Henry S Ashbaugh

List of Publications by Year in Descending Order

99 papers	3,245 citations	32 h-index	54 g-index
102 ext. papers	3,483 ext. citations	5.6 avg, IF	5.44 L-index

#	Paper	IF	Citations
99	Blending Linear and Cyclic Block Copolymers to Manipulate Nanolithographic Feature Dimensions.. *ACS Applied Polymer Materials*, **2022**, 4, 327-337	4.3	0
98	Buffer and Salt Effects in Aqueous Host-Guest Systems: Screening, Competitive Binding, or Both?. *Journal of the American Chemical Society*, **2021**, 143, 18605-18616	16.4	7
97	Cavitand Complexes in Aqueous Solution: Collaborative Experimental and Computational Studies of the Wetting, Assembly, and Function of Nanoscopic Bowls in Water. *Journal of Physical Chemistry B*, **2021**, 125, 3253-3268	3.4	8
96	Tribute to Lawrence R. Pratt. *Journal of Physical Chemistry B*, **2021**, 125, 4925-4927	3.4	
95	Evolution of the Free Energy Landscapes of -Alkane Guests Bound within Supramolecular Complexes. *Journal of Physical Chemistry B*, **2021**, 125, 7299-7310	3.4	0
94	Bridging Gaussian Density Fluctuations from Microscopic to Macroscopic Volumes: Applications to Non-Polar Solute Hydration Thermodynamics. *Journal of Physical Chemistry B*, **2021**, 125, 8152-8164	3.4	2
93	Assessment of scaled particle theory predictions of the convergence of solvation entropies. *Fluid Phase Equilibria*, **2021**, 530, 112885	2.5	2
92	Reversal of the Temperature Dependence of Hydrophobic Hydration in Supercooled Water. *Journal of Physical Chemistry Letters*, **2021**, 12, 8370-8375	6.4	0
91	Spontaneous drying of non-polar deep-cavity cavitand pockets in aqueous solution. *Nature Chemistry*, **2020**, 12, 589-594	17.6	22
90	Pressure Induced Wetting and Dewetting of the Nonpolar Pocket of Deep-Cavity Cavitands in Water. *Journal of Physical Chemistry B*, **2020**, 124, 4781-4792	3.4	3
89	Proximal charge effects on guest binding to a non-polar pocket. *Chemical Science*, **2020**, 11, 3656-3663	9.4	11
88	Emergence of non-monotonic deep cavity cavitand assembly with increasing portal methylation. *Molecular Systems Design and Engineering*, **2020**, 5, 656-665	4.6	2
87	Nonpolar solute cononsolvency in ethanol/water mixtures Connections to solvent structure. *Journal of Molecular Liquids*, **2020**, 298, 111944	6	3
86	Temperature, Pressure, and Concentration Derivatives of Nonpolar Gas Hydration: Impact on the Heat Capacity, Temperature of Maximum Density, and Speed of Sound of Aqueous Mixtures. *Journal of Physical Chemistry B*, **2020**, 124, 6924-6942	3.4	6
85	Nanostructure stability and swelling of ternary block copolymer/homopolymer blends: A direct comparison between dissipative particle dynamics and experiment. *Journal of Polymer Science, Part B: Polymer Physics*, **2019**, 57, 794-803	2.6	10
84	Electrostatic Control of Macrocyclization Reactions within Nanospaces. *Journal of the American Chemical Society*, **2019**, 141, 6740-6747	16.4	42
83	Evaluation of second osmotic virial coefficients from molecular simulation following scaled-particle theory. *Molecular Simulation*, **2019**, 45, 1403-1410	2	1

