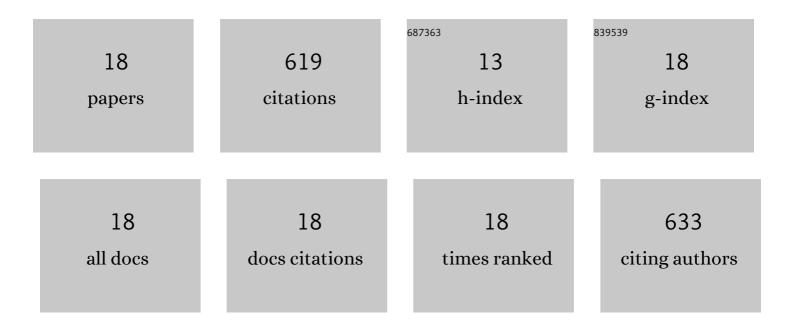
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List of Publications by Year in descending order

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#	Article	IF	CITATIONS
1	Molecular Structure and Modeling of Water–Air and Ice–Air Interfaces Monitored by Sum-Frequency Generation. Chemical Reviews, 2020, 120, 3633-3667.	47.7	97
2	Design principles for high–pressure force fields: Aqueous TMAO solutions from ambient to kilobar pressures. Journal of Chemical Physics, 2016, 144, 144104.	3.0	79
3	Water structure and solvation of osmolytes at high hydrostatic pressure: pure water and TMAO solutions at 10 kbar versus 1 bar. Physical Chemistry Chemical Physics, 2015, 17, 24224-24237.	2.8	67
4	Insights in quantum dynamical effects in the infrared spectroscopy of liquid water from a semiclassical study with an <i>ab initio</i> based flexible and polarizable force field. Journal of Chemical Physics, 2011, 135, 244503.	3.0	63
5	Orientational Distribution of Free O-H Groups of Interfacial Water is Exponential. Physical Review Letters, 2018, 121, 246101.	7.8	49
6	Toward Extreme Biophysics: Deciphering the Infrared Response of Biomolecular Solutions at High Pressures. Angewandte Chemie - International Edition, 2016, 55, 9534-9538.	13.8	47
7	Molecular origin of the difference in the HOH bend of the IR spectra between liquid water and ice. Journal of Chemical Physics, 2013, 138, 054506.	3.0	43
8	Accessing the Accuracy of Density Functional Theory through Structure and Dynamics of the Water–Air Interface. Journal of Physical Chemistry Letters, 2019, 10, 4914-4919.	4.6	43
9	Ultrafast Dynamics of Liquid Water: Energy Relaxation and Transfer Processes of the OH Stretch and the HOH Bend. Journal of Physical Chemistry B, 2015, 119, 11068-11078.	2.6	35
10	Aqueous TMAO solutions as seen by theoretical THz spectroscopy: hydrophilic <i>versus</i> hydrophobic water. Physical Chemistry Chemical Physics, 2018, 20, 6146-6158.	2.8	22
11	Hydrogen-Bonding in Liquid Water at Multikilobar Pressures. Journal of Physical Chemistry B, 2019, 123, 7748-7753.	2.6	15
12	Pressure-dependent electronic structure calculations using integral equation-based solvation models. Biophysical Chemistry, 2020, 257, 106258.	2.8	14
13	Pressure response of the THz spectrum of bulk liquid water revealed by intermolecular instantaneous normal mode analysis. Journal of Chemical Physics, 2019, 150, 084502.	3.0	13
14	Structure and Dynamics of Water at the Water–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.	5.3	12
15	Structure and thermodynamics of aqueous urea solutions from ambient to kilobar pressures: From thermodynamic modeling, experiments, and first principles simulations to an accurate force field description. Biophysical Chemistry, 2019, 254, 106260.	2.8	10
16	Toward Extreme Biophysics: Deciphering the Infrared Response of Biomolecular Solutions at High Pressures. Angewandte Chemie, 2016, 128, 9686-9690.	2.0	4
17	How Can Protons Migrate in Extremely Compressed Liquid Water?. Physical Review Letters, 2020, 125, 086001.	7.8	3
18	Aqueous TMAO solution under high hydrostatic pressure. Physical Chemistry Chemical Physics, 2021, 23, 11355-11365.	2.8	3