Susan B Rempe

List of Publications by Year
in descending order

95 papers	3,766 citations	126907 33 h-index	138484 58 g-index
97 all docs	97 docs citations	97 times ranked	4116 citing authors

#	Article	IF	Citations
1	Coordination numbers of alkali metal ions in aqueous solutions. Biophysical Chemistry, 2006, 124, 192-199.	2.8	269
2	The Hydration Number of Li+ in Liquid Water. Journal of the American Chemical Society, 2000, 122, 966-967.	13.7	219
3	Hydration Structure and Free Energy of Biomolecularly Specific Aqueous Dications, Including Zn2+ and First Transition Row Metals. Journal of the American Chemical Society, 2004, 126, 1285-1289.	13.7	155
4	The glutaminase activity of l-asparaginase is not required for anticancer activity against ASNS-negative cells. Blood, 2014, 123, 3596-3606.	1.4	150
5	Tuning Ion Coordination Architectures to Enable Selective Partitioning. Biophysical Journal, 2007, 93, 1093-1099.	0.5	142
6	The hydration number of Na+ in liquid water. Fluid Phase Equilibria, 2001, 183-184, 121-132.	2.5	137
7	K+/Na+ Selectivity in K Channels and Valinomycin: Over-coordination Versus Cavity-size constraints. Journal of Molecular Biology, 2008, 376, 13-22.	4.2	133
8	Modeling Electrochemical Decomposition of Fluoroethylene Carbonate on Silicon Anode Surfaces in Lithium Ion Batteries. Journal of the Electrochemical Society, 2014, 161, A213-A221.	2.9	132
9	Ab initio molecular dynamics calculations of ion hydration free energies. Journal of Chemical Physics, 2009, 130, 204507.	3.0	111
10	Ab initio molecular dynamics study of glycine intramolecular proton transfer in water. Journal of Chemical Physics, 2005, 122, 184506.	3.0	104
11	Density Functional Theory and DFT+U Study of Transition Metal Porphines Adsorbed on Au(111) Surfaces and Effects of Applied Electric Fields. Journal of the American Chemical Society, 2006, 128, 3659-3668.	13.7	100
12	Inner shell definition and absolute hydration free energy of K+(aq) on the basis of quasi-chemical theory and ab initio molecular dynamics. Physical Chemistry Chemical Physics, 2004, 6, 1966-1969.	2.8	88
13	Theoretical Study of Aqueous Solvation of K⁺ Comparing ab Initio, Polarizable, and Fixed-Charge Models. Journal of Chemical Theory and Computation, 2007, 3, 2068-2082.	5.3	87
14	Salt Permeation and Exclusion in Hydroxylated and Functionalized Silica Pores. Physical Review Letters, 2006, 96, 095504.	7.8	79
15	Design principles for K+ selectivity in membrane transport. Journal of General Physiology, 2011, 137, 479-488.	1.9	74
16	Ab Initio Molecular Dynamics Study of Formate Ion Hydration. Journal of the American Chemical Society, 2004, 126, 344-351.	13.7	73
17	Structural Transitions in Ion Coordination Driven by Changes in Competition for Ligand Binding. Journal of the American Chemical Society, 2008, 130, 15405-15419.	13.7	72
18	Scaling Atomic Partial Charges of Carbonate Solvents for Lithium Ion Solvation and Diffusion. Journal of Chemical Theory and Computation, 2016, 12, 5709-5718.	5.3	64

