# Henry S Ashbaugh

## List of Publications by Citations

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|---|---|---|---|
| 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 | Colloquium: Scaled particle theory and the length scales of hydrophobicity. *Reviews of Modern Physics*, **2006**, 78, 159-178 | 40.5 | 319 |
| 98 | Absolute hydration free energies of ions, ion–water clusters, and quasichemical theory. *Journal of Chemical Physics*, **2003**, 119, 2702-2708 | 3.9 | 183 |
| 97 | 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 |
| 96 | Responsive periodic mesoporous polydiacetylene/silica nanocomposites. *Journal of the American Chemical Society*, **2006**, 128, 5304-5 | 16.4 | 136 |
| 95 | A simple molecular thermodynamic theory of hydrophobic hydration. *Journal of Chemical Physics*, **2002**, 116, 2907-2921 | 3.9 | 111 |
| 94 | 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 |
| 93 | Interaction of Paraffin Wax Gels with Random Crystalline/Amorphous Hydrocarbon Copolymers. *Macromolecules*, **2002**, 35, 7044-7053 | 5.5 | 98 |
| 92 | Interaction of Paraffin Wax Gels with Ethylene/Vinyl Acetate Co-polymers. *Energy & Fuels*, **2005**, 19, 138-144 | 4.1 | 96 |
| 91 | Entropy of Hydrophobic Hydration: Extension to Hydrophobic Chains. *The Journal of Physical Chemistry*, **1996**, 100, 1900-1913 | | 86 |
| 90 | A Universal Surface Area Correlation for Molecular Hydrophobic Phenomena. *Journal of the American Chemical Society*, **1999**, 121, 9243-9244 | 16.4 | 80 |
| 89 | Convergence of Molecular and Macroscopic Continuum Descriptions of Ion Hydration. *Journal of Physical Chemistry B*, **2000**, 104, 7235-7238 | 3.4 | 77 |
| 88 | 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 |
| 87 | Thermochromatism and structural evolution of metastable polydiacetylenic crystals. *Journal of Physical Chemistry B*, **2006**, 110, 7221-5 | 3.4 | 65 |
| 86 | Assessing the thermodynamic signatures of hydrophobic hydration for several common water models. *Journal of Chemical Physics*, **2010**, 132, 124504 | 3.9 | 64 |
| 85 | 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 |
| 84 | 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 |
| 83 | 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 |

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| 82 | 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 |
| 81 | Deblurred observation of the molecular structure of an oil-water interface. *Journal of the American Chemical Society*, **2005**, 127, 2808-9 | 16.4 | 54 |
| 80 | 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 |
| 79 | Helix stabilization of poly(ethylene glycol)-peptide conjugates. *Biomacromolecules*, **2011**, 12, 2729-34 | 6.9 | 49 |
| 78 | Flow improvement of waxy oils mediated by self-aggregating partially crystallizable diblock copolymers. *Journal of Rheology*, **2002**, 46, 763 | 4.1 | 46 |
| 77 | 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 |
| 76 | The hydrophobic effect. *Current Opinion in Colloid and Interface Science*, **1996**, 1, 376-383 | 7.6 | 43 |
| 75 | Electrostatic Control of Macrocyclization Reactions within Nanospaces. *Journal of the American Chemical Society*, **2019**, 141, 6740-6747 | 16.4 | 42 |
| 74 | Conformational equilibria of alkanes in aqueous solution: relationship to water structure near hydrophobic solutes. *Biophysical Journal*, **1999**, 77, 645-54 | 2.9 | 42 |
| 73 | An analysis of molecular packing and chemical association in liquid water using quasichemical theory. *Journal of Chemical Physics*, **2006**, 124, 224502 | 3.9 | 37 |
| 72 | 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 |
| 71 | Contrasting nonaqueous against aqueous solvation on the basis of scaled-particle theory. *Journal of Physical Chemistry B*, **2007**, 111, 9330-6 | 3.4 | 36 |
| 70 | Temperature-Dependent Hydrophobic Crossover Length Scale and Water Tetrahedral Order. *Journal of Physical Chemistry Letters*, **2018**, 9, 1012-1017 | 6.4 | 35 |
| 69 | Non-van der Waals treatment of the hydrophobic solubilities of CF4. *Journal of the American Chemical Society*, **2007**, 129, 10133-40 | 16.4 | 35 |
| 68 | Hydration and conformational equilibria of simple hydrophobic and amphiphilic solutes. *Biophysical Journal*, **1998**, 75, 755-68 | 2.9 | 33 |
| 67 | Optimization of linear and branched alkane interactions with water to simulate hydrophobic hydration. *Journal of Chemical Physics*, **2011**, 135, 054510 | 3.9 | 32 |
| 66 | Gelation of "catanionic" vesicles by hydrophobically modified polyelectrolytes. *Colloid and Polymer Science*, **2002**, 280, 783-788 | 2.4 | 32 |
| 65 | 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 |

