Density, structure, and dynamics of water: The effect of

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Citation Report

#	Article	IF	Citations
1	A reactive force field for aqueous-calcium carbonate systems. Physical Chemistry Chemical Physics, 2011, 13, 16666.	1.3	87
2	Hydrogen Bonds and van der Waals Forces in Ice at Ambient and High Pressures. Physical Review Letters, 2011, 107, 185701.	2.9	193
3	Enhanced small-angle scattering connected to the Widom line in simulations of supercooled water. Journal of Chemical Physics, 2011, 134, 214506.	1.2	67
4	Application of the SCC-DFTB Method to Neutral and Protonated Water Clusters and Bulk Water. Journal of Physical Chemistry B, 2011, 115, 6790-6805.	1.2	81
5	Depolarization of water in protic ionic liquids. Physical Chemistry Chemical Physics, 2011, 13, 15083.	1.3	63
6	Van der Waals effects in ab initio water at ambient and supercritical conditions. Journal of Chemical Physics, 2011, 135, 154503.	1.2	138
7	Structural and Vibrational Properties of Liquid Water from van der Waals Density Functionals. Journal of Chemical Theory and Computation, 2011, 7, 3054-3061.	2.3	146
8	First Principles Simulations of the Infrared Spectrum of Liquid Water Using Hybrid Density Functionals. Journal of Chemical Theory and Computation, 2011, 7, 1443-1449.	2.3	139
9	Hydrogen bond dynamics in heavy water studied with quantum dynamical simulations. Physical Chemistry Chemical Physics, 2011, 13, 19865.	1.3	16
10	Ab Initio van der Waals Interactions in Simulations of Water Alter Structure from Mainly Tetrahedral to High-Density-Like. Journal of Physical Chemistry B, 2011, 115, 14149-14160.	1.2	83
11	Entropy of Liquid Water from Ab Initio Molecular Dynamics. Journal of Physical Chemistry B, 2011, 115, 14190-14195.	1.2	45
12	Simulating water with rigid non-polarizable models: a general perspective. Physical Chemistry Chemical Physics, 2011, 13, 19663.	1.3	749
13	Effects of the dispersion interaction in liquid water. Chemical Physics Letters, 2011, 513, 59-62.	1.2	20
14	Perspective on the structure of liquid water. Chemical Physics, 2011, 389, 1-34.	0.9	289
15	Deconstructing Classical Water Models at Interfaces and in Bulk. Journal of Statistical Physics, 2011, 145, 313-334.	0.5	44
16	Hydrogen bonded structure and dynamics of liquid-vapor interface of water-ammonia mixture: An ab initio molecular dynamics study. Journal of Chemical Physics, 2011, 135, 114510.	1.2	38
17	Path-integral simulation of ice I<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mi>h</mml:mi></mml:msub></mml:math>: The effect of pressure. Physical Review B, 2011, 84, .	1.1	13
18	Kinetic energy of protons in ice Ih and water: A path integral study. Physical Review B, 2011, 84, .	1.1	35

#	Article	IF	Citations
19	van der Waals density functional study of energetic, structural, and vibrational properties of small water clusters and ice<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mi>I</mml:mi><mml:mrow><mml:mi>h</mml:mi></mml:mrow></mml:msub></mml:m Physical Review B, 2011, 84, .	1.1	46
20	A tight binding model for water. Journal of Chemical Physics, 2011, 134, 044130.	1.2	10
21	The structure of ionic aqueous solutions at interfaces: An intrinsic structure analysis. Journal of Chemical Physics, 2012, 137, 114706.	1.2	39
22	Quasi-harmonic approximation of thermodynamic properties of ice Ih, II, and III. Journal of Chemical Physics, 2012, 137, 044502.	1.2	49
23	Multiscale reactive molecular dynamics. Journal of Chemical Physics, 2012, 137, 22A525.	1.2	67
24	High-density amorphous ice: A path-integral simulation. Journal of Chemical Physics, 2012, 137, 104505.	1.2	14
25	Effect of dispersion correction on the Au(1 1 1)-H2O interface: A first-principles study. Journal of Chemical Physics, 2012, 137, 114709.	1.2	49
26	The phase diagram of ice Ih, II, and III: A quasi-harmonic study. Journal of Chemical Physics, 2012, 137, 134503.	1.2	13
27	Predicting the acidity constant of a goethite hydroxyl group from first principles. Journal of Physics Condensed Matter, 2012, 24, 124105.	0.7	28
28	Isotope effects in water as investigated by neutron diffraction and path integral molecular dynamics. Journal of Physics Condensed Matter, 2012, 24, 284126.	0.7	47
29	Predicting the melting temperature of ice-Ih with only electronic structure information as input. Journal of Chemical Physics, 2012, 137, 014510.	1.2	27
30	CO2 Capture by Metalâ€“Organic Frameworks with van der Waals Density Functionals. Journal of Physical Chemistry A, 2012, 116, 4957-4964.	1.1	92
31	Exploring the influence of organic species on pre- and post-nucleation calcium carbonate. Faraday Discussions, 2012, 159, 61.	1.6	68