#	Article	IF	Citations
19	Ultra-thin enzymatic liquid membrane for CO2 separation and capture. Nature Communications, 2018, 9, 990.	12.8	62
20	Interactions and structure of poly(dimethylsiloxane) at silicon dioxide surfaces: Electronic structure and molecular dynamics studies. Journal of Chemical Physics, 2003, 118, 5132-5142.	3.0	60
21	Machine Learning-Guided Approach for Studying Solvation Environments. Journal of Chemical Theory and Computation, 2020, 16, 633-642.	5.3	52
22	Multibody Effects in Ion Binding and Selectivity. Biophysical Journal, 2010, 99, 3394-3401.	0.5	47
23	Glutaminase Activity of <scp>L</scp>-Asparaginase Contributes to Durable Preclinical Activity against Acute Lymphoblastic Leukemia. Molecular Cancer Therapeutics, 2019, 18, 1587-1592.	4.1	46
24	Hydration of krypton and consideration of clathrate models of hydrophobic effects from the perspective of quasi-chemical theory. Biophysical Chemistry, 2003, 105, 323-338.	2.8	45
25	Structural Models and Molecular Thermodynamics of Hydration ofÂIons and Small Molecules. Annual Reports in Computational Chemistry, 2012, 8, 71-127.	1.7	42
26	Role of methyl-induced polarization in ion binding. Proceedings of the National Academy of Sciences of the United States of America, 2013, 110, 12978-12983.	7.1	42
27	Dispersion- and Exchange-Corrected Density Functional Theory for Sodium Ion Hydration. Journal of Chemical Theory and Computation, 2015, 11, 2958-2967.	5.3	42
28	Dielectric Relaxation of Ethylene Carbonate and Propylene Carbonate from Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2016, 120, 1849-1853.	2.6	42
29	Ion-Specific Effects in Carboxylate Binding Sites. Journal of Physical Chemistry B, 2016, 120, 12519-12530.	2.6	41
30	Studies of the Thermodynamic Properties of Hydrogen Gas in Bulk Water. Journal of Physical Chemistry B, 2008, 112, 867-876.	2.6	40
31	A Computational Exercise Illustrating Molecular Vibrations and Normal Modes. The Chemical Educator, 1998, 3, 1-17.	0.0	36
32	Mechanism of Catalysis by <scp>l</scp>-Asparaginase. Biochemistry, 2020, 59, 1927-1945.	2.5	36
33	Quasi-chemical theory and implicit solvent models for simulations. , 1999, , .		34
34	On â€œthe complete basis set limitâ€•and plane-wave methods in first-principles simulations of water. Physical Chemistry Chemical Physics, 2008, 10, 4685.	2.8	34
35	CO2 solvation free energy using quasi-chemical theory. Journal of Chemical Physics, 2011, 134, 224506.	3.0	34
36	Octa-Coordination and the Aqueous Ba²⁺ Ion. Journal of Physical Chemistry B, 2015, 119, 8746-8753.	2.6	34

#	Article	IF	Citations
37	Ab initio rigid water: Effect on water structure, ion hydration, and thermodynamics. Physical Chemistry Chemical Physics, 2006, 8, 2153.	2.8	33
38	First Principles Calculations of Atomic Nickel Redox Potentials and Dimerization Free Energies: A Study of Metal Nanoparticle Growth. Journal of Chemical Theory and Computation, 2011, 7, 485-495.	5.3	33
39	Molecular Dynamics of Lithium Ion Transport in a Model Solid Electrolyte Interphase. Scientific Reports, 2018, 8, 10736.	3.3	33
40	Probing the Thermodynamics of Competitive Ion Binding Using Minimum Energy Structures. Journal of Physical Chemistry B, 2011, 115, 9116-9129.	2.6	32
41	Electrostatic lock in the transport cycle of the multidrug resistance transporter EmrE. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, E7502-E7511.	7.1	32
42	The Impact of Protonation on Early Translocation of Anthrax Lethal Factor: Kinetics from Molecular Dynamics Simulations and Milestoning Theory. Journal of the American Chemical Society, 2017, 139, 14837-14840.	13.7	30
43	Hydration Mimicry by Membrane Ion Channels. Annual Review of Physical Chemistry, 2020, 71, 461-484.	10.8	27
44	Ion Rejection by Nanoporous Membranes in Pressure-Driven Molecular Dynamics Simulations. Journal of Computational and Theoretical Nanoscience, 2009, 6, 1948-1955.	0.4	26
45	Catalytic Role of the Substrate Defines Specificity of Therapeutic l-Asparaginase. Journal of Molecular Biology, 2015, 427, 2867-2885.	4.2	25
46	Molecular Theory and the Effects of Solute Attractive Forces on Hydrophobic Interactions. Journal of Physical Chemistry B, 2016, 120, 1864-1870.	2.6	25
47	Thermodynamics of ion binding and occupancy in potassium channels. Chemical Science, 2021, 12, 8920-8930.	7.4	25
48	The exact quantum mechanical kinetic energy operator in internal coordinates for vibration of a hexatomic molecule. Journal of Chemical Physics, 1998, 108, 10084-10095.	3.0	24
49	Spatiotemporal pH Dynamics in Concentration Polarization near Ion-Selective Membranes. Langmuir, 2014, 30, 7902-7912.	3.5	23
50	Combined Density Functional Theory (DFT) and Continuum Calculations of pK_a in Carbonic Anhydrase. Biochemistry, 2012, 51, 5979-5989.	2.5	22
51	Statistical Analyses of Hydrophobic Interactions: A Mini-Review. Journal of Physical Chemistry B, 2016, 120, 6455-6460.	2.6	22
52	Probing key elements of teixobactinâ€“lipid II interactions in membranes. Chemical Science, 2018, 9, 6997-7008.	7.4	21
53	A Molecular Basis for Advanced Materials in Water Treatment. MRS Bulletin, 2008, 33, 42-47.	3.5	20
54	Hydration of Kr(aq) in Dilute and Concentrated Solutions. Journal of Physical Chemistry B, 2015, 119, 9098-9102.	2.6	20

