Paul E Smith

List of Publications by Year
in descending order

74 papers	5,305 citations	109321 35 h-index	91884 69 g-index
75 all docs	75 docs citations	75 times ranked	3531 citing authors

#	Article	IF	Citations
1	A generalized reaction field method for molecular dynamics simulations. Journal of Chemical Physics, 1995, 102, 5451-5459.	3.0	1,293
2	A Kirkwoodâ˜Buff Derived Force Field for Mixtures of Urea and Water. Journal of Physical Chemistry B, 2003, 107, 3891-3898.	2.6	227
3	Consistent dielectric properties of the simple point charge and extended simple point charge water models at 277 and 300 K. Journal of Chemical Physics, 1994, 100, 3169-3174.	3.0	201
4	A Kirkwoodâ€“Buff derived force field for sodium chloride in water. Journal of Chemical Physics, 2003, 119, 11342-11349.	3.0	199
5	Recent Applications of Kirkwoodâ€“Buff Theory to Biological Systems. Cell Biochemistry and Biophysics, 2008, 50, 1-22.	1.8	199
6	Peptides in ionic solutions: A comparison of the Ewald and switching function techniques. Journal of Chemical Physics, 1991, 95, 8430-8441.	3.0	156
7	Modeling Solvent in Biomolecular Systems. The Journal of Physical Chemistry, 1994, 98, 9700-9711.	2.9	144
8	Kirkwoodâ€“Buff derived force field for mixtures of acetone and water. Journal of Chemical Physics, 2003, 118, 10663-10670.	3.0	131
9	A Kirkwood-Buff Derived Force Field for Aqueous Alkali Halides. Journal of Chemical Theory and Computation, 2011, 7, 1369-1380.	5.3	128
10	The alanine dipeptide free energy surface in solution. Journal of Chemical Physics, 1999, 111, 5568-5579.	3.0	123
11	Molecular Association in Solution:â€‰ A Kirkwoodâ˜Buff Analysis of Sodium Chloride, Ammonium Sulfate, Guanidinium Chloride, Urea, and 2,2,2-Trifluoroethanol in Water. Journal of Physical Chemistry B, 2002, 106, 1491-1500.	2.6	120
12	Cosolvent Interactions with Biomolecules:â€‰ Relating Computer Simulation Data to Experimental Thermodynamic Data. Journal of Physical Chemistry B, 2004, 108, 18716-18724.	2.6	113
13	A Kirkwoodâ˜Buff Derived Force Field for Methanol and Aqueous Methanol Solutions. Journal of Physical Chemistry B, 2005, 109, 15080-15086.	2.6	110
14	Chemical Potential Derivatives and Preferential Interaction Parameters in Biological Systems from Kirkwood-Buff Theory. Biophysical Journal, 2006, 91, 849-856.	0.5	107
15	Computer Simulation of Cosolvent Effects on Hydrophobic Hydration. Journal of Physical Chemistry B, 1999, 103, 525-534.	2.6	102
16	Properties of 2,2,2-trifluoroethanol and water mixtures. Journal of Chemical Physics, 2001, 114, 426.	3.0	100
17	Ewald artifacts in liquid state molecular dynamics simulations. Journal of Chemical Physics, 1996, 105, 4289-4293.	3.0	95
18	A comparison of the properties of 2,2,2-trifluoroethanol and 2,2,2-trifluoroethanol/water mixtures using different force fields. Journal of Chemical Physics, 2001, 115, 5521-5530.	3.0	93

