <i>Journal of Biosciences</i> , 2018, 43, 499-518.	0.5	4
1627	Single-particle and collective excitations of polar water molecules confined in nano-pores within a cordierite crystal lattice. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 6890-6904.	1.3	8
1628	How do interfaces alter the dynamics of supercooled water?. <i>Nanoscale</i> , 2022, 14, 4254-4262.	2.8	4
1629	Resolution and characterization of confinement- and temperature-dependent dynamics in solvent phases that surround proteins in frozen aqueous solution by using spin-probe EPR spectroscopy. <i>Methods in Enzymology</i> , 2022, 666, 25-57.	0.4	4
1630	Introduction to Bacterial Anhydrobiosis: A General Perspective and the Mechanisms of Desiccation-Associated Damage. <i>Microorganisms</i> , 2022, 10, 432.	1.6	4
1631	Stochastic Ultralow-Frequency Oscillations of the Luminescence Intensity from the Surface of a Polymer Membrane Swelling in Aqueous Salt Solutions. <i>Polymers</i> , 2022, 14, 688.	2.0	3
1632	Self-consistent determination of long-range electrostatics in neural network potentials. <i>Nature Communications</i> , 2022, 13, 1572.	5.8	38
1633	Plasma-controlled surface wettability: recent advances and future applications. <i>International Materials Reviews</i> , 2023, 68, 82-119.	9.4	29
1634	Local Chiral Inversion of Thymine Dimers by Manipulating Single Water Molecules. <i>Journal of the American Chemical Society</i> , 2022, 144, 5023-5028.	6.6	13
1635	Future directions in physiochemical modeling of the thermodynamics of polyelectrolyte coacervates. <i>AIChE Journal</i> , 2022, 68, .	1.8	10
1636	Small-sized salt-tolerant denitrifying and phosphorus removal aerobic granular sludge cultivated with mariculture waste solids to treat synthetic mariculture wastewater. <i>Biochemical Engineering Journal</i> , 2022, 181, 108396.	1.8	10
1637	Coil-to-Bridge Transitions of Self-Assembled Water Chains Observed in a Nanoscopic Meniscus. <i>Langmuir</i> , 2022, 38, 4538-4546.	1.6	5
1638	Dielectric Properties of Water in Charged Nanopores. <i>Journal of Physical Chemistry B</i> , 2022, 126, 2688-2698.	1.2	14
1639	The local structure of water from combining diffraction and X-ray spectroscopy. <i>Journal of Non-Crystalline Solids: X</i> , 2022, 14, 100087.	0.5	3
1640	Water is a preservative of microbes. <i>Microbial Biotechnology</i> , 2022, 15, 191-214.	2.0	19
1642	The Orthodox Dry Seeds Are Alive: A Clear Example of Desiccation Tolerance. <i>Plants</i> , 2022, 11, 20.	1.6	22
1643	Thermodynamics of TMU-TMU interaction in water, ethylene glycol and formamide – From pair solvophobic interaction to cluster formation. <i>Journal of Molecular Liquids</i> , 2022, 358, 119185.	2.3	2

#	ARTICLE	IF	CITATIONS
1644	Surprising Rigidity of Functionally Important Water Molecules Buried in the Lipid Headgroup Region. <i>Journal of the American Chemical Society</i> , 2022, 144, 7881-7888.	6.6	12
1647	High-Dimensional Fluctuations in Liquid Water: Combining Chemical Intuition with Unsupervised Learning. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 3136-3150.	2.3	14
1648	Structural, dynamic, and hydration properties of quercetin and its aggregates in solution.. <i>Journal of Physics Condensed Matter</i> , 2022, , .	0.7	3
1649	Increase in the Intracellular Bulk Water Content in the Early Phase of Cell Death of Keratinocytes, Corneoptosis, as Revealed by 65 GHz Near-Field CMOS Dielectric Sensor. <i>Molecules</i> , 2022, 27, 2886.	1.7	3
