Tuesday Morning, October 16, 2007

Understanding Biointerphases and Magnetism with Neutrons Topical Conference

Room: 618 - Session NT-TuM

Applications to Biological Materials and Soft Matter

Moderator: M. Lösche, Carnegie Mellon University

8:00am **NT-TuM1 Cold and Thermal Neutrons: Suitable Probes for Biomaterials**, ***J. Katsaras***, National Research Council of Canada **INVITED**

Neutrons are electrically neutral, subatomic elementary particles whose existence had been postulated by Ernest Rutherford and discovered by James Chadwick in 1932. With the exception of hydrogen, neutrons are found in all atomic nuclei, and free neutrons are unstable with a mean lifetime of ~ 900 s. Thermal and cold neutrons, used for the study of materials ranging from engineering to biomedical applications, are typically produced by reactor- or accelerator-based sources and are the result of interacting with a given temperature moderator (e.g., graphite, water, liquid deuterium). Compared to thermal neutrons, cold neutrons possess 5 - 20 times longer wavelengths and are preferred for the study of biological materials with inherently large unit cells. Unlike x-rays, neutrons interact strongly with nuclei and the strength of their interactions varies dramatically and non-monotonically from element-to-element across the periodic table. This statement applies equally to isotopes of the same element and has been used to great advantage by biologists and polymer scientists who typically study materials rich in hydrogen. The classic example is the isotopic substitution of ^{1}H for ^{2}H (deuterium), where one can accentuate, or nullify, the scattering from particular parts of a macromolecular complex by selective deuteration. Recently, we have used a number of neutron scattering techniques to study for example, the location of cholesterol in polyunsaturated fatty acid membranes (discovered that cholesterol can reside in unexpected places within the membrane!) and the distribution of water in aligned, self-assembled lipopolysaccharide bilayers isolated from the Gram-negative bacterium, Pseudomonas aeruginosa. These results provide insights as to how molecules penetrate and assemble in biologically relevant membranes, and will be the topic of discussion. Web Site: http://neutron.nrc-cnrc.gc.ca/people/katsaras/index.html.

8:40am **NT-TuM3 Small Angle Neutron Scattering Studies of the Counterion Effects on the Molecular Conformation and Structure of Charged G4 PAMAM Dendrimers in Aqueous Solutions**, ***W.-R. Chen***, Oak Ridge National Laboratory **INVITED**

The structural properties of generation 4 (G4) poly(amidoamine) starburst dendrimers (PAMAM) with an ethylenediamine (EDA) central core in solutions have been studied by small angle neutron scattering (SANS). Upon the addition of , SANS patterns show pronounced inter-particle correlation peaks due to the strong repulsion introduced by the protonation of the amino groups of the dendrimers. By solving the Ornstein-Zernike integral equation (OZ) with hypernetted chain closure (HNC), the dendrimer-dendrimer structure factor is determined and used to fit the experimental data, where is the magnitude of the scattering wave vector Q. Quantitative information such as the effective charge per dendrimer and the radius of gyration, R_G, at different pD values is obtained. The results show that only changes by about 4 % when the pD value varies from 10.25 to 4.97, and significant counterion association/condensation occurs, strongly mediating the inter-dendrimer interaction. The influence of interplay between counterions and molecular protonation of dendrimers imposes a strong effect on the dendrimer conformation and effective interaction. Although the change of is very small, careful analyses of the high data and fitting parameters indicate a possible internal structure change of a dendrimer when the amino groups are progressively charged.

9:20am **NT-TuM5 Neutron Reflection Study of Peptides and Proteins at Interfaces**, ***J.R. Lu***, *X.B. Zhao, F. Pan, M. Yaseen*, University of Manchester, UK **INVITED**

Neutron reflection has been deployed to study the adsorption of short designed peptides and proteins at the solid/water interface, focusing on the determination of the structure of the interfacial layer. The effects of surface hydrophobicity, the size and stability of globular proteins and the solution environmental conditions on the structure and composition of the adsorbed protein layers are examined and key features highlighted. The advantegeous features of neutron reflection are described.

10:40am **NT-TuM9 Neutron Reflectivity and Scattering for Studying Biomolecules at Interfaces**, ***T. Nylander***, Lund University, Sweden **INVITED**

Neutrons are relatively more harmless to matter than X-rays and therefore they are particularly usefull to study biological material. Hydrogen scatters neutron very well and further more the scattering from hydrogen and deuterium is very different. Selective deuteration of one component and contrast matching of the aqueous solvent makes it possible to study one component at a time as the other can be made invisible. The potential of neutron scattering/reflectivity measurements will be discussed for two systems, lipid self-assembly and DNA compaction. There is an increasing demand for methods to study processes at the lipid-aqueous interface as the importance of lipids and lipid self-assembly structures as regulators for biological activity as well as for vehicles for drug delivery. Spreading of vesicles on surfaces are quite an established method to forming bilayers on hydrophilic surface, and spreading can be affected by the surface properties as well as properties that affect the stability of the vesicles. The full potential of non-lamellar liquid crystalline nano particles (LCPN) has only recently been realized, as improved methods and new lipid combinations have been introduced for producing biocompatible and structurally well-defined nano-particle dispersions of different phase structures. These include bicontinuous cubic, reverse hexagonal, and reverse cubic phases. Directly relevant for drug delivery systems is the fusion of these LCPN with a (model) membrane. Again numerous studies has been conducted on vesicle fusion, but very few on the interaction between non-lamellar LCNP and membranes. The compositional changes in the lipid bilayer will be monitored by neutron reflectivity using selective deuteration of the lipids and proper contrast matching. This has given us information on structural changes when the LCNP interacts with a surface and a bilayer. Our results show that interaction between the LCPN lipid components with the acyl chains of the bilayer, consistent with the formation of a mixed bilayer. As we observed a diffraction peak at high q after a certain time, we concluded that the interaction eventually lead to formation of multilayers on the surface. We are today fascinated of the supra-molecular structures formed by DNA packing in the cell nucleus and we are trying to understand to what extent packing regulates transcription/translation. The long-term objective of our work is to design a module for DNA packaging, where the packing and thereby the transcription can be switched on and off. This module would be a transcription competent synthetic analogue of a real cell nucleus. We are therefore study the relation between structure of the aggregate (using dynamic light scattering, small angle x-ray and neutron scattering, cryo-TEM), the degree of compaction (using fluorescence) and transcription/translation (using biochemical assays, including RNAse and luciferase production). It has been shown that DNA can be compacted by cationic lipids both in bulk and at interfaces. By using neutron scattering of DNA coated particles we have shown that the aggregate formed by CTAB when interacting with DNA is elongated and of the same structure on the surface as on the bulk.

11:20am **NT-TuM11 Roles of Carbohydrates in Fine Adjustment of Biological Interfaces**, ***M. Tanaka***, University of Heidelberg, Germany **INVITED**

In nature, cell-cell and cell-tissue contacts are madiated by various biopolymers based on carbohydrates. This paper describes some of our recent studies that physically model the active roles of carbohydrates in fine-adjustment of contacts at biological interfaces by specular and off-specular neutron scattering at defined relative humidity as well as in bulk water. The planar planar geometry of the biomembrane models containing oligo- and polysaccharides enable one to identify the in-plane and out-of-plane momentum transfers at various angles quantitatively, which can be used to determine the influence of carbohydrates on structural and mechanical properties of membranes.

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