82	Impact of Cyclic Block Copolymer Chain Architecture and Degree of Polymerization on Nanoscale Domain Spacing: A Simulation and Scaling Theory Analysis. *Macromolecules*, **2019**, 52, 9389-9397	5.5	9
81	Temperature-Dependent Hydrophobic Crossover Length Scale and Water Tetrahedral Order. *Journal of Physical Chemistry Letters*, **2018**, 9, 1012-1017	6.4	35
80	Alkane guest packing drives switching between multimeric deep-cavity cavitand assembly states. *Chemical Communications*, **2018**, 54, 2639-2642	5.8	4
79	The Thermodynamics of Anion Complexation to Nonpolar Pockets. *Journal of Physical Chemistry B*, **2018**, 122, 1702-1713	3.4	18
78	Note: Second osmotic virial coefficients of short alkanes and their alcohol counterparts in water as a function of temperature. *Journal of Chemical Physics*, **2018**, 148, 016101	3.9	1
77	Connections between the Anomalous Volumetric Properties of Alcohols in Aqueous Solution and the Volume of Hydrophobic Association. *Journal of Physical Chemistry B*, **2018**, 122, 3242-3250	3.4	7
76	Synthesis and Self-Assembly of Amphiphilic Star/Linear-Dendritic Polymers: Effect of Core versus Peripheral Branching on Reverse Micelle Aggregation. *Biomacromolecules*, **2018**, 19, 3177-3189	6.9	9
75	Methane Hydration-Shell Structure and Fragility. *Angewandte Chemie - International Edition*, **2018**, 57, 15133-15137	16.4	29
74	Methane Hydration-Shell Structure and Fragility. *Angewandte Chemie*, **2018**, 130, 15353-15357	3.6	
73	Guest Controlled Nonmonotonic Deep Cavity Cavitand Assembly State Switching. *Journal of Physical Chemistry B*, **2017**, 121, 10717-10725	3.4	10
72	Resolving solvophobic interactions inferred from experimental solvation free energies and evaluated from molecular simulations. *Chemical Physics Letters*, **2017**, 667, 62-67	2.5	1
71	Succession of Alkane Conformational Motifs Bound within Hydrophobic Supramolecular Capsular Assemblies. *Journal of Physical Chemistry B*, **2016**, 120, 10394-10402	3.4	18
70	Cooperative hydrophobe aggregation mediated by interfacially active alcohols. *Fluid Phase Equilibria*, **2016**, 407, 255-261	2.5	1
69	Communication: Stiffening of dilute alcohol and alkane mixtures with water. *Journal of Chemical Physics*, **2016**, 145, 201102	3.9	13
68	Temperature and pressure dependence of the interfacial free energy against a hard surface in contact with water and decane. *Journal of Chemical Physics*, **2016**, 145, 124710	3.9	5
67	Hydrated nonpolar solute volumes: Interplay between size, Attractiveness, and molecular structure. *Biophysical Chemistry*, **2016**, 213, 1-5	3.5	6
66	Design of Amphiphilic Polymers via Molecular Dynamics Simulations. *Journal of Physical Chemistry B* , **2016**, 120, 10603-10610	3.4	8
65	Scaled-particle theory analysis of cylindrical cavities in solution. *Physical Review E*, **2015**, 91, 042315	2.4	2

64	Effect of hydrostatic pressure on gas solubilization in micelles. *Langmuir*, **2015**, 31, 3318-25	4	6
63	Temperature and pressure dependence of methane correlations and osmotic second virial coefficients in water. *Journal of Physical Chemistry B*, **2015**, 119, 6280-94	3.4	25
62	Note: Nonpolar solute partial molar volume response to attractive interactions with water. *Journal of Chemical Physics*, **2014**, 140, 016101	3.9	2
61	Direct Evaluation of Polypeptide Partial Molar Volumes in Water Using Molecular Dynamics Simulations. *Journal of Chemical & Engineering Data*, **2014**, 59, 3130-3135	2.8	8
60	Molecular dynamics simulations of linear and cyclic amphiphilic polymers in aqueous and organic environments. *Journal of Physical Chemistry B*, **2014**, 118, 6491-7	3.4	13
59	Molecular-scale hydrophobic interactions between hard-sphere reference solutes are attractive and endothermic. *Proceedings of the National Academy of Sciences of the United States of America*, **2013**, 110, 20557-62	11.5	36
58	Simulation optimization of spherical non-polar guest recognition by deep-cavity cavitands. *Journal of Chemical Physics*, **2013**, 139, 234502	3.9	12
57	Pressure reentrant assembly: direct simulation of volumes of micellization. *Langmuir*, **2013**, 29, 14743-7	4	9
56	Solvent cavitation under solvophobic confinement. *Journal of Chemical Physics*, **2013**, 139, 064702	3.9	14
55	Numerical validation of IFT in the analysis of protein-surfactant complexes with SAXS and SANS. *Langmuir*, **2012**, 28, 12593-600	4	19
54	Confinement induced conformational changes in n-alkanes sequestered within a narrow carbon nanotube. *Physical Chemistry Chemical Physics*, **2012**, 14, 2702-9	3.6	19
53	Cosolvent preferential molecular interactions in aqueous solutions. *Journal of Physical Chemistry B*, **2011**, 115, 13633-42	3.4	9
52	Carbon microspheres as network nodes in a novel biocompatible gel. *Soft Matter*, **2011**, 7, 4170	3.6	16
51	Helix stabilization of poly(ethylene glycol)-peptide conjugates. *Biomacromolecules*, **2011**, 12, 2729-34	6.9	49
50	Optimization of linear and branched alkane interactions with water to simulate hydrophobic hydration. *Journal of Chemical Physics*, **2011**, 135, 054510	3.9	32
49	Putting the squeeze on cavities in liquids: Quantifying pressure effects on solvation using simulations and scaled-particle theory. *Journal of Chemical Physics*, **2011**, 134, 014507	3.9	15
48	Assessing the thermodynamic signatures of hydrophobic hydration for several common water models. *Journal of Chemical Physics*, **2010**, 132, 124504	3.9	64
47	Entropy crossover from molecular to macroscopic cavity hydration. *Chemical Physics Letters*, **2009**, 477, 109-111	2.5	21