1650	The spontaneous self-assembly of a molecular water pipe in 3D space. <i>IUCr</i> , 2022, 9, 364-369.	1.0	5
1651	Spatially Resolved Hydration Thermodynamics in Biomolecular Systems. <i>Journal of Physical Chemistry B</i> , 2022, 126, 3619-3631.	1.2	10
1652	Physical properties and biological effects of ceramic materials emitting infrared radiation for pain, muscular activity, and musculoskeletal conditions. <i>Photodermatology Photoimmunology and Photomedicine</i> , 2023, 39, 3-15.	0.7	8
1653	Intermolecular binding between bulk water and dissolved gases in earth's magnetic field. <i>PLoS ONE</i> , 2022, 17, e0267391.	1.1	0
1654	Aqueous Supramolecular Assemblies of Photocontrolled Molecular Amphiphiles. , 2022, , 267-308.		1
1655	Mechanic model of water-based boundary lubricated contact based on surface force effects. <i>Friction</i> , 2023, 11, 93-108.	3.4	2
1656	The structural order of protein hydration water. <i>Communications in Theoretical Physics</i> , 0, , .	1.1	1
1657	Gelation of highly entangled hydrophobic macromolecular fluid for ultrastrong underwater in situ fast tissue adhesion. <i>Science Advances</i> , 2022, 8, .	4.7	31
1658	Hydrogen-Bonding Interaction-Driven Catechin Assembly into Solvent-Free Supramolecular Adhesive with Antidrying and Antifreezing Properties. <i>ACS Applied Polymer Materials</i> , 2022, 4, 4319-4328.	2.0	10
1660	Photoinduced Electron Transfer in a Porphyrin-Fullerene Dyad at a Liquid Interface. <i>Journal of Physical Chemistry B</i> , 2022, 126, 4723-4730.	1.2	2
1661	A phenomenological model for interfacial water near hydrophilic polymers. <i>Journal of Physics Condensed Matter</i> , 0, , .	0.7	0
1662	Multidimensional insights into the repeated electromagnetic field stimulation and biosystems interaction in aging and age-related diseases. <i>Journal of Biomedical Science</i> , 2022, 29, .	2.6	6
1663	Solvent effects on the NMR shieldings of stacked DNA base pairs. <i>Physical Chemistry Chemical Physics</i> , 0, , .	1.3	0
1664	A temperature programmed desorption study of interactions between water and hydrophobes at cryogenic temperatures. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 16900-16907.	1.3	1

#	ARTICLE	IF	CITATIONS
1665	Gas phase acidity of water clusters. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 18236-18244.	1.3	4
1666	Polar liquids at charged interfaces: A dipolar shell theory. <i>Journal of Chemical Physics</i> , 2022, 156, .	1.2	8
1667	Investigating water/oil interfaces with opto-thermophoresis. <i>Nature Communications</i> , 2022, 13, .	5.8	8
1668	Statistical physics of inhomogeneous transport: Unification of diffusion laws and inference from first-passage statistics. <i>Physical Review E</i> , 2022, 106, .	0.8	6
1669	IR-Supported Thermogravimetric Analysis of Water in Hydrogels. <i>Frontiers in Materials</i> , 0, 9, .	1.2	5
1670	Comparative analysis of hydration layer reorientation dynamics of antifreeze protein and protein cytochrome P450. <i>Chinese Journal of Chemical Physics</i> , 2022, 35, 509-515.	0.6	0
1671	Proton diffusion and hydrolysis enzymatic reaction in 100â€‰nm scale biomimetic nanochannels. <i>Biomicrofluidics</i> , 2022, 16, 044109.	1.2	0
1672	Knowledge-based prediction of DNA hydration using hydrated dinucleotides as building blocks. <i>Acta Crystallographica Section D: Structural Biology</i> , 2022, 78, 1032-1045.	1.1	3