32	Anomalous Nuclear Quantum Effects in Ice. Physical Review Letters, 2012, 108, 193003.	2.9	110
33	Assessing the accuracy of quantum Monte Carlo and density functional theory for energetics of small water clusters. Journal of Chemical Physics, 2012, 136, 244105.	1.2	64
34	A Refined MS-EVB Model for Proton Transport in Aqueous Environments. Journal of Physical Chemistry B, 2012, 116, 343-352.	1.2	79
35	Ab initio parameterization of an all-atom polarizable and dissociable force field for water. Journal of Chemical Physics, 2012, 136, 114511.	1.2	26
36	Coarse-graining away electronic structure: a rigorous route to accurate condensed phase interaction potentials. Molecular Physics, 2012, 110, 935-944.	0.8	12

#	Article	IF	Citations
37	QM/MM simulation of liquid water with an adaptive quantum region. Physical Chemistry Chemical Physics, 2012, 14, 646-656.	1.3	80
38	Ab initio molecular dynamics study of water at constant pressure using converged basis sets and empirical dispersion corrections. Journal of Chemical Physics, 2012, 137, 044506.	1.2	77
39	Ab initio path integral Monte Carlo simulations for water trimer with electron correlation effects. Computational and Theoretical Chemistry, 2012, 997, 7-13.	1.1	10
40	Fluctuations in ambient water. Journal of Molecular Liquids, 2012, 176, 2-16.	2.3	86
41	Structure and Dynamics of Liquid Water from ab Initio Molecular Dynamicsâ€"Comparison of BLYP, PBE, and revPBE Density Functionals with and without van der Waals Corrections. Journal of Chemical Theory and Computation, 2012, 8, 3902-3910.	2.3	247
42	MOLECULAR BIOLOGY AT THE QUANTUM LEVEL: CAN MODERN DENSITY FUNCTIONAL THEORY FORGE THE PATH?. Nano LIFE, 2012, 02, 1230006.	0.6	8
43	A first principles molecular dynamics study of the solvation structure and migration kinetics of an excess proton and a hydroxide ion in binary water-ammonia mixtures. Journal of Chemical Physics, 2012, 136, 114509.	1.2	8
44	A simplified implementation of van der Waals density functionals for first-principles molecular dynamics applications. Journal of Chemical Physics, 2012, 136, 224107.	1.2	49
45	Assessment of density functional theory to calculate the phase transition pressure of ice. Physical Chemistry Chemical Physics, 2012, 14, 11484.	1.3	22
46	A first principles simulation study of fluctuations of hydrogen bonds and vibrational frequencies of water at liquidâ€"vapor interface. Chemical Physics, 2012, 392, 96-104.	0.9	39
47	Virtual Probes of Mineral-Water Interfaces: The More Flops, the Better!. Elements, 2013, 9, 211-216.	0.5	14
48	Microscopic properties of liquid water from combined ab initio molecular dynamics and energy decomposition studies. Physical Chemistry Chemical Physics, 2013, 15, 15746.	1.3	55
49	Anions vs. Cations of Pt13H24 Cluster Models: Ab Initio Molecular Dynamics Investigation of Electronic Properties and Photocatalytic Activity. ACS Symposium Series, 2013, , 173-185.	0.5	2
50	Dynamics of supercritical methanol of varying density from first principles simulations: Hydrogen bond fluctuations, vibrational spectral diffusion, and orientational relaxation. Journal of Chemical Physics, 2013, 138, 224501.	1.2	13
51	Machine-learning approach for one- and two-body corrections to density functional theory: Applications to molecular and condensed water. Physical Review B, 2013, 88, .	1.1	177
52	Dynamics of hydrogen bonds and vibrational spectral diffusion in liquid methanol from first principles simulations with dispersion corrected density functional. Chemical Physics, 2013, 415, 1-7.	0.9	15
53	Resonant inelastic X-ray scattering of liquid water. Journal of Electron Spectroscopy and Related Phenomena, 2013, 188, 84-100.	0.8	45
54	Tests of an Adaptive QM/MM Calculation on Free Energy Profiles of Chemical Reactions in Solution. Journal of Physical Chemistry B, 2013, 117, 12202-12211.	1.2	24

#	Article	IF	Citations
55	First-principles energetics of water clusters and ice: A many-body analysis. Journal of Chemical Physics, 2013, 139, 244504.	1.2	34
56	Bulk Liquid Water at Ambient Temperature and Pressure from MP2 Theory. Journal of Physical Chemistry Letters, 2013, 4, 3753-3759.	2.1	131
57	Hexamers and witchamers: Which hex do you choose?. Computational and Theoretical Chemistry, 2013, 1021, 70-83.	1.1	17
58	Room temperature compressibility and diffusivity of liquid water from first principles. Journal of Chemical Physics, 2013, 139, 194502.	1.2	54
59	Energy benchmarks for water clusters and ice structures from an embedded many-body expansion. Journal of Chemical Physics, 2013, 139, 114101.	1.2	60