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19	Effects of salt on the structure and dynamics of the bis(penicillamine) enkephalin zwitterion: a simulation study. Journal of the American Chemical Society, 1991, 113, 6029-6037.	13.7	88
20	Translational and Rotational Diffusion of Proteins. Journal of Molecular Biology, 1994, 236, 629-636.	4.2	80
21	Preferential Interactions of Cosolvents with Hydrophobic Solutes. Journal of Physical Chemistry B, 2001, 105, 11513-11522.	2.6	80
22	A Kirkwood-Buff derived force field for the simulation of aqueous guanidinium chloride solutions. Journal of Chemical Physics, 2004, 121, 2180-2186.	3.0	78
23	Predictions of free energy differences from a single simulation of the initial state. Journal of Chemical Physics, 1994, 100, 577-585.	3.0	72
24	A Kirkwood-Buff derived force field for amides. Journal of Computational Chemistry, 2006, 27, 1477-1485.	3.3	69
25	Molecular Dynamics Simulations of the Properties of Cosolvent Solutions. Journal of Physical Chemistry B, 2000, 104, 5854-5864.	2.6	66
26	Equilibrium Dialysis Data and the Relationships between Preferential Interaction Parameters for Biological Systems in Terms of Kirkwoodâ^'Buff Integrals. Journal of Physical Chemistry B, 2006, 110, 2862-2868.	2.6	59
27	Preferential interaction parameters in biological systems by Kirkwoodâ€“Buff theory and computer simulation. Fluid Phase Equilibria, 2007, 256, 14-19.	2.5	53
28	Developing force fields from the microscopic structure of solutions. Fluid Phase Equilibria, 2010, 290, 43-47.	2.5	53
29	On the Kirkwoodâ€“Buff inversion procedure. Journal of Chemical Physics, 2008, 129, 124509.	3.0	50
30	A Combined Simulation and Kirkwoodâ^'Buff Approach to Quantify Cosolvent Effects on the Conformational Preferences of Peptides in Solution. Journal of Physical Chemistry B, 2004, 108, 7382-7388.	2.6	47
31	On the Presence of Rotational Ewald Artifacts in the Equilibrium and Dynamical Properties of a Zwitterionic Tetrapeptide in Aqueous Solution. Journal of Physical Chemistry B, 1997, 101, 3886-3890.	2.6	46
32	Cavity formation and preferential interactions in urea solutions: Dependence on urea aggregation. Journal of Chemical Physics, 2003, 118, 5901-5910.	3.0	46
33	On the Theory of Solute Solubility in Mixed Solvents. Journal of Physical Chemistry B, 2008, 112, 7875-7884.	2.6	44
34	Kirkwoodâ€“Buff theory of molecular and protein association, aggregation, and cellular crowding. Journal of Chemical Physics, 2009, 131, 165101.	3.0	39
35	A Kirkwoodâ€“Buff force field for the aromatic amino acids. Physical Chemistry Chemical Physics, 2011, 13, 18154.	2.8	39
36	Peptides in ionic solutions: a simulation study of a bis(penicillamine) enkephalin in sodium acetate solution. Journal of the American Chemical Society, 1993, 115, 7493-7498.	13.7	33

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37	Local Chemical Potential Equalization Model for Cosolvent Effects on Biomolecular Equilibria. Journal of Physical Chemistry B, 2004, 108, 16271-16278.	2.6	32
38	Structure and stability of a model pyrimidine-purine-purine DNA triple helix with a GC.cntdot.T mismatch by simulation. Biochemistry, 1995, 34, 16269-16278.	2.5	30
39	Theory and Computer Simulation of Solute Effects on the Surface Tension of Liquids. Journal of Physical Chemistry B, 2008, 112, 8975-8984.	2.6	29
40	Conformations of nicotinamide adenine dinucleotide (NAD+) in various environments. , 2000, 13, 27-34.		27
41	Single-Molecule Imaging Revealing the Deformation-Induced Formation of a Molecular Polymer Blend. Journal of Physical Chemistry B, 2000, 104, 5221-5224.	2.6	27
42	A Kirkwoodâ^'Buff Derived Force Field for Thiols, Sulfides, and Disulfides. Journal of Physical Chemistry B, 2009, 113, 12306-12315.	2.6	27
43	Kirkwoodâ€“Buff integrals for ideal solutions. Journal of Chemical Physics, 2010, 132, 164501.	3.0	25
44	Modeling and simulation of the human Î´ opioid receptor. Protein Science, 2004, 13, 1997-2008.	7.6	23
45	Local fluctuations in solution mixtures. Journal of Chemical Physics, 2011, 135, 044506.	3.0	23
46	Preferential Solvation in Binary and Ternary Mixtures. Journal of Physical Chemistry B, 2015, 119, 15706-15717.	2.6	22
47	A conformational analysis of leucine enkephalin as a function of pH. Biopolymers, 2002, 64, 177-188.	2.4	21
48	Kirkwoodâ€“Buff theory of four and higher component mixtures. Journal of Chemical Physics, 2008, 128, 244511.	3.0	21
49	A Kirkwood-Buff derived force field for alkaline earth halide salts. Journal of Chemical Physics, 2018, 148, 222828.	3.0	21
50	Fluctuation theory of molecular association and conformational equilibria. Journal of Chemical Physics, 2011, 135, 014502.	3.0	20
51	Theory and Simulation of Multicomponent Osmotic Systems. Journal of Chemical Theory and Computation, 2012, 8, 3493-3503.	5.3	20
52	Gas or Liquid? The Supercritical Behavior of Pure Fluids. Journal of Physical Chemistry B, 2019, 123, 6554-6563.	2.6	19
53	Local Fluctuations in Solution: Theory and Applications. Advances in Chemical Physics, 2013, 153, 311-372.	0.3	18
54	Amino acid side-chain populations in aqueous and saline solution: Bis-penicillamine enkephalin. Biopolymers, 1992, 32, 1623-1629.	2.4	17

