

# Structural and Vibrational Properties of Liquid Water from Functionals

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Citation Report

#	ARTICLE	IF	CITATIONS
2	Entropy of Liquid Water from Ab Initio Molecular Dynamics. <i>Journal of Physical Chemistry B</i> , 2011, 115, 14190-14195.	1.2	45
3	Predicting the acidity constant of a goethite hydroxyl group from first principles. <i>Journal of Physics Condensed Matter</i> , 2012, 24, 124105.	0.7	28
4	Reply to "Comment on 'Structure and dynamics of liquid water on rutile TiO <sub>2</sub> (110)'" <i>Physical Review B</i> , 2012, 85, .	1.1	30
5	A Process for Visualizing Disordered Molecular Data with a Case Study in Bulk Water. , 2012, , .		1
6	CO <sub>2</sub> Capture by Metal-Organic Frameworks with van der Waals Density Functionals. <i>Journal of Physical Chemistry A</i> , 2012, 116, 4957-4964.	1.1	92
7	Dispersion Interactions and Vibrational Effects in Ice as a Function of Pressure: A First Principles Study. <i>Physical Review Letters</i> , 2012, 108, 105502.	2.9	55
8	Toward a Universal Water Model: First Principles Simulations from the Dimer to the Liquid Phase. <i>Journal of Physical Chemistry Letters</i> , 2012, 3, 3765-3769.	2.1	137
9	First-Principles Study of the Infrared Spectra of the Ice Ih (0001) Surface. <i>Journal of Physical Chemistry A</i> , 2012, 116, 9255-9260.	1.1	9
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11	Autocatalytic and Cooperatively Stabilized Dissociation of Water on a Stepped Platinum Surface. <i>Journal of the American Chemical Society</i> , 2012, 134, 19217-19222.	6.6	53
12	Improved description of soft layered materials with van der Waals density functional theory. <i>Journal of Physics Condensed Matter</i> , 2012, 24, 424216.	0.7	150
13	Structure and Dynamics of Liquid Water from ab Initio Molecular Dynamics—Comparison of BLYP, PBE, and revPBE Density Functionals with and without van der Waals Corrections. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 3902-3910.	2.3	247
14	MOLECULAR BIOLOGY AT THE QUANTUM LEVEL: CAN MODERN DENSITY FUNCTIONAL THEORY FORGE THE PATH?. <i>Nano LIFE</i> , 2012, 02, 1230006.	0.6	8
15	A simplified implementation of van der Waals density functionals for first-principles molecular dynamics applications. <i>Journal of Chemical Physics</i> , 2012, 136, 224107.	1.2	49
16	Microscopic properties of liquid water from combined ab initio molecular dynamics and energy decomposition studies. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 15746.	1.3	55
17	Raman Spectra of Liquid Water from <i>Ab Initio</i> Molecular Dynamics: Vibrational Signatures of Charge Fluctuations in the Hydrogen Bond Network. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 4124-4130.	2.3	74
18	A closer look at supercritical water. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2013, 110, 6250-6251.	3.3	29
19	First-principles energetics of water clusters and ice: A many-body analysis. <i>Journal of Chemical Physics</i> , 2013, 139, 244504.	1.2	34

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20	Coordination and Hydrolysis of Plutonium Ions in Aqueous Solution Using Carâ€Parrinello Molecular Dynamics Free Energy Simulations. Journal of Physical Chemistry A, 2013, 117, 12256-12267.	1.1	35
21	Room temperature compressibility and diffusivity of liquid water from first principles. Journal of Chemical Physics, 2013, 139, 194502.	1.2	54
22	Hydration structure of salt solutions from <i>ab initio</i> molecular dynamics. Journal of Chemical Physics, 2013, 138, 014501.	1.2	158
23	Electronic excitations in light absorbers for photoelectrochemical energy conversion: first principles calculations based on many body perturbation theory. Chemical Society Reviews, 2013, 42, 2437.	18.7	157
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