60	Microscopic structure of water at elevated pressures and temperatures. Proceedings of the National Academy of Sciences of the United States of America, 2013, 110, 6301-6306.	3.3	127
61	Structure of water layers on hydrogen-covered Pt electrodes. Catalysis Today, 2013, 202, 183-190.	2.2	90
62	Hydration structure of salt solutions from ab initio molecular dynamics. Journal of Chemical Physics, 2013, 138, 014501.	1.2	158
63	A classical density-functional theory for describing water interfaces. Journal of Chemical Physics, 2013, 138, 024509.	1.2	32
64	A Critical Assessment of Two-Body and Three-Body Interactions in Water. Journal of Chemical Theory and Computation, 2013, 9, 1103-1114.	2.3	126
65	Heat transport in liquid water at extreme pressures: A non equilibrium molecular dynamics study. Journal of Molecular Liquids, 2013, 185, 1-7.	2.3	7
66	Frequency dependence of the reorientational motion of OD bonds of deuterated methanol in liquid phase: A first principles molecular dynamics study. Journal of Molecular Liquids, 2013, 182, 43-47.	2.3	3
67	Ab initio and classical molecular dynamics studies of the structural and dynamical behavior of water near a hydrophobic graphene sheet. Journal of Chemical Physics, 2013, 138, 204702.	1.2	64
68	Clapeyron slope reversal in the melting curve of AuGa2at 5.5 GPa. Journal of Physics Condensed Matter, 2013, 25, 415401.	0.7	3
69	Optimal finite-range atomic basis sets for liquid water and ice. Journal of Physics Condensed Matter, 2013, 25, 435504.	0.7	25
70	Atypical water lattices and their possible relevance to the amorphous ices: A density functional study. AIP Advances, 2013, 3, 042119.	0.6	5
71	Communication: Energy benchmarking with quantum Monte Carlo for water nano-droplets and bulk liquid water. Journal of Chemical Physics, 2013, 138, 221102.	1.2	31
72	Development of Accurate Force Fields for the Simulation of Biomineralization. Methods in Enzymology, 2013, 532, 3-23.	0.4	10

#	Article	IF	Citations
73	On the accuracy of van der Waals inclusive density-functional theory exchange-correlation functionals for ice at ambient and high pressures. Journal of Chemical Physics, 2013, 139, 154702.	1.2	119
74	Performance Analysis of Electronic Structure Codes on HPC Systems: A Case Study of SIESTA. PLoS ONE, 2014, 9, e95390.	1.1	13
75	Many-body exchange-overlap interactions in rare gases and water. Journal of Chemical Physics, 2014, 141, 224106.	1.2	25
76	The individual and collective effects of exact exchange and dispersion interactions on the ab initio structure of liquid water. Journal of Chemical Physics, 2014, 141, 084502.	1.2	276
77	Universal tight binding model for chemical reactions in solution and at surfaces. II. Water. Journal of Chemical Physics, 2014, 141, 044504.	1.2	5
78	First-Principles Approach to Calculating Energy Level Alignment at Aqueous Semiconductor Interfaces. Physical Review Letters, 2014, 113, 176802.	2.9	72
79	Static Dielectric Permittivity of Ice from First Principles. Physical Review Letters, 2014, 113, 245501.	2.9	7
80	Dispersion corrected RPBE studies of liquid water. Journal of Chemical Physics, 2014, 141, 064501.	1.2	102
81	Density functional theory and molecular dynamics study of the uranyl ion (UO2)2+. Journal of Molecular Modeling, 2014, 20, 2150.	0.8	12
82	An ab initio molecular dynamics study of the hydrogen bonded structure, dynamics and vibrational spectral diffusion of water in the ion hydration shell of a superoxide ion. Chemical Physics, 2014, 445, 105-112.	0.9	2
83	Computational investigation of structural and electronic properties of aqueous interfaces of GaN, ZnO, and a GaN/ZnO alloy. Physical Chemistry Chemical Physics, 2014, 16, 12057-12066.	1.3	39
84	Role of Charge Transfer in Water Diffusivity in Aqueous Ionic Solutions. Journal of Physical Chemistry Letters, 2014, 5, 2711-2716.	2.1	46
85	Structure, Dynamics, and Spectral Diffusion of Water from First-Principles Molecular Dynamics. Journal of Physical Chemistry C, 2014, 118, 29401-29411.	1.5	139
86	Analyzing the errors of DFT approximations for compressed water systems. Journal of Chemical Physics, 2014, 141, 014104.	1.2	16
87	Hydration structure of Na⁺and K⁺fromab initiomolecular dynamics based on modern density functional theory. Molecular Physics, 2014, 112, 1448-1456.	0.8	37
88	The random phase approximation applied to ice. Journal of Chemical Physics, 2014, 140, 084502.	1.2	45
89	A thermodynamic adsorption/entrapment model for selenium(IV) coprecipitation with calcite. Geochimica Et Cosmochimica Acta, 2014, 134, 16-38.	1.6	46
90	Quantum Monte Carlo Benchmark of Exchange-Correlation Functionals for Bulk Water. Journal of Chemical Theory and Computation, 2014, 10, 2355-2362.	2.3	39

