Structure, Dynamics, and Spectral Diffusion of Water fr Dynamics

Journal of Physical Chemistry C

118, 29401-29411

DOI: 10.1021/jp506120t

Citation Report

#	Article	IF	Citations
2	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
3	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
4	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
5	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
6	Local structure analysis in ab initio liquid water. Molecular Physics, 2015, 113, 2829-2841.	0.8	96
7	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
8	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
9	The interplay between dynamic heterogeneities and structure of bulk liquid water: A molecular dynamics simulation study. Journal of Chemical Physics, 2015, 142, 244507.	1.2	4
10	Ultrafast Vibrational Echo Spectroscopy of Liquid Water from First-Principles Simulations. Journal of Physical Chemistry B, 2015, 119, 11215-11228.	1.2	24
11	Ionic Hydrogen Bonding Vibration in OH^{â^'}(H₂O)₂₋₄. Journal of Computer Chemistry Japan, 2016, 15, 192-198.	0.0	2
12	Can dispersion corrections annihilate the dispersion-driven nano-aggregation of non-polar groups? An ab initio molecular dynamics study of ionic liquid systems. Journal of Chemical Physics, 2016, 145, 204502.	1.2	13
13	Perspective: How good is DFT for water?. Journal of Chemical Physics, 2016, 144, 130901.	1.2	571
14	From single molecules to water networks: Dynamics of water adsorption on Pt(111). Journal of Chemical Physics, 2016, 145, 094703.	1.2	18
15	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
16	Pressure Dependence of Hydrogen-Bond Dynamics in Liquid Water Probed by Ultrafast Infrared Spectroscopy. Journal of Physical Chemistry Letters, 2016, 7, 3579-3584.	2.1	16
17	HBP Builder: A Tool to Generate Hyperbranched Polymers and Hyperbranched Multi-Arm Copolymers for Coarse-grained and Fully Atomistic Molecular Simulations. Scientific Reports, 2016, 6, 26264.	1.6	10
18	Guanidinium Pairing Facilitates Membrane Translocation. Journal of Physical Chemistry B, 2016, 120, 143-153.	1.2	22
19	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

#	Article	IF	Citations
20	Ab initio molecular dynamics simulations of liquid water using high quality meta-GGA functionals. Chemical Science, 2017, 8, 3554-3565.	3.7	95
21	Revisiting the hydration structure of aqueous Na+. Journal of Chemical Physics, 2017, 146, 084504.	1.2	90
22	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
23	Benchmark Relative Energies for Large Water Clusters with the Generalized Energy-Based Fragmentation Method. Journal of Chemical Theory and Computation, 2017, 13, 2696-2704.	2.3	34
24	Probing the dynamics of N-methylacetamide in methanol via ab initio molecular dynamics. Physical Chemistry Chemical Physics, 2017, 19, 12868-12875.	1.3	12
25	Ab initio molecular dynamics simulations of SO 2 solvation in choline chloride/glycerol deep eutectic solvent. Fluid Phase Equilibria, 2017, 448, 59-68.	1.4	56
26	Quantum Dynamics and Spectroscopy of Ab Initio Liquid Water: TheÂInterplay of Nuclear and Electronic Quantum Effects. Journal of Physical Chemistry Letters, 2017, 8, 1545-1551.	2.1	163
27	Time-dependent vibrational spectral analysis of first principles trajectory of methylamine with wavelet transform. Physical Chemistry Chemical Physics, 2017, 19, 9912-9922.	1.3	17
28	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
29	Formaldehyde-mediated spectroscopic properties of heavy water from first principles simulation. Computational and Theoretical Chemistry, 2017, 1122, 9-15.	1.1	8
30	Theoretical investigation of the solidâ€“liquid phase transition in protonated water clusters. Physical Chemistry Chemical Physics, 2017, 19, 27288-27298.	1.3	11
31	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
32	A First-Principles Molecular Dynamics Study of the Solvation Shell Structure, Vibrational Spectra, Polarity, and Dynamics around a Nitrate Ion in Aqueous Solution. Journal of Physical Chemistry B, 2017, 121, 9032-9044.	1.2	32
33	Structure and polarization near the Li+ ion in ethylene and propylene carbonates. Journal of Chemical Physics, 2017, 147, 161710.	1.2	20
34	Communication: Influence of external static and alternating electric fields on water from long-time non-equilibrium ab initio molecular dynamics. Journal of Chemical Physics, 2017, 147, 031102.	1.2	57
35	Toward chemical accuracy in the description of ionâ€“water interactions through many-body representations. Alkali-water dimer potential energy surfaces. Journal of Chemical Physics, 2017, 147, 161715.	1.2	57
36	Computational Insight into Calciumâ€“Sulfate Ion Pair Formation. Journal of Physical Chemistry C, 2017, 121, 25956-25966.	1.5	31
37	Ab Initio Molecular Dynamics Simulation of the Phosphate Ion in Water: Insights into Solvation Shell Structure, Dynamics, and Kosmotropic Activity. Journal of Physical Chemistry B, 2017, 121, 10519-10529.	1.2	16

