

# CHEMISTRY DEPARTMENT COLLOQUIUM

*PROFESSOR JAMES L. SKINNER*



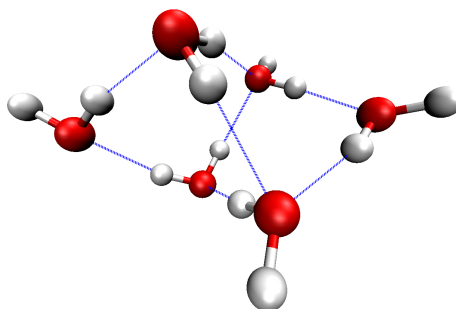
**Friday, March 1  
3:30 pm  
Room 1315  
Chemistry Building**



DEPARTMENT OF  
**Chemistry**

## **Hydrogen bonding in water: liquid, surface, clusters, ice**

While the water molecule itself is quite simple, small and large collections of water molecules in clusters and condensed phases are exceptionally complex. I will describe our efforts to understand the structure and dynamics of water in clusters, liquid water, the liquid/vapor interface, and ice, through classical molecular dynamics simulation of a model with explicit two- and three-body interactions. I will also focus on cooperative hydrogen bonding in water, and its relationship to several types of frequency- and time-domain vibrational spectroscopy. Extensive comparison with experiment will be presented.



**RECEPTION TO FOLLOW IN SHAIN ATRIUM**