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55	Protein volume changes on cosolvent denaturation. Biophysical Chemistry, 2005, 113, 299-302.	2.8	16
56	The effect of urea on the morphology of NaCl crystals: A combined theoretical and simulation study. Fluid Phase Equilibria, 2010, 290, 36-42.	2.5	15
57	Particle and Energy Pair and Triplet Correlations in Liquids and Liquid Mixtures from Experiment and Simulation. Journal of Physical Chemistry B, 2015, 119, 7761-7777.	2.6	15
58	To Polarize or Not to Polarize? Charge-on-Spring versus KBFF Models for Water and Methanol Bulk and Vaporâ€“Liquid Interfacial Mixtures. Journal of Chemical Theory and Computation, 2016, 12, 2373-2387.	5.3	15
59	Rationally designed peptide nanosponges for cell-based cancer therapy. Nanomedicine: Nanotechnology, Biology, and Medicine, 2017, 13, 2555-2564.	3.3	14
60	Kirkwoodâ€“Buff-Derived Force Field for Peptides and Proteins: Philosophy and Development of KBFF20. Journal of Chemical Theory and Computation, 2021, 17, 2964-2990.	5.3	14
61	Fluctuation Solution Theory. , 2013, , 1-34.		13
62	How Osmolytes Counteract Pressure Denaturation on a Molecular Scale. ChemPhysChem, 2017, 18, 2243-2249.	2.1	13
63	Infinitely Dilute Partial Molar Properties of Proteins from Computer Simulation. Journal of Physical Chemistry B, 2014, 118, 12844-12854.	2.6	11
64	Fluctuation solution theory of pure fluids. Journal of Chemical Physics, 2017, 146, .	3.0	11
65	Experimental triplet and quadruplet fluctuation densities and spatial distribution function integrals for pure liquids. Journal of Chemical Physics, 2015, 142, 044502.	3.0	9
66	Experimental triplet and quadruplet fluctuation densities and spatial distribution function integrals for liquid mixtures. Journal of Chemical Physics, 2015, 142, 094504.	3.0	8
67	A simple two-dimensional representation for the common secondary structural elements of polypeptides and proteins. , 1997, 27, 227-233.		7
68	Gaussian and non-Gaussian fluctuations in pure classical fluids. Journal of Chemical Physics, 2017, 146, 094509.	3.0	7
69	Simulated pressure denaturation thermodynamics of ubiquitin. Biophysical Chemistry, 2017, 231, 135-145.	2.8	6
70	Kirkwoodâ€“Buff-Derived Force Field for Peptides and Proteins: Applications of KBFF20. Journal of Chemical Theory and Computation, 2021, 17, 2991-3009.	5.3	6
71	The Effects of Internal Water Molecules on the Structure and Dynamics of Chymotrypsin Inhibitor 2. Journal of Physical Chemistry B, 2003, 107, 1395-1402.	2.6	3
72	Classical harmonic model for the behavior of pure fluids at the critical point. Physical Chemistry Chemical Physics, 2019, 21, 8004-8014.	2.8	2

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73	Experimental investigation of triplet correlation approximations for fluid water. Fluid Phase Equilibria, 2018, 470, 38-50.	2.5	0
74	The flexible connection of the Nâ€terminal domain in ClpB supports substrate binding and controls the aggregate reactivation efficiency. FASEB Journal, 2011, 25, 907.7.	0.5	0