#	Article	IF	Citations
55	Partitioning of Seven Different Classes of Antibiotics into LPS Monolayers Supports Three Different Permeation Mechanisms through the Outer Bacterial Membrane. Langmuir, 2021, 37, 1372-1385.	3.5	19
56	Molecular basis of endosomal-membrane association for the dengue virus envelope protein. Biochimica Et Biophysica Acta - Biomembranes, 2015, 1848, 1041-1052.	2.6	18
57	Strontium and barium in aqueous solution and a potassium channel binding site. Journal of Chemical Physics, 2018, 148, 222831.	3.0	18
58	Atomistic Study of Intramolecular Interactions in the Closed-State Channelrhodopsin Chimera, C1C2. Biophysical Journal, 2017, 112, 943-952.	0.5	17
59	Utility of chemical computations in predicting solution free energies of metal ions. Molecular Simulation, 2018, 44, 110-116.	2.0	16
60	Assessment of Simple Models for Molecular Simulation of Ethylene Carbonate and Propylene Carbonate as Solvents for Electrolyte Solutions. Topics in Current Chemistry, 2018, 376, 7.	5.8	15
61	First-principles modeling of chemistry in mixed solvents: Where to go from here?. Journal of Chemical Physics, 2020, 152, 130902.	3.0	15
62	Quasi-chemical theory of Fâ˜(aq): The â€œno split occupancies ruleâ€•revisited. Journal of Chemical Physics, 2017, 147, 161728.	3.0	12
63	Insertion of Dengue E into lipid bilayers studied by neutron reflectivity and molecular dynamics simulations. Biochimica Et Biophysica Acta - Biomembranes, 2018, 1860, 1216-1230.	2.6	12
64	Polyelectrolyte layer-by-layer deposition on nanoporous supports for ion selective membranes. RSC Advances, 2018, 8, 32992-32999.	3.6	12
65	Quasi-Chemical Theory with Cluster Sampling from Ab Initio Molecular Dynamics: Fluoride (F^{â€“}) Anion Hydration. Journal of Physical Chemistry A, 2018, 122, 9806-9812.	2.5	12
66	Role of Solute Attractive Forces in the Atomic-Scale Theory of Hydrophobic Effects. Journal of Physical Chemistry B, 2018, 122, 6272-6276.	2.6	12
67	An Information Theory Approach to Nonlinear, Nonequilibrium Thermodynamics. Journal of Statistical Physics, 2011, 145, 385-409.	1.2	11
68	Evaluation of Electrodialysis Desalination Performance of Novel Bioinspired and Conventional Ion Exchange Membranes with Sodium Chloride Feed Solutions. Membranes, 2021, 11, 217.	3.0	11
69	<I>Ab Initio</I> Study of Hydrogen Storage in Water Clathrates. Journal of Computational and Theoretical Nanoscience, 2010, 7, 2602-2606.	0.4	9
70	Hydrated Anions: From Clusters to Bulk Solution with Quasi-Chemical Theory. Accounts of Chemical Research, 2022, 55, 2201-2212.	15.6	9
71	Response to â€œComment on â€˜Ab initio molecular dynamics calculation of ion hydration free energiesâ€™â€‰ [J. Chem. Phys. 133, 047103 (2010)]â€• Journal of Chemical Physics, 2010, 133, .	3.0	8
72	Simulation Study of the Silicon Oxide and Water Interface. Journal of Computational and Theoretical Nanoscience, 2010, 7, 2586-2601.	0.4	8

