Shawn M Kathmann

List of Publications by Year
in descending order

23	815	623734	677142
papers	citations	14 h-index	22 g-index

23	23	23	1073
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Understanding the Surface Potential of Water. Journal of Physical Chemistry B, 2011, 115, 4369-4377.	2.6	157
2	Molecular simulations of heterogeneous ice nucleation. I. Controlling ice nucleation through surface hydrophilicity. Journal of Chemical Physics, 2015, 142, 184704.	3.0	122
3	Molecular simulations of heterogeneous ice nucleation. II. Peeling back the layers. Journal of Chemical Physics, 2015, 142, 184705.	3.0	72
4	Charge and Electric Field Fluctuations in Aqueous NaCl Electrolytes. Journal of Physical Chemistry B, 2013, 117, 10869-10882.	2.6	62
5	Understanding the sensitivity of nucleation kinetics: A case study on water. Journal of Chemical Physics, 2002, 116, 5046.	3.0	61
6	Thermodynamics and Kinetics of Nanoclusters Controlling Gas-to-Particle Nucleation. Journal of Physical Chemistry C, 2009, 113, 10354-10370.	3.1	59
7	Analysis of the Activation and Heterolytic Dissociation of H₂ by Frustrated Lewis Pairs: NH₃/BX₃ (X = H, F, and Cl). Journal of Physical Chemistry A, 2012, 116, 7228-7237.	2.5	51
8	Isomers and Conformers of H(NH2BH2)nH Oligomers:â€‰ Understanding the Geometries and Electronic Structure of Boronâ^'Nitrogenâ^'Hydrogen Compounds as Potential Hydrogen Storage Materials. Journal of Physical Chemistry C, 2007, 111, 3294-3299.	3.1	38
9	Molecular-level origin of the carboxylate head group response to divalent metal ion complexation at the airâ€“water interface. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 14874-14880.	7.1	37
10	Mean Inner Potential of Liquid Water. Physical Review Letters, 2020, 124, 065502.	7.8	32
11	Multicomponent dynamical nucleation theory and sensitivity analysis. Journal of Chemical Physics, 2004, 120, 9133-9141.	3.0	26
12	Isotopomer-selective spectra of a single intact H2O molecule in the Cs+(D2O)5H2O isotopologue: Going beyond pattern recognition to harvest the structural information encoded in vibrational spectra. Journal of Chemical Physics, 2016, 144, 074305.	3.0	23
13	Toward a First-Principles Framework for Predicting Collective Properties of Electrolytes. Accounts of Chemical Research, 2021, 54, 2833-2843.	15.6	21
14	A matter of quantum voltages. Journal of Chemical Physics, 2014, 141, 18C534.	3.0	17
15	Nanometer-Scale Correlations in Aqueous Salt Solutions. Journal of Physical Chemistry Letters, 2020, 11, 2598-2604.	4.6	10
16	Experimental and Theoretical Study of Molecular Response of Amine Bases in Organic Solvents. Journal of Physical Chemistry B, 2014, 118, 4883-4888.	2.6	9
17	A classical reactive potential for molecular clusters of sulphuric acid and water. Molecular Physics, 2016, 114, 172-185.	1.7	8
18	Electric Potentials of Metastable Salt Clusters. Journal of Physical Chemistry C, 2019, 123, 14010-14023.	3.1	4

#	Article	IF	Citations
19	Investigating the significance of zero-point motion in small molecular clusters of sulphuric acid and water. Journal of Chemical Physics, 2014, 140, 024306.	3.0	2
20	Electric fields and potentials in condensed phases. Physical Chemistry Chemical Physics, 2021, 23, 23836-23849.	2.8	2
21	Dynamical consequences of a constraint on the Langevin thermostat in molecular cluster simulation. Molecular Physics, 2014, 112, 2920-2923.	1.7	1
22	Developing New Measurement Capabilities with Nanochannel Liquid Phase TEM. Microscopy and Microanalysis, 2018, 24, 256-257.	0.4	1
23	Measuring Surface Charge on a Single Nanoparticle in Liquids using Off-Axis Electron Holography. Microscopy and Microanalysis, 2018, 24, 1460-1461.	0.4	0