

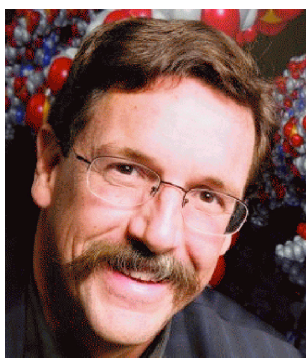
# Joint ChemBio/Physical Chemistry Seminar

Tuesday,  
September 22, 2015

11:00 am

Room 1315  
Chemistry Building

## Surface tension and solubility vs hydrophobicity



Professor B. Montgomery Pettitt

*Department of Biophysics  
University of Texas Medical Branch  
Sealy Center for Structural Biology & Molecular*

Host: Professor Qiang Cui

Surface tension models of contact angles provide a rigorous definition of wetting and dewetting in surface science. The case of atomically rough and chemically heterogeneous boundaries between solvent and flexible solutes is less straightforward. The mechanism of protein folding and association is often described in terms of hydrogen bonding, side chain packing and the hydrophobic effect. In this study we compare the solution properties of alkanes, peptides and proteins from theory and simulation with experiment. Classical concepts involving dependence on surface area as used in surface science are found to be inadequate for peptides and proteins by free energy calculations. We use the properties of oligoglycines, oligoalanines and protein dimers in water at varying concentrations in order to understand the structural and thermodynamic changes that occur during aggregation. Aggregation often manifests as a liquid-liquid, phase separation at the solubility limit. Thermodynamic signatures of this aggregation of short oligoglycines is remarkably similar to the thermodynamics of folding or collapse of longer oligoglycines in water. We compare the gradients of the free energy with respect to geometry and find anomalous behavior which explains the failure of surface area based descriptions of nonpolar solvation in biochemistry.

Refreshments will be available prior to the seminar at 10:45 a.m. outside room 1315

Graduate Students may meet with the speaker at 1:00 p.m. in Room 8305F