#	Article	IF	Citations
91	Density functional tight binding: application to organic and biological molecules. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2014, 4, 49-61.	6.2	157
92	Simulating liquid water for determining its structural and transport properties. Applied Radiation and Isotopes, 2014, 83, 115-121.	0.7	4
93	Assessing the accuracy of the van der Waals density functionals for rare-gas and small molecular systems. Physical Review B, 2015, 91, .	1.1	34
94	Nature of the Volume Isotope Effect in Ice. Physical Review Letters, 2015, 115, 173005.	2.9	22
95	Role of van der Waals corrections in first principles simulations of alkali metal ions in aqueous solutions. Journal of Chemical Physics, 2015, 143, 194510.	1.2	30
96	Probing the structural and dynamical properties of liquid water with models including non-local electron correlation. Journal of Chemical Physics, 2015, 143, 054506.	1.2	89
97	Structural Properties of Liquid Water and Ice Ih from Ab-Initio Molecular Dynamics with a Non-Local Correlation Functional. Energies, 2015, 8, 9383-9391.	1.6	20
98	Density and Compressibility of Liquid Water and Ice from First-Principles Simulations with Hybrid Functionals. Journal of Physical Chemistry Letters, 2015, 6, 2902-2908.	2.1	77
99	Ab initio molecular dynamics studies of hydrogen bonded structure, molecular motion, and frequency fluctuations of water in the vicinity of azide ions. Journal of Chemical Physics, 2015, 142, 164505.	1.2	5
100	A systematic study of chloride ion solvation in water using van der Waals inclusive hybrid density functional theory. Molecular Physics, 2015, 113, 2842-2854.	0.8	47
101	Local structure analysis in ab initio liquid water. Molecular Physics, 2015, 113, 2829-2841.	0.8	96
102	Water: one molecule, two surfaces, one mistake. Molecular Physics, 2015, 113, 1145-1163.	0.8	51
103	Nuclear quantum effects in liquid water from path-integral simulations using anab initioforce-matching approach. Molecular Physics, 2015, 113, 808-822.	0.8	32
104	The adaptive buffered force <scp>QM/MM</scp> method in the <scp>CP2K</scp> and <scp>AMBER</scp> software packages. Journal of Computational Chemistry, 2015, 36, 633-648.	1.5	39
105	¹H Nuclear Spin Relaxation of Liquid Water from Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2015, 119, 1966-1973.	1.2	39
106	Isobaric first-principles molecular dynamics of liquid water with nonlocal van der Waals interactions. Journal of Chemical Physics, 2015, 142, 034501.	1.2	68
107	Dispersion- and Exchange-Corrected Density Functional Theory for Sodium Ion Hydration. Journal of Chemical Theory and Computation, 2015, 11, 2958-2967.	2.3	42
108	Ab initio study of the structural properties of acetonitrileâ€“water mixtures. Chemical Physics, 2015, 457, 87-97.	0.9	22

#	Article	IF	Citations
109	First-Principles Simulation Study of Vibrational Spectral Diffusion and Hydrogen Bond Fluctuations in Aqueous Solution of N-Methylacetamide. Journal of Physical Chemistry B, 2015, 119, 9858-9867.	1.2	31
110	Water in Hydration Shell of an Iodide Ion: Structure and Dynamics of Solute-Water Hydrogen Bonds and Vibrational Spectral Diffusion from First-Principles Simulations. Journal of Physical Chemistry B, 2015, 119, 8561-8572.	1.2	36
111	Local order of liquid water at metallic electrode surfaces. Journal of Chemical Physics, 2015, 142, 034706.	1.2	36
112	van der Waals forces in density functional theory: a review of the vdW-DF method. Reports on Progress in Physics, 2015, 78, 066501.	8.1	615
113	Liquid Polyamorphous Transition and Self-Organization in Aqueous Solutions of Ionic Surfactants. Langmuir, 2015, 31, 8535-8547.	1.6	18
114	Proton reduction at surface of transition metal nanocatalysts. Molecular Simulation, 2015, 41, 134-145.	0.9	13
115	Ultrafast Vibrational Echo Spectroscopy of Liquid Water from First-Principles Simulations. Journal of Physical Chemistry B, 2015, 119, 11215-11228.	1.2	24
116	Ab initio molecular dynamics simulation of liquid water by quantum Monte Carlo. Journal of Chemical Physics, 2015, 142, 144111.	1.2	59
117	Path-integral simulation of ice VII: Pressure and temperature effects. Chemical Physics, 2015, 461, 125-136.	0.9	10
118	The structure of water; from ambient to deeply supercooled. Journal of Non-Crystalline Solids, 2015, 407, 399-417.	1.5	51
119	Enabling simulation at the fifth rung of DFT: Large scale RPA calculations with excellent time to solution. Computer Physics Communications, 2015, 187, 120-129.	3.0	42
120	Assessing the accuracy of improved forceâ€matched water models derived from Ab initio molecular dynamics simulations. Journal of Computational Chemistry, 2016, 37, 1828-1838.	1.5	11
