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	Toward a First-Principles Framework for Predicting Collective Properties of Electrolytes. Accounts of Chemical Research, 2021, 54, 2833-2843.	15.6	21
2	Electric fields and potentials in condensed phases. Physical Chemistry Chemical Physics, 2021, 23, 23836-23849.	2.8	2
3	Nanometer-Scale Correlations in Aqueous Salt Solutions. Journal of Physical Chemistry Letters, 2020, 11, 2598-2604.	4.6	10
4	Mean Inner Potential of Liquid Water. Physical Review Letters, 2020, 124, 065502.	7.8	32
5	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
6	Electric Potentials of Metastable Salt Clusters. Journal of Physical Chemistry C, 2019, 123, 14010-14023.	3.1	4
7	Developing New Measurement Capabilities with Nanochannel Liquid Phase TEM. Microscopy and Microanalysis, 2018, 24, 256-257.	0.4	1
8	Measuring Surface Charge on a Single Nanoparticle in Liquids using Off-Axis Electron Holography. Microscopy and Microanalysis, 2018, 24, 1460-1461.	0.4	0
9	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
10	A classical reactive potential for molecular clusters of sulphuric acid and water. Molecular Physics, 2016, 114, 172-185.	1.7	8
11	Molecular simulations of heterogeneous ice nucleation. I. Controlling ice nucleation through surface hydrophilicity. Journal of Chemical Physics, 2015, 142, 184704.	3.0	122
12	Molecular simulations of heterogeneous ice nucleation. II. Peeling back the layers. Journal of Chemical Physics, 2015, 142, 184705.	3.0	72
13	A matter of quantum voltages. Journal of Chemical Physics, 2014, 141, 18C534.	3.0	17
14	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
15	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
16	Dynamical consequences of a constraint on the Langevin thermostat in molecular cluster simulation. Molecular Physics, 2014, 112, 2920-2923.	1.7	1
17	Charge and Electric Field Fluctuations in Aqueous NaCl Electrolytes. Journal of Physical Chemistry B, 2013, 117, 10869-10882.	2.6	62
18	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

#	Article	IF	Citations
19	Understanding the Surface Potential of Water. Journal of Physical Chemistry B, 2011, 115, 4369-4377.	2.6	157
20	Thermodynamics and Kinetics of Nanoclusters Controlling Gas-to-Particle Nucleation. Journal of Physical Chemistry C, 2009, 113, 10354-10370.	3.1	59
21	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
22	Multicomponent dynamical nucleation theory and sensitivity analysis. Journal of Chemical Physics, 2004, 120, 9133-9141.	3.0	26
23	Understanding the sensitivity of nucleation kinetics: A case study on water. Journal of Chemical Physics, 2002, 116, 5046.	3.0	61