1673	Water as the often neglected medium at the interface between materials and biology. <i>Nature Communications</i> , 2022, 13, .	5.8	20
1674	The Role of Water Network Chemistry in Proteins: A Structural Bioinformatics Perspective in Drug Discovery and Development.. <i>Current Topics in Medicinal Chemistry</i> , 2022, 22, .	1.0	2
1675	Importance of Hydrogen Bonding in Crowded Environments: A Physical Chemistry Perspective. <i>Journal of Physical Chemistry A</i> , 2022, 126, 5881-5889.	1.1	9
1676	Using Metadynamics To Explore the Free Energy of Dewetting in Biologically Relevant Nanopores. <i>Journal of Physical Chemistry B</i> , 2022, 126, 6428-6437.	1.2	3
1677	Walking on water: revisiting the role of water in articular cartilage biomechanics in relation to tissue engineering and regenerative medicine. <i>Journal of the Royal Society Interface</i> , 2022, 19, .	1.5	6
1679	Biological Tissue Interaction with Sub-Terahertz Wave. <i>Biological and Medical Physics Series</i> , 2022, , 57-92.	0.3	0
1680	X-Ray absorption spectroscopy of H ₃ O ⁺ . <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 23119-23127.	1.3	4
1681	Addition of cholesterol alters the hydration at the surface of model lipids: a spectroscopic investigation. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 20381-20389.	1.3	5
1682	Effects of hydrogen bonds on the single-chain mechanics of chitin. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 24535-24541.	1.3	5
1684	Three-Dimensional Confinement of Water: H ₂ O Exhibits Long-Range (>50 nm) Structure while D ₂ O Does Not. <i>Nano Letters</i> , 2022, 22, 7394-7400.	4.5	4

#	ARTICLE	IF	CITATIONS
1685	Arrangement of Hydrogen Bonds in Aqueous Solutions of Different Globular Proteins. <i>International Journal of Molecular Sciences</i> , 2022, 23, 11381.	1.8	1
1686	Toxic Effect of Metal Doping on Diatoms as Probed by Broadband Terahertz Time-Domain Spectroscopy. <i>Molecules</i> , 2022, 27, 5897.	1.7	0
1687	Connecting Non-Gaussian Water Density Fluctuations to the Lengthscale Dependent Crossover in Hydrophobic Hydration. <i>Journal of Physical Chemistry B</i> , 2022, 126, 7604-7614.	1.2	4
1688	Innermost Ion Association Configuration Is a Key Structural Descriptor of Ionic Liquids at Electrified Interfaces. <i>Journal of Physical Chemistry Letters</i> , 2022, 13, 9464-9472.	2.1	3
1689	The pathway from the solution to the steps. <i>Journal of Crystal Growth</i> , 2022, 599, 126870.	0.7	2
1690	Spatial reorganization of analytes in charged aqueous microdroplets. <i>Chemical Science</i> , 2022, 13, 13321-13329.	3.7	3
1691	Analysis of the Site-Specific Myoglobin Modifications in the Melibiose-Derived Novel Advanced Glycation End-Product. <i>International Journal of Molecular Sciences</i> , 2022, 23, 13036.	1.8	1
1692	Application of Fundamental Chemical Principles for Solvation Effects: A Unified Perspective for Interaction Patterns in Solution. <i>Journal of Physical Chemistry B</i> , 2022, 126, 8864-8872.	1.2	2
1693	The Hydrophobic Effects: Our Current Understanding. <i>Molecules</i> , 2022, 27, 7009.	1.7	14
1694	The Global Polarity of Alcoholic Solvents and Water – Importance of the Collectively Acting Factors Density, Refractive Index and Hydrogen Bonding Forces. <i>ChemistryOpen</i> , 2022, 11, .	0.9	2
1695	Guest Binding with Sulfated Cyclodextrins: Does the Size of Cavity Matter?. <i>ChemPhysChem</i> , 2023, 24, .	1.0	2
