



## SEMINAIRE ISMO

**Yuki Nagata**

*Max Planck Institute for Polymer Research  
Ackermannweg 1055128 Mainz, Germany*

### **Water/Lipid Interface Viewed from Simulated Sum – Frequency Generation Spectroscopy**

Water-lipid interface emerges in various biological/chemical/physical phenomena. For example, oil does not mix with water, but oil is mixed with soap solution. Membrane (bi)layer is stabilized by the water-lipid interactions against increase in the entropy. Further, lipid interfaces play a catalytic role on the aggregation of amyloid beta protein.

To probe such interfacial molecules, sum-frequency generation (SFG) spectroscopy is a powerful experimental technique. I will describe the simulation procedure for calculating the SFG spectra of water at the water/lipid interfaces and discuss interfacial water structure and hydrogen bond dynamics by analyzing the spectra.

In addition, the SFG spectra for transient protein structures at the water/lipid interface will be discussed.

\* \* \* \* \*

**Mardi 13 décembre 2011 à 11 h 00**  
**Bât. 210 – Amphi 1 (2<sup>ème</sup> étage)**  
*Université Paris-Sud 91405 ORSAY Cedex*