#	Article	IF	Citations
38	Orientational order and dynamics of interfacial water near a hexagonal boron-nitride sheet: An ab initio molecular dynamics study. Journal of Chemical Physics, 2017, 147, 164704.	1.2	13
39	Mass density fluctuations in quantum and classical descriptions of liquid water. Journal of Chemical Physics, 2017, 146, 244501.	1.2	44
40	Structure of Hydrated Gibbsite and Brucite Edge Surfaces: DFT Results and Further Development of the ClayFF Classical Force Field with Metalâ€“Oâ€“H Angle Bending Terms. Journal of Physical Chemistry C, 2017, 121, 14757-14771.	1.5	91
41	Interstitial Voids and Resultant Density of Liquid Water: A First-Principles Molecular Dynamics Study. ACS Omega, 2018, 3, 2010-2017.	1.6	23
42	The dissociation mechanism and thermodynamic properties of HCl(aq) in hydrothermal fluids (to) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 226, 84-106.	1.6	29
43	Bornâ€“Oppenheimer Molecular Dynamics Simulations of a Bromate Ion in Water Reveal Its Dual Kosmotropic and Chaotropic Behavior. Journal of Physical Chemistry B, 2018, 122, 2090-2101.	1.2	11
44	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
45	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
46	Structural and Dynamical Nature of Hydration Shells of the Carbonate Ion in Water: An Ab Initio Molecular Dynamics Study. Journal of Physical Chemistry B, 2018, 122, 1495-1504.	1.2	34
47	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
48	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
49	Structuration and Dynamics of Interfacial Liquid Water at Hydrated Î³-Alumina Determined by ab Initio Molecular Simulations: Implications for Nanoparticle Stability. ACS Applied Nano Materials, 2018, 1, 191-199.	2.4	37
50	Water Structure, Dynamics and Ion Adsorption at the Aqueous {010} Brushite Surface. Minerals (Basel, Switzerland), 2018, 8, 334.	0.8	8
51	Vibrational spectral diffusion in supercritical deuterated ammonia from first principles simulations: Roles of hydrogen bonds, free ND modes and inertial rotation of ammonia molecules. Journal of Molecular Liquids, 2018, 269, 896-904.	2.3	2
52	Contribution of the Covalent Component of the Hydrogen-Bond Network to the Properties of Liquid Water. Journal of Physical Chemistry A, 2018, 122, 7482-7490.	1.1	8
53	Dynamics of vibrational frequency fluctuations in deuterated liquid ammonia: roles of fluctuating hydrogen bonds and free ND modes. Molecular Simulation, 2018, 44, 1210-1219.	0.9	1
54	Pressure dependence of structural properties of ice VII: An ab initio molecular-dynamics study. Journal of Chemical Physics, 2018, 148, 204505.	1.2	7
55	Evaluating the London Dispersion Coefficients of Protein Force Fields Using the Exchange-Hole Dipole Moment Model. Journal of Physical Chemistry B, 2018, 122, 6690-6701.	1.2	32

