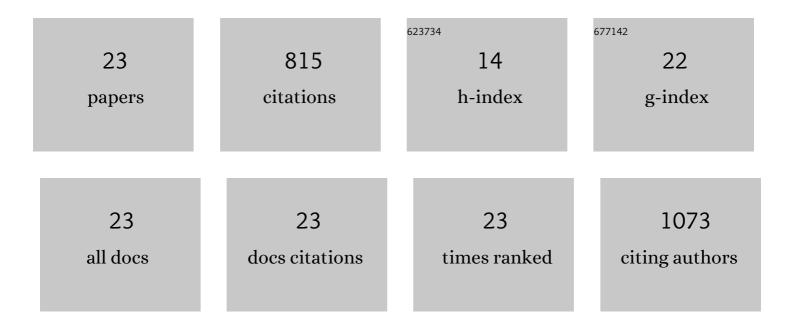
Shawn M Kathmann

List of Publications by Year in descending order

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#	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 H ₂ by Frustrated Lewis Pairs: NH ₃ /BX ₃ (X = H, F, and Cl). Journal of Physical Chemistry A, 2012, 116, 7228-7237.	2.5	51
8	lsomers and Conformers of H(NH2BH2)nH Oligomers:  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 air–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	lsotopomer-selective spectra of a single <i>intact</i> 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	Ο