121	How van der Waals interactions determine the unique properties of water. Proceedings of the National Academy of Sciences of the United States of America, 2016, 113, 8368-8373.	3.3	312
122	Structural and configurational properties of nanoconfined monolayer ice from first principles. Scientific Reports, 2016, 6, 18651.	1.6	61
123	Optimization of an exchange-correlation density functional for water. Journal of Chemical Physics, 2016, 144, 224101.	1.2	27
124	Perspective: How good is DFT for water?. Journal of Chemical Physics, 2016, 144, 130901.	1.2	571
125	Pressure-induced Transformations of Dense Carbonyl Sulfide to Singly Bonded Amorphous Metallic Solid. Scientific Reports, 2016, 6, 31594.	1.6	2
126	Structure and dynamics of aqueous solutions from PBE-based first-principles molecular dynamics simulations. Journal of Chemical Physics, 2016, 145, 154501.	1.2	87

#	Article	IF	Citations
127	The structure of water at a Pt(111) electrode and the potential of zero charge studied from first principles. Journal of Chemical Physics, 2016, 144, 194701.	1.2	127
128	Adsorption-Induced Surface Stresses of the Water/Quartz Interface: Ab Initio Molecular Dynamics Study. Langmuir, 2016, 32, 5259-5266.	1.6	18
129	Ab initio molecular dynamics study of Se(<scp>iv</scp>) species in aqueous environment. Physical Chemistry Chemical Physics, 2016, 18, 26755-26763.	1.3	4
130	Liquid Water through Density-Functional Molecular Dynamics: Plane-Wave vs Atomic-Orbital Basis Sets. Journal of Chemical Theory and Computation, 2016, 12, 3456-3462.	2.3	23
131	AbÂinitio Electronic Structure of Liquid Water. Physical Review Letters, 2016, 117, 186401.	2.9	64
132	Thermal conductivity switch: Optimal semiconductor/metal melting transition. Physical Review B, 2016, 94, .	1.1	21
133	Why Is MP2-Water â€œCoolerâ€•and â€œDenserâ€•than DFT-Water?. Journal of Physical Chemistry Letters, 2016, 7, 680-684.	2.1	47
134	Two Dimensional Ice from First Principles: Structures and Phase Transitions. Physical Review Letters, 2016, 116, 025501.	2.9	167
135	Real-Time Quantum Dynamics Reveals Complex, Many-Body Interactions in Solvated Nanodroplets. Journal of Chemical Theory and Computation, 2016, 12, 1862-1871.	2.3	39
136	Anisotropic structure and dynamics of the solvation shell of a benzene solute in liquid water from ab initio molecular dynamics simulations. Physical Chemistry Chemical Physics, 2016, 18, 6132-6145.	1.3	20
137	Modelling heterogeneous interfaces for solar water splitting. Nature Materials, 2017, 16, 401-408.	13.3	252
138	Divide-and-Conquer-Type Density-Functional Tight-Binding Simulations of Hydroxide Ion Diffusion in Bulk Water. Journal of Physical Chemistry B, 2017, 121, 1362-1371.	1.2	38
139	First-Principles Models for van der Waals Interactions in Molecules and Materials: Concepts, Theory, and Applications. Chemical Reviews, 2017, 117, 4714-4758.	23.0	408
140	Dehydrogenation Free Energy of Co²⁺(aq) from Density Functional Theory-Based Molecular Dynamics. Journal of Chemical Theory and Computation, 2017, 13, 974-981.	2.3	7
141	Ab initio molecular dynamics simulations of liquid water using high quality meta-GGA functionals. Chemical Science, 2017, 8, 3554-3565.	3.7	95
142	Vibrational Modes of Hydrogen Hydrates: A First-Principles Molecular Dynamics and Raman Spectra Study. Journal of Physical Chemistry C, 2017, 121, 3690-3696.	1.5	29
143	Performance of the AMOEBA Water Model in the Vicinity of QM Solutes: A Diagnosis Using Energy Decomposition Analysis. Journal of Chemical Theory and Computation, 2017, 13, 1963-1979.	2.3	28
144	Phase diagram of carbonyl sulfide: An analogy to carbon dioxide and carbon disulfide. Japanese Journal of Applied Physics, 2017, 56, 05FA04.	0.8	2

#	Article	IF	Citations
145	Understanding the structure and hydrogen bonding network of (H₂O)₃₂ and (H₂O)₃₃: an improved Monte Carlo temperature basin paving (MCTBP) method and quantum theory of atoms in molecules (QTAIM) analysis. RSC Advances, 2017, 7, 18401-18417.	1.7	16
146	Exploring Solvation Effects in Ligand-Exchange Reactions via Static and Dynamic Methods. Journal of Chemical Theory and Computation, 2017, 13, 3348-3358.	2.3	18
147	Quantum and classical inter-cage hopping of hydrogen molecules in clathrate hydrate: temperature and cage-occupation effects. Physical Chemistry Chemical Physics, 2017, 19, 717-728.	1.3	28
148	Ab initio theory and modeling of water. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, 10846-10851.	3.3	340
149	X-ray absorption of liquid water by advanced ab initio methods. Physical Review B, 2017, 96, .	1.1	11
150	optPBE-vdW density functional theory study of liquid water and pressure-induced structural evolution in ice Ih. Canadian Journal of Chemistry, 2017, 95, 1205-1211.	0.6	6