46	Tuning the globular assembly of hydrophobic/hydrophilic heteropolymer sequences. *Journal of Physical Chemistry B*, **2009**, 113, 14043-6	3.4	19
45	Blowing bubbles in Lennard-Jonesium along the saturation curve. *Journal of Chemical Physics*, **2009**, 130, 204517	3.9	20
44	Natively unfolded protein stability as a coil-to-globule transition in charge/hydropathy space. *Journal of the American Chemical Society*, **2008**, 130, 9536-42	16.4	56
43	Aqueous Partial Molar Volumes from Simulation and Individual Group Contributions. *Industrial & Engineering Chemistry Research*, **2008**, 47, 5169-5174	3.9	19
42	Digging a hole: Scaled-particle theory and cavity solvation in organic solvents. *Journal of Chemical Physics*, **2008**, 129, 174505	3.9	15
41	Single ion hydration free energies: a consistent comparison between experiment and classical molecular simulation. *Journal of Chemical Physics*, **2008**, 129, 204501	3.9	29
40	Contrasting nonaqueous against aqueous solvation on the basis of scaled-particle theory. *Journal of Physical Chemistry B*, **2007**, 111, 9330-6	3.4	36
39	Non-van der Waals treatment of the hydrophobic solubilities of CF4. *Journal of the American Chemical Society*, **2007**, 129, 10133-40	16.4	35
38	An analysis of molecular packing and chemical association in liquid water using quasichemical theory. *Journal of Chemical Physics*, **2006**, 124, 224502	3.9	37
37	Mesoscopically ordered organosilica and carbon-silica hybrids with uniform morphology by surfactant-assisted self-assembly of organo bis-silanetriols. *Chemical Communications*, **2006**, 1545-7	5.8	14
36	Thermochromatism and structural evolution of metastable polydiacetylenic crystals. *Journal of Physical Chemistry B*, **2006**, 110, 7221-5	3.4	65
35	Colloquium: Scaled particle theory and the length scales of hydrophobicity. *Reviews of Modern Physics*, **2006**, 78, 159-178	40.5	319
34	Monomer Hydrophobicity as a Mechanism for the LCST Behavior of Poly(ethylene oxide) in Water. *Industrial & Engineering Chemistry Research*, **2006**, 45, 5531-5537	3.9	52
33	Responsive periodic mesoporous polydiacetylene/silica nanocomposites. *Journal of the American Chemical Society*, **2006**, 128, 5304-5	16.4	136
32	Deblurred observation of the molecular structure of an oil-water interface. *Journal of the American Chemical Society*, **2005**, 127, 2808-9	16.4	54
31	Polydiacetylene/silica nanocomposites with tunable mesostructure and thermochromatism from diacetylenic assembling molecules. *Journal of the American Chemical Society*, **2005**, 127, 12782-3	16.4	99
30	Interaction of Paraffin Wax Gels with Ethylene/Vinyl Acetate Co-polymers. *Energy & Fuels*, **2005**, 19, 138-144	4.1	96
29	Mesoscale model of polymer melt structure: self-consistent mapping of molecular correlations to coarse-grained potentials. *Journal of Chemical Physics*, **2005**, 122, 104908	3.9	59

