



## ~~Special Polymer Physics Seminar ~~

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Norman, OK 73019

**10:00 AM Tuesday,  
September 27<sup>th</sup>, 2011  
301 Steidle Bldg.**

### **Aqueous Systems at Interfaces: Water and Ions Properties, Surfactant Aggregates, and Hydrodynamics**

A number of experimental and simulation results consistently show that a solid surface perturbs interfacial water for up to 1-2 nm. Our group is interested in understanding how it is possible that such short-ranged perturbation results in macroscopic observations that include hydrodynamic slip, salt-specific effects relevant for protein folding and precipitation, self assembly of lipids and nanoparticles, and even the preservation of artistic heritage. (For example, Giotto's frescos in the Scrovegni's chapel, Padua, Italy, and the Mogao caves, in Dunhuang, China, a lasting but frail testimony to the Buddhist influences on modern Chinese culture, are endangered by the humidity caused by the breathing visitors.)

Our philosophy consists in employing molecular simulations to provide the details needed for interpreting, and when possible predicting macroscopic observations. In this seminar we will discuss the results for structure and dynamics of water on a few solid-liquid interfaces, how such predictions could be tested by AFM, and we will then present three practical applications. In the first we suggest that the structure of the hydration layer might be responsible for hydrodynamic boundary conditions; based on our results, it appears that appropriate hydrophilic surfaces could be fabricated to sustain hydrodynamic slip. In the second we discuss how the partition of aqueous NaCl vs. CsCl electrolytes within narrow slit-shaped silica pores; the resultant self-diffusion coefficients for the various ions are so different that chromatographic separations appear feasible. In the third application we will discuss how aqueous surfactants could be employed to stabilize dispersions of carbon nanostructures (nanotubes and graphene), thus enabling their practical applications.