## Invited Contribution from AIChE Area 1a Alkanes + Cavitands: Some Assembly Required

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Cavitands are supra-molecular bowl shaped molecules composed of a hydrophobic pocket ringed by acidic groups that make them water soluble. These biomimetic molecules actively bind hydrophobic species in aqueous solution, finding applications in gas separations, delivery vehicles, yoctoliter reactors, etc. The stoichiometry of cavitand hosts bound to hydrophobic guests and the structures formed has been experimentally found to depend sensitively on the size of the hydrophobic guests and the chemistry of the cavitand. In an effort to piece apart the molecular rationale for the assembly of cavitands with hydrophobic guests, we present here a simulation study of the complexes formed between alkanes of varying length and cavitands that differ simply by degree of methylation. We will present results from our thermodynamic investigations of the assembly of these supramolecular hosts into a range of distinct multimeric complexes, the packing of hydrophobic guests within those complexes, and the wetting of individual cavitands in aqueous solution.