First-principles study of the infrared spectrum in liquid improved description of H-bond network

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Citation Report

#	Article	IF	Citations
1	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
2	Accurate Water Properties from an Efficient ab Initio Method. Journal of Chemical Theory and Computation, 2020, 16, 974-987.	2.3	15
3	First-Principles Calculation of Water pK_a Using the Newly Developed SCAN Functional. Journal of Physical Chemistry Letters, 2020, 11, 54-59.	2.1	19
4	A multivariate analysis for enhancing the interpretation of infrared spectra of plant residues on lithic artefacts. Journal of Archaeological Science: Reports, 2020, 33, 102526.	0.2	5
5	Effect of Oxidation Level on the Interfacial Water at the Graphene Oxideâ€“Water Interface: From Spectroscopic Signatures to Hydrogen-Bonding Environment. Journal of Physical Chemistry B, 2020, 124, 8167-8178.	1.2	27
6	Selective CO2 electrocatalysis at the pseudocapacitive nanoparticle/ordered-ligand interlayer. Nature Energy, 2020, 5, 1032-1042.	19.8	99
7	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
8	Vibrational mode frequency correction of liquid water in density functional theory molecular dynamics simulations with van der Waals correction. Physical Chemistry Chemical Physics, 2020, 22, 12785-12793.	1.3	9
9	Enabling Large-Scale Condensed-Phase Hybrid Density Functional Theory Based Ab Initio Molecular Dynamics. 1. Theory, Algorithm, and Performance. Journal of Chemical Theory and Computation, 2020, 16, 3757-3785.	2.3	29
10	Hydrogen bonding interactions between arsenious acid and dithiothreitol/dithioerythritol at different pH values: a computational study with an explicit solvent model. New Journal of Chemistry, 2021, 45, 20181-20192.	1.4	4
11	Effects of applied voltage on water at a gold electrode interface from ab initio molecular dynamics. Chemical Science, 2021, 12, 5865-5873.	3.7	29
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13	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
14	Hydration structures of barium ions: Ab initio molecular dynamics simulations using the SCAN meta-GGA density functional and EXAFS spectroscopy studies. Chemical Physics Letters, 2021, 780, 138945.	1.2	5
15	Isotope effects in molecular structures and electronic properties of liquid water via deep potential molecular dynamics based on the SCAN functional. Physical Review B, 2020, 102, .	1.1	22
16	Temperature-Induced Change of Water Structure in Aqueous Solutions of Some Kosmotropic and Chaotropic Salts. International Journal of Molecular Sciences, 2021, 22, 12896.	1.8	4
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18	Structural and Dynamic Properties of Solvated Hydroxide and Hydronium Ions in Water from Ab Initio Modeling. Journal of Chemical Physics, 0, , .	1.2	8

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19	Extended X-ray absorption fine structure spectroscopy measurements and ab initio molecular dynamics simulations reveal the hydration structure of the radium(II) ion. IScience, 2022, 25, 104763.	1.9	9
20	Superhydrophilicity of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si22.svg"><mml:mrow><mml:mi>Î±</mml:mi></mml:mrow></mml:math>-alumina surfaces results from tight binding of interfacial waters to specific aluminols. Journal of Colloid and Interface Science, 2022, 628, 943-954.	5.0	7