#	Article	IF	Citations
56	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
57	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
58	Ab initio spectroscopy of water under electric fields. Physical Chemistry Chemical Physics, 2019, 21, 21205-21212.	1.3	44
59	Dynamics and Spectral Response of Water Molecules around Tetramethylammonium Cation. Journal of Physical Chemistry B, 2019, 123, 8753-8766.	1.2	24
60	Interfacial Water at Graphene Oxide Surface: Ordered or Disordered?. Journal of Physical Chemistry B, 2019, 123, 1636-1649.	1.2	12
61	Liquid water is a dynamic polydisperse branched polymer. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 1998-2003.	3.3	42
62	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
63	Ion Association in Lanthanide Chloride Solutions. Chemistry - A European Journal, 2019, 25, 8725-8740.	1.7	5
64	Heterogeneous Occupancy and Vibrational Dynamics of Spatially Patterned Water Molecules. Journal of Physical Chemistry B, 2019, 123, 4278-4290.	1.2	2
65	Urea in Water: Structure, Dynamics, and Vibrational Echo Spectroscopy from First-Principles Simulations. Journal of Physical Chemistry B, 2019, 123, 3325-3336.	1.2	15
66	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
67	The dielectric constant: Reconciling simulation and experiment. Journal of Chemical Physics, 2019, 150, 084108.	1.2	28
68	Vibration Spectral Dynamics of Weakly Coordinating Water Molecules near an Anion: FPMD Simulations of an Aqueous Solution of Tetrafluoroborate. Journal of Physical Chemistry B, 2019, 123, 2135-2146.	1.2	4
69	Self-diffusion coefficient of bulk and confined water: a critical review of classical molecular simulation studies. Molecular Simulation, 2019, 45, 425-453.	0.9	130
70	Polarization Corrections and the Hydration Free Energy of Water. Journal of Chemical Theory and Computation, 2019, 15, 1065-1078.	2.3	29
71	Structure and Dynamics of Water at the Waterâ€“Air Interface Using First-Principles Molecular Dynamics Simulations within Generalized Gradient Approximation. Journal of Chemical Theory and Computation, 2019, 15, 595-602.	2.3	18
72	A reactive force field molecular dynamics simulation of the dynamic properties of hydrogen bonding in supercritical water. Journal of Molecular Liquids, 2019, 276, 83-92.	2.3	18
73	ReaxFF molecular dynamics simulations on the structure and dynamics of electrolyte water systems at ambient temperature. Computational Materials Science, 2020, 172, 109349.	1.4	21

#	Article	IF	Citations
74	The role of sulfur in molybdenum transport in hydrothermal fluids: Insight from in situ synchrotron XAS experiments and molecular dynamics simulations. Geochimica Et Cosmochimica Acta, 2020, 290, 162-179.	1.6	12
75	Conformational dynamics of aqueous hydrogen peroxide from first principles molecular dynamics simulations. Physical Chemistry Chemical Physics, 2020, 22, 28286-28296.	1.3	9
76	Calcite (104) Surfaceâ€“Electrolyte Structure: A 3D Comparison of Surface X-ray Diffraction and Simulations. Journal of Physical Chemistry C, 2020, 124, 18564-18575.	1.5	23
77	Temperature dependence of nuclear quantum effects on liquid water via artificial neural network model based on SCAN meta-GGA functional. Journal of Chemical Physics, 2020, 153, 044114.	1.2	22
78	Solvation Shell of the Nitrite Ion in Water: An Ab Initio Molecular Dynamics Study. Journal of Physical Chemistry B, 2020, 124, 7194-7204.	1.2	11
79	Hydrogenâ€Bond Structure and Lowâ€Frequency Dynamics of Electrolyte Solutions: Hydration Numbers from ab Initio Water Reorientation Dynamics and Dielectric Relaxation Spectroscopy. ChemPhysChem, 2020, 21, 2334-2346.	1.0	20
80	Ab Initio Molecular Dynamics Study of Methanol-Water Mixtures under External Electric Fields. Molecules, 2020, 25, 3371.	1.7	15
81	Does Confinement Modify Preferential Solvation and H-Bond Fluctuation Dynamics? A Molecular Level Investigation through Simulations of a Bulk and Confined Three-Component Mixture. Journal of Physical Chemistry B, 2020, 124, 11718-11729.	1.2	10
82	Anomalous Facile Carbamate Formation at High Stripping Temperatures from Carbon Dioxide Reaction with 2-Amino-2-methyl-1-propanol in Aqueous Solution. ACS Sustainable Chemistry and Engineering, 2020, 8, 18671-18677.	3.2	10
83	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
84	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
85	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
86	Dynamics of Water in the Solvation Shell of an Iodate Ion: A Bornâ€“Oppenheimer Molecular Dynamics Study. Journal of Physical Chemistry B, 2020, 124, 2618-2631.	1.2	3
87	Distinctive behavior and two-dimensional vibrational dynamics of water molecules inside glycine solvation shell. RSC Advances, 2020, 10, 6658-6670.	1.7	12
88	Structure and stretching dynamics of water molecules around an amphiphilic amide from FPMD simulations: A case study of N,N-dimethylformamide. Journal of Molecular Liquids, 2020, 302, 112524.	2.3	20
89	Computational modeling of metal ions removal by a modified polypropylene membrane. Chemical Physics Letters, 2020, 749, 137452.	1.2	0
90	Hydration structure and water exchange kinetics at xenotimeâ€“water interfaces: implications for rare earth minerals separation. Physical Chemistry Chemical Physics, 2020, 22, 7719-7727.	1.3	10
91	Yttrium complexation and hydration in chloride-rich hydrothermal fluids: A combined ab initio molecular dynamics and in situ X-ray absorption spectroscopy study. Geochimica Et Cosmochimica Acta, 2020, 281, 168-189.	1.6	18

