CHEMICAL ENGINEERING

SEMINAR SERIES

HANK ASHBAUGH

Associate Professor
Chemical & Biomolecular Engineering
Tulane University

Monday, May 2, 2016

Caught in a Hydrophobic Bind: Alkane Assembly in Cavitand Complexes

ABSTRACT: 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 cavtiands that differ simply by degree of methylation. To begin we examine the hydrophobic driving forces for association between a single cavitand and alkane and its relationship to the wetting of the cavitand,Äôs hydrophobic pocket. Next we examine the impact of guest confinement within a dimeric cavitand capsule on the succession of alkane conformational motifs observed with increasing chain length. In the final part of the talk we examine for a methylated cavitand how the length of the encapsulated alkanes impacts the structure of the complex formed from dimeric, to tetrameric, to hexameric cavitand complexes.

RECEPTION 3:30 • LECTURE 4:00 – 5:00
PHYSICS ASTRONOMY BLDG. (PAA) A118

CHEMICAL ENGINEERING
UNIVERSITY of WASHINGTON
Knowledge and solutions for a changing world

BIOGRAPHY: Hank Ashbaugh grew up in Charlotte, North Carolina. He obtained his Bachelors degree in 1992 from North Carolina State University and his Doctorate degree in Chemical Engineering from the University of Delaware in 1998. After finishing his PhD, Hank went on to post-doctoral assignments at Lund University in Sweden, Princeton University, and Los Alamo National Laboratory. Hank joined the Department of Chemical Engineering at Tulane University as an Assistant Professor in 2004 and was promoted to Associate Professor in 2010. His current research interests include the multiscale simulation and theory of self-assembly and hierarchical organization in complex fluids including surfactant solutions, polymer melts and solutions, and biopolymer gels and networks to advance self-assembly as a labile tool for building tailored nanostructured materials.