

# Marcel D Baer

## List of Publications by Year in descending order

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Version: 2024-02-01

49  
papers

2,152  
citations

201674

27  
h-index

223800

46  
g-index

49  
all docs

49  
docs citations

49  
times ranked

2420  
citing authors

#	ARTICLE	IF	CITATIONS
1	Regioselectivity mechanism of the <i>Thunbergia alata</i> 6-16:0-acyl carrier protein desaturase. <i>Plant Physiology</i> , 2022, 188, 1537-1549.	4.8	3
2	Highly Bright and Photostable Two-Dimensional Nanomaterials Assembled from Sequence-Defined Peptoids. <i>ACS Nano</i> , 2021, 3, 420-427.		16
3	Early-Stage Aggregation and Crystalline Interactions of Peptoid Nanomembranes. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 6126-6133.	4.6	14
4	Atomistic insight on structure and dynamics of spinach acyl carrier protein with substrate length. <i>Biophysical Journal</i> , 2021, 120, 3841-3853.	0.5	1
5	The Statistical Mechanics of Solution-Phase Nucleation: CaCO <sub>3</sub> Revisited. <i>Molecular Modeling and Simulation</i> , 2021, , 101-122.	0.2	1
6	Role of Hydration in Magnesium versus Calcium Ion Pairing with Carboxylate: Solution and the Aqueous Interface. <i>Journal of Physical Chemistry B</i> , 2021, 125, 11308-11319.	2.6	13
7	Quantifying the hydration structure of sodium and potassium ions: taking additional steps on Jacob's Ladder. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 10641-10652.	2.8	38
8	Solvent reaction coordinate for an SN2 reaction. <i>Journal of Chemical Physics</i> , 2020, 153, 024103.	3.0	11
9	Resolving Heterogeneous Dynamics of Excess Protons in Aqueous Solution with Rate Theory. <i>Journal of Physical Chemistry B</i> , 2020, 124, 5665-5675.	2.6	17
10	Visualization of Aluminum Ions at the Mica Water Interface Links Hydrolysis State-to-Surface Potential and Particle Adhesion. <i>Journal of the American Chemical Society</i> , 2020, 142, 6093-6102.	13.7	24
11	Experimental and DFT Calculated IR Spectra of Guests in Zeolites: Acyclic Olefins and Host-Guest Interactions. <i>Journal of Physical Chemistry C</i> , 2020, 124, 10561-10572.	3.1	8
12	Molecular-level origin of the carboxylate head group response to divalent metal ion complexation at the air-water interface. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2019, 116, 14874-14880.	7.1	37
13	The Diverse Nature of Ion Speciation at the Nanoscale Hydrophobic/Water Interface. <i>Journal of Physical Chemistry B</i> , 2019, 123, 2414-2423.	2.6	16
14	Direct Observation of the Orientational Anisotropy of Buried Hydroxyl Groups inside Muscovite Mica. <i>Journal of the American Chemical Society</i> , 2019, 141, 2135-2142.	13.7	23
15	Water Lone Pair Delocalization in Classical and Quantum Descriptions of the Hydration of Model Ions. <i>Journal of Physical Chemistry B</i> , 2018, 122, 3519-3527.	2.6	27
16	Peptoid Backbone Flexibility Dictates Its Interaction with Water and Surfaces: A Molecular Dynamics Investigation. <i>Biomacromolecules</i> , 2018, 19, 1006-1015.	5.4	28
17	Supersaturated calcium carbonate solutions are classical. <i>Science Advances</i> , 2018, 4, eaao6283.	10.3	116
18	Detecting the undetectable: The role of trace surfactant in the Jones-Ray effect. <i>Journal of Chemical Physics</i> , 2018, 149, 194702.	3.0	27

