Marcel D Baer

List of Publications by Year
in descending order

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49 papers	2,152 citations	201575 27 h-index	223716 46 g-index
49 all docs	49 docs citations	49 times ranked	2420 citing authors

#	Article	IF	Citations
1	Simulation and Theory of Ions at Atmospherically Relevant Aqueous Liquid-Air Interfaces. Annual Review of Physical Chemistry, 2013, 64, 339-359.	4.8	151
2	Highly stable and self-repairing membrane-mimetic 2D nanomaterials assembled from lipid-like peptoids. Nature Communications, 2016, 7, 12252.	5.8	124
3	Tuning crystallization pathways through sequence engineering of biomimetic polymers. Nature Materials, 2017, 16, 767-774.	13.3	116
4	Supersaturated calcium carbonate solutions are classical. Science Advances, 2018, 4, eaao6283.	4.7	116
5	Toward an Understanding of the Specific Ion Effect Using Density Functional Theory. Journal of Physical Chemistry Letters, 2011, 2, 1088-1093.	2.1	114
6	Toward a Unified Picture of the Water Self-Ions at the Airâ€“Water Interface: A Density Functional Theory Perspective. Journal of Physical Chemistry B, 2014, 118, 8364-8372.	1.2	90
7	Re-examining the properties of the aqueous vaporâ€“liquid interface using dispersion corrected density functional theory. Journal of Chemical Physics, 2011, 135, 124712.	1.2	82
8	Probing the Hydration Structure of Polarizable Halides: A Multiedge XAFS and Molecular Dynamics Study of the Iodide Anion. Journal of Physical Chemistry B, 2010, 114, 12926-12937.	1.2	78
9	The Role of Broken Symmetry in Solvation of a Spherical Cavity in Classical and Quantum Water Models. Journal of Physical Chemistry Letters, 2014, 5, 2767-2774.	2.1	71
10	Is Iodate a Strongly Hydrated Cation?. Journal of Physical Chemistry Letters, 2011, 2, 2650-2654.	2.1	68
11	Electrochemical Surface Potential Due to Classical Point Charge Models Drives Anion Adsorption to the Airâ€“Water Interface. Journal of Physical Chemistry Letters, 2012, 3, 1565-1570.	2.1	67
12	Real single ion solvation free energies with quantum mechanical simulation. Chemical Science, 2017, 8, 6131-6140.	3.7	63
13	Generalized Normal Coordinates for the Vibrational Analysis of Molecular Dynamics Simulations. Journal of Chemical Theory and Computation, 2011, 7, 2028-2039.	2.3	56
14	Persistent Ion Pairing in Aqueous Hydrochloric Acid. Journal of Physical Chemistry B, 2014, 118, 7211-7220.	1.2	53
15	Marcus Theory of Ion-Pairing. Journal of Chemical Theory and Computation, 2017, 13, 3470-3477.	2.3	53
16	An ab initio approach to understanding the specific ion effect. Faraday Discussions, 2013, 160, 89-101.	1.6	49
17	Infrared Spectroscopy of Fluxional Molecules from (ab Initio) Molecular Dynamics: Resolving Large-Amplitude Motion, Multiple Conformations, and Permutational Symmetries. Journal of Chemical Theory and Computation, 2012, 8, 224-234.	2.3	48
18	Mass density fluctuations in quantum and classical descriptions of liquid water. Journal of Chemical Physics, 2017, 146, 244501.	1.2	44