1696	A Molecular View of the Surface Pressure/Area Per Lipid Isotherms Assessed by FTIR/ATR Spectroscopy. <i>Colloids and Interfaces</i> , 2022, 6, 54.	0.9	1
1697	Difference in the hydration state of water at the hydrophobic interface of structural isomers of propanol investigated by U.V visible absorption and Raman spectroscopic study. <i>Journal of Molecular Liquids</i> , 2022, 368, 120530.	2.3	1
1698	Grazing incidence neutron scattering for the study of solid–liquid interfaces. , 2024, , 305-323.		0
1699	Biophysical principles of liquid–liquid phase separation. , 2023, , 3-82.		1
1701	Hydration Free Energies of Polypeptides from Popular Implicit Solvent Models versus All-Atom Simulation Results Based on Molecular Quasichemical Theory. <i>Journal of Physical Chemistry B</i> , 0, , .	1.2	1
1702	Guanidinium–amino acid hydrogen-bonding interactions in protein crystal structures: implications for guanidinium-induced protein denaturation. <i>Physical Chemistry Chemical Physics</i> , 2022, 25, 857-869.	1.3	3
1703	The effect of electric field on the structural order of water molecules around chitosan between nano gold plates determined by molecular dynamics simulations. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 30035-30043.	1.3	0

#	ARTICLE	IF	CITATIONS
1704	Thermal tuning of protein hydration in a hyperthermophilic enzyme. <i>Frontiers in Molecular Biosciences</i> , 0, 9, .	1.6	1
1705	Hydrophobicity of arginine leads to reentrant liquid-liquid phase separation behaviors of arginine-rich proteins. <i>Nature Communications</i> , 2022, 13, .	5.8	27
1707	Small Hydropower Plantsâ€™ Impacts on the Ecological Status Indicators of Urban Rivers. <i>Applied Sciences (Switzerland)</i> , 2022, 12, 12882.	1.3	13
1708	Large Oscillatory Forces and Self-Assembled Water Chains. , 2023, , 99-122.		0
1709	High-field/High-frequency EPR Spectroscopy in Protein Research: Principles and Examples. <i>Applied Magnetic Resonance</i> , 2023, 54, 207-287.	0.6	4
1710	Computational investigation of functional water molecules in GPCRs bound to G protein or arrestin. <i>Journal of Computer-Aided Molecular Design</i> , 2023, 37, 91-105.	1.3	3
1711	Multiverse Predictions for Habitability: Element Abundances. <i>Universe</i> , 2022, 8, 651.	0.9	3
1713	Assisting role of water molecules in ionic recognition by 18-crown-6 ether in aqueous solutions. <i>Journal of Molecular Liquids</i> , 2023, 371, 121127.	2.3	4
1714	Temperature-dependent dielectric relaxation and hydrophobicity of aqueous alanine using time domain reflectometry. <i>Journal of Biomolecular Structure and Dynamics</i> , 2023, 41, 10690-10701.	2.0	6
1715	What happens when chitin becomes chitosan? A single-molecule study. <i>RSC Advances</i> , 2023, 13, 2294-2300.	1.7	2
1718	The Hydrophobic Effect Studied by Using Interacting Colloidal Suspensions. <i>International Journal of Molecular Sciences</i> , 2023, 24, 2003.	1.8	0
1719	Local Molecular Field Theory for Coulomb Interactions in Aqueous Solutions. <i>Journal of Physical Chemistry B</i> , 2023, 127, 809-821.	1.2	3
1720	Impact of an Ionic Liquid on Amino Acid Side Chains: A Perspective from Molecular Simulation Studies. <i>Journal of Chemical Information and Modeling</i> , 2023, 63, 959-972.	2.5	2
1721	Elucidating the Sluggish Water Dynamics at the Ice-Binding Surface of the Hyperactive <i>Tenebrio molitor</i> Antifreeze Protein. <i>Journal of Physical Chemistry B</i> , 2023, 127, 121-132.	1.2	1