#	Article	IF	Citations
92	Ion Pairing and Multiple Ion Binding in Calcium Carbonate Solutions Based on a Polarizable AMOEBA Force Field and Ab Initio Molecular Dynamics. Journal of Physical Chemistry B, 2020, 124, 3568-3582.	1.2	30
93	Self-consistent electrostatic embedding for liquid phase polarization. Journal of Molecular Liquids, 2021, 322, 114550.	2.3	7
94	Predicting Vibrational Spectroscopy for Flexible Molecules and Molecules with Nonâ€Idle Environments. Advanced Theory and Simulations, 2021, 4, 2000223.	1.3	19
95	Conformation-induced vibrational spectral dynamics of hydrogen peroxide and vicinal water molecules. Physical Chemistry Chemical Physics, 2021, 23, 6665-6676.	1.3	10
96	Unraveling the Hydroxide Ion Transportation Mechanism along the Surface of Two-Dimensional Layered Double Hydroxide Nanosheets. Journal of Physical Chemistry C, 2021, 125, 1240-1248.	1.5	10
97	When do short-range atomistic machine-learning models fall short?. Journal of Chemical Physics, 2021, 154, 034111.	1.2	61
98	Reactive uptake of N ₂ O ₅ by atmospheric aerosol is dominated by interfacial processes. Science, 2021, 371, 921-925.	6.0	71
99	Quantum Simulations of Hydrogen Bonding Effects in Glycerol Carbonate Electrolyte Solutions. Journal of Physical Chemistry B, 2021, 125, 2157-2166.	1.2	7
100	Intrinsically Polar Piezoelectric Selfâ€Assembled Oligopeptide Monolayers. Advanced Materials, 2021, 33, e2007486.	11.1	12
101	Electric Field and Temperature Effects on the Ab Initio Spectroscopy of Liquid Methanol. Applied Sciences (Switzerland), 2021, 11, 5457.	1.3	1
102	Dynamics of Ionic Liquid through Intrinsic Vibrational Probes Using the Dispersion-Corrected DFT Functionals. Journal of Physical Chemistry B, 2021, 125, 6994-7008.	1.2	11
103	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
104	Electric-field-promoted photo-electrochemical production of hydrogen from water splitting. Journal of Molecular Liquids, 2021, 342, 116949.	2.3	11
105	Nuclear Quantum Effect and Its Temperature Dependence in Liquid Water from Random Phase Approximation via Artificial Neural Network. Journal of Physical Chemistry Letters, 2021, 12, 6354-6362.	2.1	16
106	Possibility of realizing superionic ice VII in external electric fields of planetary bodies. Science Advances, 2020, 6, eaaz2915.	4.7	18
107	Deconstructing waterâ€™s diffuse OH stretching vibrational spectrum with cold clusters. Science, 2019, 364, 275-278.	6.0	53
108	Dielectric properties of ice VII under the influence of time-alternating external electric fields. Physical Chemistry Chemical Physics, 2021, , .	1.3	1
109	Revisiting OD-stretching dynamics of methanolâ€‘d4, ethanol-d6 and dilute HOD/H2O mixture with predefined potentials and wavelet transform spectra. Chemical Physics, 2022, 553, 111385.	0.9	7

