K Thor Wikfeldt

List of Publications by Year
in descending order

31 papers	2,594 citations	279798 23 h-index	434195 31 g-index
31 all docs	31 docs citations	31 times ranked	2881 citing authors

#	Article	IF	Citations
1	Radial distribution functions of water: Models vs experiments. Journal of Chemical Physics, 2019, 151, 044502.	3.0	25
2	Translational and rotational dynamics of high and low density TIP4P/2005 water. Journal of Chemical Physics, 2019, 150, 224507.	3.0	20
3	Coherent X-rays reveal the influence of cage effects on ultrafast water dynamics. Nature Communications, 2018, 9, 1917.	12.8	59
4	Probing the triplet correlation function in liquid water by experiments and molecular simulations. Physical Chemistry Chemical Physics, 2017, 19, 3265-3278.	2.8	14
5	Long-Time Scale Simulations of Tunneling-Assisted Diffusion of Hydrogen on Ice Surfaces at Low Temperature. Journal of Physical Chemistry C, 2017, 121, 1648-1657.	3.1	17
6	Mechanism of enhancement of ferroelectricity of croconic acid with temperature. Physical Chemistry Chemical Physics, 2017, 19, 32216-32225.	2.8	7
7	The structural validity of various thermodynamical models of supercooled water. Journal of Chemical Physics, 2016, 145, 134507.	3.0	41
8	The temperature dependence of intermediate range oxygen-oxygen correlations in liquid water. Journal of Chemical Physics, 2016, 145, 084503.	3.0	33
9	Modeling Molecular Interactions in Water: From Pairwise to Many-Body Potential Energy Functions. Chemical Reviews, 2016, 116, 7501-7528.	47.7	314
10	Requirements of first-principles calculations of X-ray absorption spectra of liquid water. Physical Chemistry Chemical Physics, 2016, 18, 566-583.	2.8	30
11	Molecular reordering processes on ice (0001) surfaces from long timescale simulations. Journal of Chemical Physics, 2014, 141, 234706.	3.0	17
12	Communication: Ab initio simulations of hydrogen-bonded ferroelectrics: Collective tunneling and the origin of geometrical isotope effects. Journal of Chemical Physics, 2014, 140, 041103.	3.0	19
13	Triplet correlation functions in liquid water. Journal of Chemical Physics, 2014, 141, 174504.	3.0	25
14	Ultrafast X-ray probing of water structure below the homogeneous ice nucleation temperature. Nature, 2014, 510, 381-384.	27.8	385
15	A transferable H2O interaction potential based on a single center multipole expansion: SCME. Physical Chemistry Chemical Physics, 2013, 15, 16542.	2.8	32
16	Quantum Effects in the Diffusion of Hydrogen on Ru(0001). Journal of Physical Chemistry Letters, 2013, 4, 1565-1569.	4.6	59
17	The Boson peak in supercooled water. Scientific Reports, 2013, 3, 1980.	3.3	47
18	Selective Probing of the OH or OD Stretch Vibration in Liquid Water Using Resonant Inelastic Soft-X-Ray Scattering. Physical Review Letters, 2013, 111, 193001.	7.8	90

#	Article	IF	Citations
19	In situ X-ray probing reveals fingerprints of surface platinum oxide. Physical Chemistry Chemical Physics, 2011, 13, 262-266.	2.8	110
20	Spatially inhomogeneous bimodal inherent structure of simulated liquid water. Physical Chemistry Chemical Physics, 2011, 13, 19918.	2.8	136
21	Enhanced small-angle scattering connected to the Widom line in simulations of supercooled water. Journal of Chemical Physics, 2011, 134, 214506.	3.0	67
22	Ab Initio van der Waals Interactions in Simulations of Water Alter Structure from Mainly Tetrahedral to High-Density-Like. Journal of Physical Chemistry B, 2011, 115, 14149-14160.	2.6	83
23	Wide-angle X-ray diffraction and molecular dynamics study of medium-range order in ambient and hot water. Physical Chemistry Chemical Physics, 2011, 13, 19997.	2.8	63
24	Reply to Soper et al.: Fluctuations in water around a bimodal distribution of local hydrogen-bonded structural motifs. Proceedings of the National Academy of Sciences of the United States of America, 2010, 107, .	7.1	44
25	Oxygen-oxygen correlations in liquid water: Addressing the discrepancy between diffraction and extended x-ray absorption fine-structure using a novel multiple-data set fitting technique. Journal of Chemical Physics, 2010, 132, 104513.	3.0	37
26	SpecSwap-RMC: a novel reverse Monte Carlo approach using a discrete set of local configurations and pre-computed properties. Journal of Physics Condensed Matter, 2010, 22, 135001.	1.8	12
27	Increasing correlation length in bulk supercooled H2O, D2O, and NaCl solution determined from small angle x-ray scattering. Journal of Chemical Physics, 2010, 133, 134504.	3.0	84
28	Complementarity between high-energy photoelectron and L-edge spectroscopy for probing the electronic structure of 5d transition metal catalysts. Physical Chemistry Chemical Physics, 2010, 12, 5694.	2.8	23
29	The inhomogeneous structure of water at ambient conditions. Proceedings of the National Academy of Sciences of the United States of America, 2009, 106, 15214-15218.	7.1	526
30	On the Range of Water Structure Models Compatible with X-ray and Neutron Diffraction Data. Journal of Physical Chemistry B, 2009, 113, 6246-6255.	2.6	81
31	Diffraction and IR/Raman data do not prove tetrahedral water. Journal of Chemical Physics, 2008, 129, 084502.	3.0	94