1722	Hunting for environments favorable to life on planets, moons, dwarf planets, and meteorites. , 2023, , 737-772.		0
1724	Investigation of Glucoseâ€“Water Mixtures as a Function of Concentration and Temperature by Infrared Spectroscopy. <i>International Journal of Molecular Sciences</i> , 2023, 24, 2564.	1.8	0
1725	Preparation of pure active water for auto-catalytic reactions performed in it. <i>Nanoscale</i> , 0, , .	2.8	0
1726	A new apparatus and the relevant method to retrieve IR spectra of solutes from the corresponding aqueous solutions. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2023, 296, 122598.	2.0	0

#	ARTICLE	IF	CITATIONS
1727	A new perspective in understanding the processing mechanisms of traditional Chinese medicine by near-infrared spectroscopy with Aquaphotomics. <i>Journal of Molecular Structure</i> , 2023, 1284, 135401.	1.8	0
1728	Small hydropower plants's impacts in urban areas: Assessment of water quality from an environmental, social, and economic perspective. , 2022, , .		0
1729	Reinforced Hydrophobic Molecular Layer Promoting Waterproof Lithium for High-Performance Lithium-Metal Batteries. <i>Key Engineering Materials</i> , 0, 939, 117-122.	0.4	0
1730	Ordered/Disordered Structures of Water at Solid/Liquid Interfaces. <i>Crystals</i> , 2023, 13, 263.	1.0	1
1731	Prediction of hydrophilic and hydrophobic hydration structure of protein by neural network optimized using experimental data. <i>Scientific Reports</i> , 2023, 13, .	1.6	0
1732	Evolution of Solute's Water Interactions in the Benzaldehyde-(H ₂ O) ₆ Clusters by Rotational Spectroscopy. <i>Journal of the American Chemical Society</i> , 2023, 145, 4119-4128.	6.6	11
1733	Scientific novelty beyond the experiment. <i>Microbial Biotechnology</i> , 2023, 16, 1131-1173.	2.0	30
1734	Molecular dynamics simulation of infrared absorption spectra of one-dimensional ordered single-file water. <i>Wuli Xuebao/Acta Physica Sinica</i> , 2023, 72, 084207.	0.2	0
1735	REVIEW ON DRYING PROCESSES AND DAMAGE PROTECTION MECHANISM OF LIQUOR YEAST. <i>INMATEH - Agricultural Engineering</i> , 2022, , 735-746.	0.1	1
1736	Heterogeneous and Allosteric Role of Surface Hydration for Protein's Ligand Binding. <i>Journal of Chemical Theory and Computation</i> , 2023, 19, 1875-1887.	2.3	3
1737	Thermodynamics of the self-assembly of <i>N</i> -annulated perylene bisimides in water. Disentangling the enthalpic and entropic contributions. <i>Organic Chemistry Frontiers</i> , 2023, 10, 1959-1967.	2.3	5
1738	Quantifying the Molecular Polarization Response of Liquid Water Interfaces at Heterogeneously Charged Surfaces. <i>Journal of Chemical Theory and Computation</i> , 2023, 19, 1843-1852.	2.3	1
1739	Synthesis, crystal structure and electrocatalytic hydrogen evolution reaction studies of cobaloximes with diphenylglyoxime and carboxylic acid functionalized neutral bases. <i>Polyhedron</i> , 2023, 238, 116394.	1.0	4
1740	Acidic Conditions Impact Hydrophobe Transfer across the Oil's Water Interface in Unusual Ways. <i>Journal of Physical Chemistry B</i> , 0, , .	1.2	0
1762	Water, Solvent of Life. , 2023, , 3234-3237.		0
1771	Terahertz spectroscopy as a method for investigation of hydration shells of biomolecules. <i>Biophysical Reviews</i> , 2023, 15, 833-849.	1.5	2
1807	The dawn of hydrogen and halogen bonds and their crucial role in collisional processes probing long-range intermolecular interactions. <i>Physical Chemistry Chemical Physics</i> , 2024, 26, 7971-7987.	1.3	0