28	Effects of nonpolar solutes on the thermodynamic response functions of aqueous mixtures. *Journal of Chemical Physics*, **2005**, 123, 164503	3.9	25
27	Response to Comment on A simple molecular thermodynamic theory of hydrophobic hydration [J. Chem. Phys. 119, 10448 (2003)]. *Journal of Chemical Physics*, **2003**, 119, 10450-10451	3.9	4
26	Absolute hydration free energies of ions, ion water clusters, and quasichemical theory. *Journal of Chemical Physics*, **2003**, 119, 2702-2708	3.9	183
25	Hydration of krypton and consideration of clathrate models of hydrophobic effects from the perspective of quasi-chemical theory. *Biophysical Chemistry*, **2003**, 105, 323-38	3.5	45
24	Alkane Adsorption at the Water Vapor Interface. *Langmuir*, **2003**, 19, 7638-7645	4	27
23	Self-consistent molecular field theory for packing in classical liquids. *Physical Review E*, **2003**, 68, 021505	2.4	20
22	Gelation of "catanionic" vesicles by hydrophobically modified polyelectrolytes. *Colloid and Polymer Science*, **2002**, 280, 783-788	2.4	32
21	Conformational equilibria of polar and charged flexible polymer chains in water. *Polymer*, **2002**, 43, 559-565	3.9	2
20	A simple molecular thermodynamic theory of hydrophobic hydration. *Journal of Chemical Physics*, **2002**, 116, 2907-2921	3.9	111
19	Interaction of Paraffin Wax Gels with Random Crystalline/Amorphous Hydrocarbon Copolymers. *Macromolecules*, **2002**, 35, 7044-7053	5.5	98
18	Flow improvement of waxy oils mediated by self-aggregating partially crystallizable diblock copolymers. *Journal of Rheology*, **2002**, 46, 763	4.1	46
17	Temperature dependence of hydrophobic hydration and entropy convergence in an isotropic model of water. *Journal of Chemical Physics*, **2001**, 115, 977-982	3.9	61
16	Swelling and Structural Changes of Oppositely Charged Polyelectrolyte Gel Mixed Surfactant Complexes. *Macromolecules*, **2001**, 34, 1522-1525	5.5	22
15	Effect of solute size and solute-water attractive interactions on hydration water structure around hydrophobic solutes. *Journal of the American Chemical Society*, **2001**, 123, 10721-8	16.4	164
14	Convergence of Molecular and Macroscopic Continuum Descriptions of Ion Hydration. *Journal of Physical Chemistry B*, **2000**, 104, 7235-7238	3.4	77
13	Interactions of Cationic/Nonionic Surfactant Mixtures with an Anionic Hydrogel: Absorption Equilibrium and Thermodynamic Modeling. *Langmuir*, **2000**, 16, 2529-2538	4	25
12	Influence of potential truncation on anisotropic systems. *Molecular Physics*, **1999**, 97, 433-437	1.7	8
11	A Universal Surface Area Correlation for Molecular Hydrophobic Phenomena. *Journal of the American Chemical Society*, **1999**, 121, 9243-9244	16.4	80

10	Conformational equilibria of alkanes in aqueous solution: relationship to water structure near hydrophobic solutes. *Biophysical Journal*, **1999**, 77, 645-54	2.9	42
9	Continuum Corrections to the Polarization and Thermodynamic Properties of Ewald Sum Simulations for Ions and Ion Pairs at Infinite Dilution. *Journal of Physical Chemistry B*, **1998**, 102, 5673-5682	3.4	60
8	A Molecular/Continuum Thermodynamic Model of Hydration. *Journal of Physical Chemistry B*, **1998**, 102, 5029-5032	3.4	5
7	Reply to Comment on Electrostatic Potentials and Free Energies of Solvation of Polar and Charged Molecules *Journal of Physical Chemistry B*, **1998**, 102, 3844-3845	3.4	32
6	Hydration and conformational equilibria of simple hydrophobic and amphiphilic solutes. *Biophysical Journal*, **1998**, 75, 755-68	2.9	33
5	Effects of long-range electrostatic potential truncation on the free energy of ionic hydration. *Journal of Chemical Physics*, **1997**, 106, 8135-8139	3.9	70
4	Entropy of Hydrophobic Hydration: Extension to Hydrophobic Chains. *The Journal of Physical Chemistry*, **1996**, 100, 1900-1913		86
3	The hydrophobic effect. *Current Opinion in Colloid and Interface Science*, **1996**, 1, 376-383	7.6	43
2	The entropy of hydration of simple hydrophobic solutes. *Biophysical Chemistry*, **1994**, 51, 349-357	3.5	17
1	Influence of potential truncation on anisotropic systems		3