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| 64 | Single ion hydration free energies: a consistent comparison between experiment and classical molecular simulation. *Journal of Chemical Physics*, **2008**, 129, 204501 | 3.9 | 29 |
| 63 | Methane Hydration-Shell Structure and Fragility. *Angewandte Chemie - International Edition*, **2018**, 57, 15133-15137 | 16.4 | 29 |
| 62 | Alkane Adsorption at the Water Vapor Interface. *Langmuir*, **2003**, 19, 7638-7645 | 4 | 27 |
| 61 | 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 |
| 60 | Effects of nonpolar solutes on the thermodynamic response functions of aqueous mixtures. *Journal of Chemical Physics*, **2005**, 123, 164503 | 3.9 | 25 |
| 59 | Interactions of Cationic/Nonionic Surfactant Mixtures with an Anionic Hydrogel: Absorption Equilibrium and Thermodynamic Modeling. *Langmuir*, **2000**, 16, 2529-2538 | 4 | 25 |
| 58 | Spontaneous drying of non-polar deep-cavity cavitand pockets in aqueous solution. *Nature Chemistry*, **2020**, 12, 589-594 | 17.6 | 22 |
| 57 | Swelling and Structural Changes of Oppositely Charged Polyelectrolyte Gel Mixed Surfactant Complexes. *Macromolecules*, **2001**, 34, 1522-1525 | 5.5 | 22 |
| 56 | Entropy crossover from molecular to macroscopic cavity hydration. *Chemical Physics Letters*, **2009**, 477, 109-111 | 2.5 | 21 |
| 55 | Blowing bubbles in Lennard-Jonesium along the saturation curve. *Journal of Chemical Physics*, **2009**, 130, 204517 | 3.9 | 20 |
| 54 | Self-consistent molecular field theory for packing in classical liquids. *Physical Review E*, **2003**, 68, 021505 | 2.4 | 20 |
| 53 | Numerical validation of IFT in the analysis of protein-surfactant complexes with SAXS and SANS. *Langmuir*, **2012**, 28, 12593-600 | 4 | 19 |
| 52 | Confinement induced conformational changes in n-alkanes sequestered within a narrow carbon nanotube. *Physical Chemistry Chemical Physics*, **2012**, 14, 2702-9 | 3.6 | 19 |
| 51 | Tuning the globular assembly of hydrophobic/hydrophilic heteropolymer sequences. *Journal of Physical Chemistry B*, **2009**, 113, 14043-6 | 3.4 | 19 |
| 50 | Aqueous Partial Molar Volumes from Simulation and Individual Group Contributions. *Industrial & Engineering Chemistry Research*, **2008**, 47, 5169-5174 | 3.9 | 19 |
| 49 | The Thermodynamics of Anion Complexation to Nonpolar Pockets. *Journal of Physical Chemistry B*, **2018**, 122, 1702-1713 | 3.4 | 18 |
| 48 | Succession of Alkane Conformational Motifs Bound within Hydrophobic Supramolecular Capsular Assemblies. *Journal of Physical Chemistry B*, **2016**, 120, 10394-10402 | 3.4 | 18 |
| 47 | The entropy of hydration of simple hydrophobic solutes. *Biophysical Chemistry*, **1994**, 51, 349-357 | 3.5 | 17 |