#	Article	IF	Citations
73	Density Functional Theory and Conductivity Studies of Boron-Based Anion Receptors. Journal of the Electrochemical Society, 2015, 162, A1927-A1934.	2.9	8
74	Molecular Dynamics Simulations of Lithium Ion Transport through a Model Solid Electrolyte Interphase (SEI) Layer. ECS Transactions, 2017, 77, 1155-1162.	0.5	8
75	Ab initio and force field molecular dynamics study of bulk organophosphorus and organochlorine liquid structures. Journal of Chemical Physics, 2021, 154, 084503.	3.0	8
76	Atomic Layer Deposition of <scp>l</scp>-Alanine Polypeptide. Journal of the American Chemical Society, 2014, 136, 15821-15824.	13.7	7
77	Dielectric Properties of Ethylene Carbonate and Propylene Carbonate Using Molecular Dynamics Simulations. ECS Transactions, 2015, 69, 107-111.	0.5	7
78	Molecular Simulation Results on Charged Carbon Nanotube Forestâ€Based Supercapacitors. ChemSusChem, 2018, 11, 1927-1932.	6.8	7
79	The convergence properties of hindered rotor energy levels. Chemical Physics Letters, 1997, 269, 455-463.	2.6	6
80	Irreversible Thermodynamics. Journal of Physics: Conference Series, 2012, 402, 012014.	0.4	6
81	Probing Translocation in Mutants of the Anthrax Channel: Atomically Detailed Simulations with Milestoning. Journal of Physical Chemistry B, 2018, 122, 10296-10305.	2.6	6
82	Design principles for K+ selectivity in membrane transport. Journal of General Physiology, 2011, 138, 279-279.	1.9	5
83	Reduction and Increase in Thermal Conductivity of Si Irradiated with Ga⁺ via Focused Ion Beam. ACS Applied Materials & Interfaces, 2018, 10, 37679-37684.	8.0	5
84	Free Energies of Hydrated Halide Anions: High Through-Put Computations on Clusters to Treat Rough Energy-Landscapes. Molecules, 2021, 26, 3087.	3.8	5
85	Bio-inspired incorporation of phenylalanine enhances ionic selectivity in layer-by-layer deposited polyelectrolyte films. Soft Matter, 2021, 17, 6315-6325.	2.7	5
86	Computing Potential of the Mean Force Profiles for Ion Permeation Through Channelrhodopsin Chimera, C1C2. Methods in Molecular Biology, 2021, 2191, 17-28.	0.9	3
87	Reply to â€œComment on â€˜Probing the Thermodynamics of Competitive Ion Binding Using Minimum Energy Structuresâ€™â€•. Journal of Physical Chemistry B, 2012, 116, 7994-7995.	2.6	2
88	Method for measuring the unbinding energy of strongly-bound membrane-associated proteins. Biochimica Et Biophysica Acta - Biomembranes, 2016, 1858, 2753-2762.	2.6	2
89	Nanoporous Hydrogels for the Observation of Anthrax Exotoxin Translocation Dynamics. ACS Applied Materials & Interfaces, 2018, 10, 13342-13349.	8.0	2
90	Channelrhodopsin C1C2: Photocycle kinetics and interactions near the central gate. Biophysical Journal, 2021, 120, 1835-1845.	0.5	2

#	Article	IF	Citations
91	Enhancing Paraoxon Binding to Organophosphorus Hydrolase Active Site. International Journal of Molecular Sciences, 2021, 22, 12624.	4.1	2
92	Editorial for special issue on ions. Biophysical Chemistry, 2006, 124, 169-170.	2.8	1
93	Tribute to Lawrence R. Pratt. Journal of Physical Chemistry B, 2021, 125, 4925-4927.	2.6	0
94	Quantum Calculations of VX Ammonolysis and Hydrolysis Pathways via Hydrated Lithium Nitride. International Journal of Molecular Sciences, 2021, 22, 8653.	4.1	0
95	Active Role of the Substrate During Catalysis by the Therapeutic Enzyme Lâ€Asparaginase II. FASEB Journal, 2015, 29, 573.51.	0.5	0