#	Article	IF	Citations
110	Dynamics and Surface Propensity of H+ and OHâ€“ within Rigid Interfacial Water: Implications for Electrocatalysis. Journal of Physical Chemistry Letters, 2021, 12, 10128-10134.	2.1	4
111	Molecular dissociation and proton transfer in aqueous methane solution under an electric field. Physical Chemistry Chemical Physics, 2021, 23, 25649-25657.	1.3	2
112	Simulating the binding of key organic functional groups to aqueous calcium carbonate species. Physical Chemistry Chemical Physics, 2021, 23, 27253-27265.	1.3	7
113	2D IR spectra of the intrinsic vibrational probes of ionic liquid from dispersion corrected DFT-MD simulations. Journal of Molecular Liquids, 2022, 348, 118390.	2.3	4
114	Computational Insights into Mg²⁺ Dehydration in the Presence of Carbonate. ACS Earth and Space Chemistry, 2022, 6, 733-745.	1.2	11
115	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
116	Connection between waterâ€™s dynamical and structural properties: Insights from ab initio simulations. Proceedings of the National Academy of Sciences of the United States of America, 2022, 119, e2121641119.	3.3	9
117	Structure and Interactions at the Mg(0001)/Water Interface: An ab initio Study. Journal of Chemical Physics, 0, , .	1.2	2
118	Microheterogeneity-Induced Vibrational Spectral Dynamics of Aqueous 1-Alkyl-3-methylimidazolium Tetrafluoroborate Ionic Liquids of Different Cationic Chain Lengths. Journal of Physical Chemistry B, 0, , .	1.2	4
119	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
120	Equilibrium and Dynamical Characteristics of Hydrogen Bond Bifurcations in Waterâ€“Water and Waterâ€“Ammonia Dimers: A Path Integral Molecular Dynamics Study. Journal of Physical Chemistry A, 2022, 126, 4721-4733.	1.1	5
121	Ionic Dynamics and Vibrational Spectral Diffusion of a Protic Alkylammonium Ionic Salt through Intrinsic Cationic Nâ€“H Vibrational Probe from FPMD Simulations. Journal of Physical Chemistry A, 2022, 126, 5134-5147.	1.1	1
122	Multiple Ensembles of the Hydrogenâ€bonded Network in Ethylammonium Nitrate versus Water from Vibrational Spectral Dynamics of SCNâ€•Probe. ChemPhysChem, 0, , .	1.0	0
123	Understanding speciation and solvation of glyphosate from first principles simulations. Journal of Molecular Liquids, 2022, 365, 120154.	2.3	4
124	Molecular dynamics study of structure and reactions at the hydroxylated Mg(0001)/bulk water interface. Journal of Chemical Physics, 2022, 157, .	1.2	1
125	Quantifying the Structure of Water and Hydrated Monovalent Ions by Density Functional Theory-Based Molecular Dynamics. Journal of Physical Chemistry B, 2022, 126, 10471-10480.	1.2	11
126	Mixed Molecular and Dissociative Water Adsorption on Hydroxylated TiO₂(110): An Infrared Spectroscopy and Ab Initio Molecular Dynamics Study. Journal of Physical Chemistry C, 2022, 126, 21616-21627.	1.5	2
127	A cellulose-derived supramolecule for fast ion transport. Science Advances, 2022, 8, .	4.7	25

#	Article	IF	Citations
128	Data-driven many-body potentials from density functional theory for aqueous phase chemistry. Chemical Physics Reviews, 2023, 4, .	2.6	4
129	Direct Correlation between Short-Range Vibrational Spectral Diffusion and Localized Ion-Cage Dynamics of Water-in-Salt Electrolytes. Journal of Physical Chemistry B, 2023, 127, 236-248.	1.2	1
130	Nature and coordination geometry of geologically relevant aqueous Uranium(VI) complexes up to 400 Â°C: A review and new data. Journal of Hazardous Materials, 2023, 452, 131309.	6.5	0
131	Collective Proton Transfers in Cyclic Waterâ€“Ammonia Tetramers: A Path Integral Machine-Learning Study. Journal of Physical Chemistry A, 2023, 127, 1839-1848.	1.1	0
132	Improved and Always Improving: Reference Formulations for Thermophysical Properties of Water. Journal of Physical and Chemical Reference Data, 2023, 52, .	1.9	9