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19	Understanding the scale of the single ion free energy: A critical test of the tetra-phenyl arsonium and tetra-phenyl borate assumption. <i>Journal of Chemical Physics</i> , 2018, 148, 222819.	3.0	18
20	Tuning crystallization pathways through sequence engineering of biomimetic polymers. <i>Nature Materials</i> , 2017, 16, 767-774.	27.5	116
21	Electrostatic solvation free energies of charged hard spheres using molecular dynamics with density functional theory interactions. <i>Journal of Chemical Physics</i> , 2017, 147, 161716.	3.0	42
22	Marcus Theory of Ion-Pairing. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 3470-3477.	5.3	53
23	Real single ion solvation free energies with quantum mechanical simulation. <i>Chemical Science</i> , 2017, 8, 6131-6140.	7.4	63
24	Mass density fluctuations in quantum and classical descriptions of liquid water. <i>Journal of Chemical Physics</i> , 2017, 146, 244501.	3.0	44
25	Reaction Rate Theory in Coordination Number Space: An Application to Ion Solvation. <i>Journal of Physical Chemistry C</i> , 2016, 120, 7597-7605.	3.1	36
26	Ions interacting in solution: Moving from intrinsic to collective properties. <i>Current Opinion in Colloid and Interface Science</i> , 2016, 23, 58-65.	7.4	29
27	Highly stable and self-repairing membrane-mimetic 2D nanomaterials assembled from lipid-like peptoids. <i>Nature Communications</i> , 2016, 7, 12252.	12.8	124
28	Divalent Ion Parameterization Strongly Affects Conformation and Interactions of an Anionic Biomimetic Polymer. <i>Journal of Physical Chemistry B</i> , 2016, 120, 2198-2208.	2.6	18
29	Dependence of the Rate of LiF Ion-Pairing on the Description of Molecular Interaction. <i>Journal of Physical Chemistry B</i> , 2016, 120, 1749-1758.	2.6	13
30	Local Aqueous Solvation Structure Around $\text{Ca}^{2+}$ During $\text{Ca}^{2+} \cdot \text{Cl}^{-}$ Pair Formation. <i>Journal of Physical Chemistry B</i> , 2016, 120, 1885-1893.	2.6	40
31	Aqueous Cation-Amide Binding: Free Energies and IR Spectral Signatures by Ab Initio Molecular Dynamics. <i>Journal of Physical Chemistry Letters</i> , 2014, 5, 2235-2240.	4.6	37
32	The Role of Broken Symmetry in Solvation of a Spherical Cavity in Classical and Quantum Water Models. <i>Journal of Physical Chemistry Letters</i> , 2014, 5, 2767-2774.	4.6	71
33	Toward a Unified Picture of the Water Self-Ions at the Air-Water Interface: A Density Functional Theory Perspective. <i>Journal of Physical Chemistry B</i> , 2014, 118, 8364-8372.	2.6	90
34	Persistent Ion Pairing in Aqueous Hydrochloric Acid. <i>Journal of Physical Chemistry B</i> , 2014, 118, 7211-7220.	2.6	53
35	An ab initio approach to understanding the specific ion effect. <i>Faraday Discussions</i> , 2013, 160, 89-101.	3.2	49
36	Simulation and Theory of Ions at Atmospherically Relevant Aqueous Liquid-Air Interfaces. <i>Annual Review of Physical Chemistry</i> , 2013, 64, 339-359.	10.8	151

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37	Infrared Spectroscopy of Fluxional Molecules from (ab Initio) Molecular Dynamics: Resolving Large-Amplitude Motion, Multiple Conformations, and Permutational Symmetries. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 224-234.	5.3	48
38	Electrochemical Surface Potential Due to Classical Point Charge Models Drives Anion Adsorption to the Air-Water Interface. <i>Journal of Physical Chemistry Letters</i> , 2012, 3, 1565-1570.	4.6	67
39	Generalized Normal Coordinates for the Vibrational Analysis of Molecular Dynamics Simulations. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 2028-2039.	5.3	56
40	Toward an Understanding of the Specific Ion Effect Using Density Functional Theory. <i>Journal of Physical Chemistry Letters</i> , 2011, 2, 1088-1093.	4.6	114
41	Is Iodate a Strongly Hydrated Cation?. <i>Journal of Physical Chemistry Letters</i> , 2011, 2, 2650-2654.	4.6	68
42	Assigning Predissociation Infrared Spectra of Microsolvated Hydronium Cations $H_3O^+ \cdots (H_2)_n$ ( $n=0, 1, 2, 3$ ) by Ab Initio Molecular Dynamics. <i>ChemPhysChem</i> , 2011, 12, 1906-1915.	2.1	22
43	Re-examining the properties of the aqueous vapor-liquid interface using dispersion corrected density functional theory. <i>Journal of Chemical Physics</i> , 2011, 135, 124712.	3.0	82
44	Theoretical Messenger Spectroscopy of Microsolvated Hydronium and Zundel Cations. <i>Angewandte Chemie - International Edition</i> , 2010, 49, 7346-7349.	13.8	38
45	Interpreting Vibrational Sum-Frequency Spectra of Sulfur Dioxide at the Air/Water Interface: A Comprehensive Molecular Dynamics Study. <i>Journal of Physical Chemistry B</i> , 2010, 114, 7245-7249.	2.6	27
46	Probing the Hydration Structure of Polarizable Halides: A Multiedge XAFS and Molecular Dynamics Study of the Iodide Anion. <i>Journal of Physical Chemistry B</i> , 2010, 114, 12926-12937.	2.6	78
47	Interfacial Behavior of Perchlorate versus Chloride Ions in Aqueous Solutions. <i>Journal of Physical Chemistry B</i> , 2009, 113, 15843-15850.	2.6	36
48	Potential Proton Release Channels in Bacteriorhodopsin. <i>ChemPhysChem</i> , 2008, 9, 2751-2758.	2.1	17
49	Spectral Signatures of the Pentagonal Water Cluster in Bacteriorhodopsin. <i>ChemPhysChem</i> , 2008, 9, 2703-2707.	2.1	32