The adage “oil and water don’t mix” underlies many phenomena of the aqueous environment, including surfactant assembly, folding of globular proteins, biological membrane formation, and the fate of pollutants in nature. If one examines the interaction of hydrophobic/non-polar substances with water more closely, however, one sees that the actual situation is more subtle. For example, many soluble proteins are globular at one temperature but unfold upon both heating and cooling. Simpler examples are the solubilities of inert gases and non-polar oils in water that exhibit solubility minima with increasing temperature, attributable to thermodynamic signatures characteristic of hydrophobic hydration. The application of pressure, on the other hand, can mollify the hydrophobic driving forces for assembly and denature proteins, while surfactant micelles exhibit maxima in their critical micelle concentrations with pressure, indicative of significant volumetric differences with protein folding. The distinctions between water and organic solvents are generic and are a central puzzle of hydrophobic hydration. Molecular simulations applied in conjunction with statistical thermodynamic tools have proven to be invaluable in piecing apart the molecular origins of hydrophobic hydration. In this talk I discuss the application of simulations in my group to examine hydrophobic phenomena from molecularly detailed models of assembly to more simplified descriptions that permit examination of the atomistic-to-macroscopic length scales relevant to assembly. Specific examples that will be discussed include: The unfavorable dissolution of non-polar species in aqueous solution on the molecular scale, the heat induced collapse of poly(N-isopropylacrylamide) in aqueous solution, the re-entrant micellization of ionic and non-ionic micelles with increasing pressure, and the long-range attraction between hydrophobic surfaces in solution.

About the Speaker: 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.