151	Molecular polarizability of water from local dielectric response theory. Physical Review B, 2017, 96, .	1.1	15
152	Simulations of water nano-confined between corrugated planes. Journal of Chemical Physics, 2017, 147, 194509.	1.2	7
153	The hydration structure of carbon monoxide byab initiomethods. Journal of Chemical Physics, 2017, 146, 034503.	1.2	5
154	Mass density fluctuations in quantum and classical descriptions of liquid water. Journal of Chemical Physics, 2017, 146, 244501.	1.2	44
155	Interstitial Voids and Resultant Density of Liquid Water: A First-Principles Molecular Dynamics Study. ACS Omega, 2018, 3, 2010-2017.	1.6	23
156	Insights into the Structure of Liquid Water from Nuclear Quantum Effects on the Density and Compressibility of Ice Polymorphs. Journal of Physical Chemistry B, 2018, 122, 5694-5706.	1.2	11
157	Equilibration and analysis of first-principles molecular dynamics simulations of water. Journal of Chemical Physics, 2018, 148, 124501.	1.2	41
158	Effects of dispersion interactions on the structure, polarity, and dynamics of liquid-vapor interface of an aqueous NaCl solution: Results of first principles simulations at room temperature. Journal of Chemical Physics, 2018, 148, 024702.	1.2	4
159	Dynamics of vibrational spectral diffusion in water: Effects of dispersion interactions, temperature, density, system size and fictitious orbital mass. Journal of Molecular Liquids, 2018, 249, 169-178.	2.3	4
160	Study of hydrogen-molecule guests in type II clathrate hydrates using a force-matched potential model parameterised from ab initio molecular dynamics. Journal of Chemical Physics, 2018, 148, 102323.	1.2	18
161	Nuclear quantum effects of light and heavy water studied by all-electron first principles path integral simulations. Journal of Chemical Physics, 2018, 148, 102324.	1.2	21
162	Water in the human body: An anesthesiologist's perspective on the connection between physicochemical properties of water and physiologic relevance. Annals of Medicine and Surgery, 2018, 26, 1-8.	0.5	13

#	Article	IF	Citations
163	Structural, electronic, and dynamical properties of liquid water by ab initio molecular dynamics based on SCAN functional within the canonical ensemble. Journal of Chemical Physics, 2018, 148, 164505.	1.2	58
164	Water under Supercritical Conditions: Hydrogen Bonds, Polarity, and Vibrational Frequency Fluctuations from Ab Initio Simulations with a Dispersion Corrected Density Functional. ACS Omega, 2018, 3, 3453-3462.	1.6	9
165	Bias-dependent local structure of water molecules at a metallic interface. Chemical Science, 2018, 9, 62-69.	3.7	19
166	The structure of metal-water interface at the potential of zero charge from density functional theory-based molecular dynamics. Journal of Electroanalytical Chemistry, 2018, 819, 87-94.	1.9	50
167	Simulation of Calcium Phosphate Species in Aqueous Solution: Force Field Derivation. Journal of Physical Chemistry B, 2018, 122, 1471-1483.	1.2	26
168	Electrowetting on 2D dielectrics: a quantum molecular dynamics investigation. Journal of Physics Condensed Matter, 2018, 30, 375001	0.7	3
169	Wettability Alteration and Enhanced Oil Recovery Induced by Proximal Adsorption of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline" overflow="scroll"><mml:msup><mml:mi>Na</mml:mi><mml:mo>+</mml:mo></mml:msup></mml:math> , <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline" overflow="scroll"><mml:msup><mml:mi>Cl</mml:mi><mml:mo>â^'</mml:mo></mml:msup></mml:math> , <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline" overflow="scroll"><m	1.5	42
170	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
171	First-Principles Simulations of Liquid Water Using a Dielectric-Dependent Hybrid Functional. Journal of Physical Chemistry Letters, 2018, 9, 3068-3073.	2.1	82
172	Role of solvent in metal-on-metal surface diffusion: A case for rational solvent selection for materials synthesis. Surface Science, 2018, 675, 54-63.	0.8	9
173	Water wettability of graphene: interplay between the interfacial water structure and the electronic structure. RSC Advances, 2018, 8, 16918-16926.	1.7	24
174	Computational Modeling of Electrocatalytic Reactions. , 2018, , 455-465.		0
175	Solvent effects on the decarboxylation of trichloroacetic acid: insights from ab initio molecular dynamics simulations. Physical Chemistry Chemical Physics, 2018, 20, 21988-21998.	1.3	15
176	Pressure dependence of structural properties of ice VII: An ab initio molecular-dynamics study. Journal of Chemical Physics, 2018, 148, 204505.	1.2	7
177	MP2- and RPA-Based Ab Initio Molecular Dynamics and Monte Carlo Sampling. , 2018, , 1-21.		1