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19	Electrostatic solvation free energies of charged hard spheres using molecular dynamics with density functional theory interactions. Journal of Chemical Physics, 2017, 147, 161716.	1.2	42
20	Local Aqueous Solvation Structure Around Ca²⁺ During Ca²⁺Â·Â·Â·Cl^{â€“} Pair Formation. Journal of Physical Chemistry B, 2016, 120, 1885-1893.	1.2	40
21	Theoretical Messenger Spectroscopy of Microsolvated Hydronium and Zundel Cations. Angewandte Chemie - International Edition, 2010, 49, 7346-7349.	7.2	38
22	Quantifying the hydration structure of sodium and potassium ions: taking additional steps on Jacob's Ladder. Physical Chemistry Chemical Physics, 2020, 22, 10641-10652.	1.3	38
23	Aqueous Cation-Amide Binding: Free Energies and IR Spectral Signatures by Ab Initio Molecular Dynamics. Journal of Physical Chemistry Letters, 2014, 5, 2235-2240.	2.1	37
24	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.	3.3	37
25	Interfacial Behavior of Perchlorate versus Chloride Ions in Aqueous Solutions. Journal of Physical Chemistry B, 2009, 113, 15843-15850.	1.2	36
26	Reaction Rate Theory in Coordination Number Space: An Application to Ion Solvation. Journal of Physical Chemistry C, 2016, 120, 7597-7605.	1.5	36
27	Spectral Signatures of the Pentagonal Water Cluster in Bacteriorhodopsin. ChemPhysChem, 2008, 9, 2703-2707.	1.0	32
28	Ions interacting in solution: Moving from intrinsic to collective properties. Current Opinion in Colloid and Interface Science, 2016, 23, 58-65.	3.4	29
29	Peptoid Backbone Flexibilility Dictates Its Interaction with Water and Surfaces: A Molecular Dynamics Investigation. Biomacromolecules, 2018, 19, 1006-1015.	2.6	28
30	Interpreting Vibrational Sum-Frequency Spectra of Sulfur Dioxide at the Air/Water Interface: A Comprehensive Molecular Dynamics Study. Journal of Physical Chemistry B, 2010, 114, 7245-7249.	1.2	27
31	Water Lone Pair Delocalization in Classical and Quantum Descriptions of the Hydration of Model Ions. Journal of Physical Chemistry B, 2018, 122, 3519-3527.	1.2	27
32	Detecting the undetectable: The role of trace surfactant in the Jones-Ray effect. Journal of Chemical Physics, 2018, 149, 194702.	1.2	27
33	Visualization of Aluminum Ions at the Mica Water Interface Links Hydrolysis State-to-Surface Potential and Particle Adhesion. Journal of the American Chemical Society, 2020, 142, 6093-6102.	6.6	24
34	Direct Observation of the Orientational Anisotropy of Buried Hydroxyl Groups inside Muscovite Mica. Journal of the American Chemical Society, 2019, 141, 2135-2142.	6.6	23
35	Assigning Predissociation Infrared Spectra of Microsolvated Hydronium Cations H₃O⁺â‹…(H₂)_n (n=0, 1, 2, 3) by Ab Initio Molecular Dynamics. ChemPhysChem, 2011, 12, 1906-1915.	1.0	22
36	Divalent Ion Parameterization Strongly Affects Conformation and Interactions of an Anionic Biomimetic Polymer. Journal of Physical Chemistry B, 2016, 120, 2198-2208.	1.2	18

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37	Understanding the scale of the single ion free energy: A critical test of the tetra-phenyl arsonium and tetra-phenyl borate assumption. Journal of Chemical Physics, 2018, 148, 222819.	1.2	18
38	Potential Protonâ€Release Channels in Bacteriorhodopsin. ChemPhysChem, 2008, 9, 2751-2758.	1.0	17
39	Resolving Heterogeneous Dynamics of Excess Protons in Aqueous Solution with Rate Theory. Journal of Physical Chemistry B, 2020, 124, 5665-5675.	1.2	17
40	The Diverse Nature of Ion Speciation at the Nanoscale Hydrophobic/Water Interface. Journal of Physical Chemistry B, 2019, 123, 2414-2423.	1.2	16
41	Highly Bright and Photostable Two-Dimensional Nanomaterials Assembled from Sequence-Defined Peptoids. , 2021, 3, 420-427.		16
42	Early-Stage Aggregation and Crystalline Interactions of Peptoid Nanomembranes. Journal of Physical Chemistry Letters, 2021, 12, 6126-6133.	2.1	14
43	Dependence of the Rate of LiF Ion-Pairing on the Description of Molecular Interaction. Journal of Physical Chemistry B, 2016, 120, 1749-1758.	1.2	13
44	Role of Hydration in Magnesium versus Calcium Ion Pairing with Carboxylate: Solution and the Aqueous Interface. Journal of Physical Chemistry B, 2021, 125, 11308-11319.	1.2	13
45	Solvent reaction coordinate for an SN2 reaction. Journal of Chemical Physics, 2020, 153, 024103.	1.2	11
46	Experimental and DFT Calculated IR Spectra of Guests in Zeolites: Acyclic Olefins and Hostâ€“Guest Interactions. Journal of Physical Chemistry C, 2020, 124, 10561-10572.	1.5	8
47	Regioselectivity mechanism of the Thunbergia alata Î”6-16:0-acyl carrier protein desaturase. Plant Physiology, 2022, 188, 1537-1549.	2.3	3
48	Atomistic insight on structure and dynamics of spinach acyl carrier protein with substrate length. Biophysical Journal, 2021, 120, 3841-3853.	0.2	1
49	The Statistical Mechanics ofÂSolution-Phase Nucleation: CaCO$$_3$$ Revisited. Molecular Modeling and Simulation, 2021, , 101-122.	0.2	1