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| 46 | Carbon microspheres as network nodes in a novel biocompatible gel. *Soft Matter*, **2011**, 7, 4170 | 3.6 | 16 |
| 45 | 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 |
| 44 | Digging a hole: Scaled-particle theory and cavity solvation in organic solvents. *Journal of Chemical Physics*, **2008**, 129, 174505 | 3.9 | 15 |
| 43 | Solvent cavitation under solvophobic confinement. *Journal of Chemical Physics*, **2013**, 139, 064702 | 3.9 | 14 |
| 42 | 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 |
| 41 | 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 |
| 40 | Communication: Stiffening of dilute alcohol and alkane mixtures with water. *Journal of Chemical Physics*, **2016**, 145, 201102 | 3.9 | 13 |
| 39 | Simulation optimization of spherical non-polar guest recognition by deep-cavity cavitands. *Journal of Chemical Physics*, **2013**, 139, 234502 | 3.9 | 12 |
| 38 | Proximal charge effects on guest binding to a non-polar pocket. *Chemical Science*, **2020**, 11, 3656-3663 | 9.4 | 11 |
| 37 | 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 |
| 36 | Guest Controlled Nonmonotonic Deep Cavity Cavitand Assembly State Switching. *Journal of Physical Chemistry B*, **2017**, 121, 10717-10725 | 3.4 | 10 |
| 35 | 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 |
| 34 | Pressure reentrant assembly: direct simulation of volumes of micellization. *Langmuir*, **2013**, 29, 14743-7 | 4 | 9 |
| 33 | Cosolvent preferential molecular interactions in aqueous solutions. *Journal of Physical Chemistry B*, **2011**, 115, 13633-42 | 3.4 | 9 |
| 32 | 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 |
| 31 | 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 |
| 30 | Influence of potential truncation on anisotropic systems. *Molecular Physics*, **1999**, 97, 433-437 | 1.7 | 8 |
| 29 | 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 |

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| 28 | Design of Amphiphilic Polymers via Molecular Dynamics Simulations. *Journal of Physical Chemistry B* , **2016**, 120, 10603-10610 | 3.4 | 8 |
| 27 | 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 |
| 26 | 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 |
| 25 | Effect of hydrostatic pressure on gas solubilization in micelles. *Langmuir*, **2015**, 31, 3318-25 | 4 | 6 |
| 24 | 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 |
| 23 | Hydrated nonpolar solute volumes: Interplay between size, Attractiveness, and molecular structure. *Biophysical Chemistry*, **2016**, 213, 1-5 | 3.5 | 6 |
| 22 | A Molecular/Continuum Thermodynamic Model of Hydration. *Journal of Physical Chemistry B*, **1998**, 102, 5029-5032 | 3.4 | 5 |
| 21 | 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 |
| 20 | Alkane guest packing drives switching between multimeric deep-cavity cavitand assembly states. *Chemical Communications*, **2018**, 54, 2639-2642 | 5.8 | 4 |
| 19 | 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 |
| 18 | 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 |
| 17 | Influence of potential truncation on anisotropic systems | | 3 |
| 16 | Nonpolar solute cononsolvency in ethanol/water mixtures □Connections to solvent structure. *Journal of Molecular Liquids*, **2020**, 298, 111944 | 6 | 3 |
| 15 | Scaled-particle theory analysis of cylindrical cavities in solution. *Physical Review E*, **2015**, 91, 042315 | 2.4 | 2 |
| 14 | Note: Nonpolar solute partial molar volume response to attractive interactions with water. *Journal of Chemical Physics*, **2014**, 140, 016101 | 3.9 | 2 |
| 13 | Conformational equilibria of polar and charged flexible polymer chains in water. *Polymer*, **2002**, 43, 559-565 | 3.9 | 2 |
| 12 | Emergence of non-monotonic deep cavity cavitand assembly with increasing portal methylation. *Molecular Systems Design and Engineering*, **2020**, 5, 656-665 | 4.6 | 2 |
| 11 | 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 |

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| 10 | Assessment of scaled particle theory predictions of the convergence of solvation entropies. *Fluid Phase Equilibria*, **2021**, 530, 112885 | 2.5 | 2 |
| 9 | 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 |
| 8 | Cooperative hydrophobe aggregation mediated by interfacially active alcohols. *Fluid Phase Equilibria*, **2016**, 407, 255-261 | 2.5 | 1 |
| 7 | Evaluation of second osmotic virial coefficients from molecular simulation following scaled-particle theory. *Molecular Simulation*, **2019**, 45, 1403-1410 | 2 | 1 |
| 6 | Resolving solvophobic interactions inferred from experimental solvation free energies and evaluated from molecular simulations. *Chemical Physics Letters*, **2017**, 667, 62-67 | 2.5 | 1 |
| 5 | 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 |
| 4 | Reversal of the Temperature Dependence of Hydrophobic Hydration in Supercooled Water. *Journal of Physical Chemistry Letters*, **2021**, 12, 8370-8375 | 6.4 | 0 |
| 3 | Blending Linear and Cyclic Block Copolymers to Manipulate Nanolithographic Feature Dimensions.. *ACS Applied Polymer Materials*, **2022**, 4, 327-337 | 4.3 | 0 |
| 2 | Tribute to Lawrence R. Pratt. *Journal of Physical Chemistry B*, **2021**, 125, 4925-4927 | 3.4 | |
| 1 | Methane Hydration-Shell Structure and Fragility. *Angewandte Chemie*, **2018**, 130, 15353-15357 | 3.6 | |