178	Structure, polarity, dynamics, and vibrational spectral diffusion of liquidâ€"vapour interface of a waterâ€"methanol mixture from first principles simulation using dispersion corrected density functional. Indian Journal of Physics, 2018, 92, 1337-1346.	0.9	2
179	OH radical in water from ab initio molecular dynamics simulation employing hybrid functionals. Journal of Chemical Physics, 2019, 151, 064111.	1.2	8
180	Classical and path-integral molecular-dynamics study on liquid water and ice melting using non-empirical TTM2.1-F model. Molecular Physics, 2019, 117, 3241-3253.	0.8	1

#	Article	IF	Citations
181	An ab initio molecular dynamics study of benzene in water at supercritical conditions: Structure, dynamics, and polarity of hydration shell water and the solute. Journal of Chemical Physics, 2019, 151, 044508.	1.2	6
182	Interatomic potentials of Mg ions in aqueous solutions: structure and dehydration kinetics. European Journal of Mineralogy, 2019, 31, 275-287.	0.4	13
183	Isotope effects in liquid water via deep potential molecular dynamics. Molecular Physics, 2019, 117, 3269-3281.	0.8	52
184	Using a monomer potential energy surface to perform approximate path integral molecular dynamics simulation of ab initio water at near-zero added cost. Physical Chemistry Chemical Physics, 2019, 21, 409-417.	1.3	1
185	Structure and Dynamics of Water at the Waterâ€“Air Interface Using First-Principles Molecular Dynamics Simulations. II. NonLocal vs Empirical van der Waals Corrections. Journal of Chemical Theory and Computation, 2019, 15, 3836-3843.	2.3	12
186	Unraveling the metastability of the SI and SII carbon monoxide hydrate with a combined DFT-neutron diffraction investigation. Journal of Chemical Physics, 2019, 150, 184705.	1.2	12
187	Importance of van der Waals effects on the hydration of metal ions from the Hofmeister series. Journal of Chemical Physics, 2019, 150, 124505.	1.2	11
188	Temperature dependence of the ultrafast vibrational echo spectroscopy of OD modes in liquid water from first principles simulations. Physical Chemistry Chemical Physics, 2019, 21, 6485-6498.	1.3	10
189	Ensemble first-principles molecular dynamics simulations of water using the SCAN meta-GGA density functional. Journal of Chemical Physics, 2019, 151, 164101.	1.2	24
190	Ab initio simulations of liquid electrolytes for energy conversion and storage. International Journal of Quantum Chemistry, 2019, 119, e25795.	1.0	14
191	Sampling Potential Energy Surfaces in the Condensed Phase with Manyâ€Body Electronic Structure Methods. Chemistry - A European Journal, 2020, 26, 362-368.	1.7	7
192	Nuclear Quantum Effects Largely Influence Molecular Dissociation and Proton Transfer in Liquid Water under an Electric Field. Journal of Physical Chemistry Letters, 2020, 11, 8983-8988.	2.1	63
193	Vibrational Spectra of the OH Radical in Water: Ab Initio Molecular Dynamics Simulations and Quantum Chemical Calculations Using Hybrid Functionals. Advanced Theory and Simulations, 2020, 3, 2000174.	1.3	5
194	Isotope effects in x-ray absorption spectra of liquid water. Physical Review B, 2020, 102, .	1.1	6
195	Hydrogen Intramolecular Stretch Redshift in the Electrostatic Environment of Type II Clathrate Hydrates from SchrÃ¶dinger Equation Treatment. Applied Sciences (Switzerland), 2020, 10, 8504.	1.3	1
196	Self-interaction error overbinds water clusters but cancels in structural energy differences. Proceedings of the National Academy of Sciences of the United States of America, 2020, 117, 11283-11288.	3.3	57
197	Spatially resolved hydration shells and dynamics of different sulfur species in water from first-principle molecular dynamics simulations. Journal of Molecular Liquids, 2020, 312, 113387.	2.3	1
198	Hydration Properties of H_nPO₄^{nâ^'3} (n = 0â^'3) From Ab Initio Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2020, 124, 5454-5464.	1.2	4

#	Article	IF	Citations
199	S<scp>iesta</scp>: Recent developments and applications. Journal of Chemical Physics, 2020, 152, 204108.	1.2	229
200	Thermophysical Properties and Angular Jump Dynamics of Water: A Comparative DFT and DFT-Dispersion-Based Molecular Dynamics Study. Journal of Physical Chemistry A, 2020, 124, 6039-6049.	1.1	5
201	Water on surfaces from first-principles molecular dynamics. Chinese Physics B, 2020, 29, 116804.	0.7	1
202	Accurate SCC-DFTB Parametrization for Bulk Water. Journal of Chemical Theory and Computation, 2020, 16, 1768-1778.	2.3	17
203	Bornâ€“Oppenheimer molecular dynamics simulations on structures of high-density and low-density water: a comparison of the SCAN meta-GGA and PBE GGA functionals. Physical Chemistry Chemical Physics, 2021, 23, 2298-2304.	1.3	9
