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Accessing the Accuracy of Density Functional Theory through Structure and Dynamics of the Water-Air Interface

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Journal of Physical Chemistry Letters, 2019, 10, 4914-4919.

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#	Paper	IF	Citations
26	Nature of Excess Hydrated Proton at the Water-Air Interface.		
25	First-Principles Calculation of Water p Using the Newly Developed SCAN Functional. <i>Journal of Physical Chemistry Letters</i> , 2020 , 11, 54-59	6.4	12
24	Nature of Excess Hydrated Proton at the Water-Air Interface. <i>Journal of the American Chemical Society</i> , 2020 , 142, 945-952	16.4	16
23	"On-The-Fly" Calculation of the Vibrational Sum-Frequency Generation Spectrum at the Air-Water Interface. <i>Molecules</i> , 2020 , 25,	4.8	4
22	Self-interaction error overbinds water clusters but cancels in structural energy differences. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2020 , 117, 11283-11288	11.5	37
21	Vibrational mode frequency correction of liquid water in density functional theory molecular dynamics simulations with van der Waals correction. <i>Physical Chemistry Chemical Physics</i> , 2020 , 22, 12785-12793	3.6	12793
20	CP2K: An electronic structure and molecular dynamics software package - Quickstep: Efficient and accurate electronic structure calculations. <i>Journal of Chemical Physics</i> , 2020 , 152, 194103	3.9	421
19	Molecular Structure and Modeling of Water-Air and Ice-Air Interfaces Monitored by Sum-Frequency Generation. <i>Chemical Reviews</i> , 2020 , 120, 3633-3667	68.1	43
18	Molecular Dynamics Simulation: Methods and Application. 2020 , 213-238		1
17	Current investigations in theoretical studies of nanostructure-liquid interfaces. <i>Chinese Journal of Physics</i> , 2020 , 65, 93-107	3.5	4
16	Existence of weakly interacting OH bond at air/water interface. <i>Journal of Chemical Physics</i> , 2020 , 152, 134703	3.9	5
15	Decoding the molecular water structure at complex interfaces through surface-specific spectroscopy of the water bending mode. <i>Physical Chemistry Chemical Physics</i> , 2020 , 22, 10934-10940	3.6	9
14	Hydrogen bond dynamics of interfacial water molecules revealed from two-dimensional vibrational sum-frequency generation spectroscopy. <i>Scientific Reports</i> , 2021 , 11, 2456	4.9	1
13	Suitable acid groups and density in electrolytes to facilitate proton conduction. <i>Physical Chemistry Chemical Physics</i> , 2021 , 23, 23778-23786	3.6	0
12	Investigations of water/oxide interfaces by molecular dynamics simulations. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2021 , 11, e1537	7.9	4
11	Predicting the substituent effects in the optical and electrochemical properties of N,N-substituted isoindigos. <i>Photochemical and Photobiological Sciences</i> , 2021 , 20, 927-938	4.2	1
10	Efficient Quantum Vibrational Spectroscopy of Water with High-Order Path Integrals: From Bulk to Interfaces. <i>Journal of Physical Chemistry Letters</i> , 2021 , 12, 9108-9114	6.4	3

9	H/D isotope effect between adsorbed water (H ₂ O, D ₂ O, and HDO) and H ₂ O- and D ₂ O-ice Ih(0 0 0 1) basal surfaces based on the combined plane wave and localized basis set method. <i>Applied Surface Science</i> , 2021 , 561, 150100	6.7	
8	Accurate molecular orientation at interfaces determined by multimode polarization-dependent heterodyne-detected sum-frequency generation spectroscopy via multidimensional orientational distribution function.. <i>Journal of Chemical Physics</i> , 2022 , 156, 094703	3.9	2
7	Effects of stearyl alcohol monolayer on the structure, dynamics and vibrational sum frequency generation spectroscopy of interfacial water.. <i>Physical Chemistry Chemical Physics</i> , 2022 ,	3.6	0
6	New insights into hydrophobicity at nanostructured surfaces: Experiments and computational models. <i>Nanomaterials and Nanotechnology</i> , 2022 , 12, 184798042110623	2.9	1
5	Molecular Features of Hydration Layers: Insights from Simulation, Microscopy, and Spectroscopy. <i>Journal of Physical Chemistry C</i> ,	3.8	0
4	Polarization-Dependent Heterodyne-Detected Sum-Frequency Generation Spectroscopy as a Tool to Explore Surface Molecular Orientation and Ångström-Scale Depth Profiling. <i>Journal of Physical Chemistry B</i> ,	3.4	0
3	Solvent Exchange around Aqueous Zn(II) from Ab Initio Molecular Dynamics Simulations. 2022 , 2, 243-257		0
2	On the Fresnel Factor Correction of Sum-Frequency Generation Spectra of Interfacial Water.		1
1	On the Propensity of Excess Hydroxide Ions at the Alcohol Monolayer/Water Interface.		0