Amgen Seminar Series in Chemical Engineering

in

Cherry Auditorium, Kirk Hall, 1 PM

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THERMODYNAMICS OF HYDRATION ACROSS MULTIPLE LENGTH SCALES

By

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Confining geometries that contain thin water films are ubiquitous in nature, materials science and engineering. Examples include ion channels, zeolites, mineral inclusions, and mesoscopic surfactant assemblies. Understanding the influence of the confining surfaces on the structure, dynamics and thermodynamics of water is therefore of interest in applications such as corrosion inhibition, the design of super-hydrophobic surfaces and heterogeneous catalysis. I will discuss recent computational studies of hydration phenomena in which the characteristic length scale of the problem is of the order of a few nanometers. Specific problems to be addressed include water structure on surfaces with patterned hydrophobicity and hydrophilicity, the phase behavior of water in hydrophobic confinement, the mechanical properties of glassy water confined by surfaces of tunable polarity, and the roles of chemistry and geometry in the hydration of biological surfaces. I will also discuss recent computational investigations of solubility and molecular conformations of hydrocarbon chains in water, and their implications for our understanding of self-assembly and the folding of globular proteins.

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