204	p-Aminobenzoic acid protonation dynamics in an evaporating droplet by ab initio molecular dynamics. Physical Chemistry Chemical Physics, 2021, 23, 19659-19672.	1.3	13
205	Self-interaction correction in waterâ€“ion clusters. Journal of Chemical Physics, 2021, 154, 094302.	1.2	16
206	Role of water model on ion dissociation at ambient conditions. Journal of Chemical Physics, 2021, 154, 194502.	1.2	6
207	Water Breakup at Fe₂O₃â€“Hematite/Water Interfaces: Influence of External Electric Fields from Nonequilibrium Ab Initio Molecular Dynamics. Journal of Physical Chemistry Letters, 2021, 12, 6818-6826.	2.1	9
208	Modeling Liquid Water by Climbing up Jacobâ€™s Ladder in Density Functional Theory Facilitated by Using Deep Neural Network Potentials. Journal of Physical Chemistry B, 2021, 125, 11444-11456.	1.2	40
209	Using Neural Network Force Fields to Ascertain the Quality of Ab Initio Simulations of Liquid Water. Journal of Physical Chemistry B, 2021, 125, 10772-10778.	1.2	13
210	Structure and Dynamics of Liquid Water from ab Initio Molecular Dynamicsâ€”Comparison of BLYP, PBE, and revPBE Density Functionals with and without van der Waals Corrections. Journal of Chemical Theory and Computation, 2012, 8, 3902-3910.	2.3	116
211	A Two-State Picture of Water and the Funnel of Life. Springer Proceedings in Physics, 2019, , 3-39.	0.1	8
212	Equation of state of water based on the SCAN meta-GGA density functional. Physical Chemistry Chemical Physics, 2020, 22, 4626-4631.	1.3	9
213	Possibility of realizing superionic ice VII in external electric fields of planetary bodies. Science Advances, 2020, 6, eaaz2915.	4.7	18
215	Structure of Micelles of Sodium Dodecyl Sulphate in Water: an X-ray and Dynamic Light Scattering Study. Chemistry Journal of Moldova, 2019, 14, 107-119.	0.3	8
216	Dielectric properties of ice VII under the influence of time-alternating external electric fields. Physical Chemistry Chemical Physics, 2021, , .	1.3	1
217	The microscopic origin of the anomalous isotopic properties of ice relies on the strong quantum anharmonic regime of atomic vibration. Journal of Chemical Physics, 2021, 155, 184502.	1.2	8

#	Article	IF	Citations
218	Photocatalytic Zâ€Scheme Overall Water Splitting: Recent Advances in Theory and Experiments. Advanced Materials, 2021, 33, e2105195.	11.1	123
219	An Introduction to Water. , 2014, , 1-58.		0
220	MP2- and RPA-Based Ab Initio Molecular Dynamics and Monte Carlo Sampling. , 2020, , 523-543.		0
221	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
222	Ab initio 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
223	Ab Initio Simulations of Water/Metal Interfaces. Chemical Reviews, 2022, 122, 10746-10776.	23.0	72
224	Electrocatalysis in Alkaline Media and Alkaline Membrane-Based Energy Technologies. Chemical Reviews, 2022, 122, 6117-6321.	23.0	195
225	Solution and Interface Structure and Dynamics in Geochemistry: Gateway to Link Elementary Processes to Mineral Nucleation and Growth. Crystal Growth and Design, 2022, 22, 853-870.	1.4	8
226	Ordering of a Nanoconfined Water Network around Zinc Ions Induces High Proton Conductivity in Layered Titanate. Chemistry of Materials, 2022, 34, 3967-3975.	3.2	3
227	Assessing the Interplay between Functional-Driven and Density-Driven Errors in DFT Models of Water. Journal of Chemical Theory and Computation, 2022, 18, 3410-3426.	2.3	14
228	Structural and Dynamic Properties of Solvated Hydroxide and Hydronium Ions in Water from Ab Initio Modeling. Journal of Chemical Physics, 0, , .	1.2	8
229	A Deep Neural Network Potential for Water Confined in Graphene Nanocapillaries. Journal of Physical Chemistry C, 2022, 126, 10546-10553.	1.5	7
230	Accurate diffusion coefficients of the excess proton and hydroxide in water via extensive ab initio simulations with different schemes. Journal of Chemical Physics, 2022, 157, .	1.2	2
231	Phase stability, phonon, electronic, and optical properties of not-yet-synthesized CsScS2, CsYS2, and APmS2 (A= Li, Na, K, Rb, Cs) materials: Insights from first-principles calculations. Materials Science in Semiconductor Processing, 2022, 150, 106936.	1.9	4
232	Recent advances in solvation modeling applications: Chemical properties, reaction mechanisms and catalysis. Annual Reports in Computational Chemistry, 2022, , 53-121.	0.9	1
233	Perspectives on weak interactions in complex materials at different length scales. Physical Chemistry Chemical Physics, 2023, 25, 2671-2705.	1.3	10
234	Transport properties in liquids from first-principles: The case of liquid water and liquid argon. Journal of Chemical Physics, 2023, 158, .	1.2	2