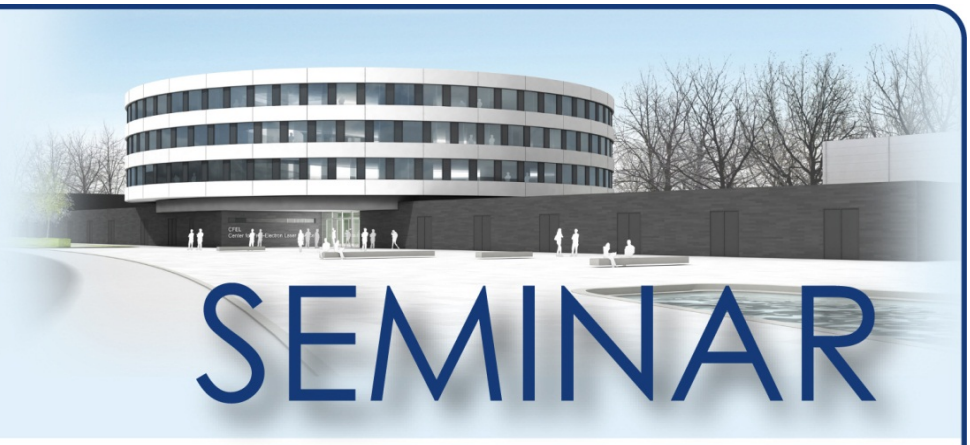
CFEL SCIENCE



SEMINAR

21st of May 2012 – 2:00 pm

Bld. 49a - Seminar Room111

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Sum-frequency generation spectra of water at the hydrophilic and superhydrophilic interfaces: A molecular dynamics simulation study

A living eukaryotic cell is bounded by the plasma membrane, and the ions are actively transported to a cell cytoplasm across the membrane. Since the structures of membranes are stabilized by the water- lipid headgroup interactions against the increase in entropy, understanding the water structure and dynamics at the lipid interface is crucial. Sum-frequency generation (SFG) spectroscopy is suitable for probing the interfacial water structure, because it does not contain the bulk contribution due to the symmetry rule. SFG spectra of water OH vibrational bond at the lipid interfaces show 3200-3300 cm^{-1} and 3400-3500 cm^{-1} peaks. We have conducted the molecular dynamics simulation for the water/lipid interface and have revealed the 3200-3300 cm^{-1} peak is contributed by the OH stretching mode non-adjacent to the lipid headgroup but ordered along the surface normal due to the electrostatic interaction of lipid, while the 3400-3500 cm^{-1} peak is contributed by the OH stretching mode adjacent to the lipid headgroup. [1] Moreover, we have shown that we can reveal the fast spectral diffusion for the 3200-3300 cm^{-1} and slow spectral diffusion for the 3400-3500 cm^{-1} by using two-dimensional SFG spectroscopy. [2] This newly proposed spectroscopic experiment was very recently done. [3]

Beyond the hydrophilic interfaces, we are investigating the water structure and dynamics at the superhydrophilic TiO_2 interface and are calculating the SFG spectra to check the accuracy of our modeling and interpret the experimental data. Final goals are to study the mechanism of the superhydrophilic interface and the hydrogen-bond dynamics of interfacial water by collaborating with the experimental group at the same department in the Max-Planck institute for polymer researches.

[1] Y. Nagata, S. Mukamel, J. Am. Chem. Soc., 132, 6434 (2010).
[2] Y. Nagata, S. Mukamel, J. Am. Chem. Soc., 133, 3276 (2011).
[3] Z. Zhang, L. Piatkowski, H. J. Bakker, M. Bonn, Nature Chem. 3, 888 (2011).

Host: Dwayne Miller, CFEL/ MPSD