Biomaterial Interfaces
Room 313 - Session BI-MoM

BioMaterials and Neutrons (BioMaN) I

Moderator: M. Grunze, Universität Heidelberg, Germany

8:20am **BI-MoM1 Neutron Scattering Tutorial**, ***J.K. Zhao,*** Oak Ridge National Laboratory

We will give an introduction to the neutron scattering techniques relevant to the current session. Topics will include Reflectometry, Small Angle Neutron Scattering and Inelastic Scattering. We will briefly describe these methods and introduce various technical terms that will be used by the subsequent talks. These subsequent presentations will concentrate on scientific achievements or potentials of neutron scattering in biomaterials. We will also distribute handouts as technical references during session.

8:40am **BI-MoM2 Compositional Depth Profiles of Biomaterial Interfaces by Specular Neutron Reflection**, ***C.F. Majkrzak,*** *S.K. Krueger, U. Perez-Salas, N.F. Berk,* National Institute of Standards and Technology

We present the results of recent studies which illustrate the power of specular neutron reflectivity and diffraction for determining the compositional depth profiles of thin films and multilayered structures of interest in biology and biotechnology. Research discussed includes: probing the interactions of melittin (a model peptide for antibiotics and membrane proteins) with hybrid bilayers; the structural characterization of a polyelectrolyte/terpolymer/phospholipid sandwich; the orientation of adsorbed biomineralization proteins; and the location of cholesterol within lipid membranes. Using specular neutron reflection from single-repeat lamellar assemblies or diffraction from periodic multilayers as probes, cross sectional composition depth profiles, with spatial resolutions of the order of a nanometer and Angstrom, respectively, can now be obtained. We demonstrate, in the context of the aforementioned work, how the neutron's sensitivity to different isotopes, in particular hydrogen and deuterium, enables detailed structural information -- for example, the water concentration profile across the thickness of a film -- to be revealed through selective substitution in organic materials. We also show how the high transmission of neutrons through inorganic single crystals, e.g., silicon, sapphire, and quartz, allows such crystals to serve as both substrate for the film of interest as well as fronting medium for the incident and specularly reflected neutron beams. This in turn makes it possible to study the film in intimate contact with a fluid reservoir -- which may be, for instance, part of a functioning electrochemical cell. Finally, the uniqueness of a depth profile obtained from neutron reflection data is considered, together with the degree of uncertainty in the density and the spatial resolution.

9:00am **BI-MoM3 Neutron Scattering and Diffraction for Molecular-Scale Characterization of Biomimetic Membranes**, ***M. Loesche,*** Johns Hopkins University and CNBT at the NIST Center for Neutron Research

Nanotechnology and molecular bioengineering are making ever deepening inroads into our daily lives. Physicochemical and biotechnological achievements in the design of physiologically active supramolecular assemblies have brought about an urgent need for new means of characterizing them at the molecular and submolecular levels. Because surfaces and interfaces play a pivotal role in this field, surface-sensitive neutron and x-ray scattering techniques have become particularly important for characterization. The CNBT consortium, located at the NCNR, is a biophysics partnership that utilizes neutron scattering, tightly interfaced with MD simulations, for advanced research in membrane biology and biotechnology. A new neutron spectrometer – the Advanced Neutron Reflectometer and Diffractometer, AND/R – has been commissioned which is optimized for surface-sensitive neutron scattering. In this talk, I will discuss current highlights of research performed on the AND/R, including investigations of peptidemembrane interactions and the molecular-scale characterization of model bilayer membranes tethered to solid supports.

9:20am **BI-MoM4 Towards a Deeper Understanding of Protein Resistance: Characterizing Water/Surface and Protein/Surface Interactions by In Situ Neutron Reflectometry**, ***R. Dahint,*** Universität Heidelberg, Germany*; M. Skoda, F. Schreiber,* Universität Tübingen, Germany*; M. Himmelhaus, M. Grunze,* Universität Heidelberg, Germany

Materials which are resistant towards adsorption of proteins from biological media are of crucial importance in biotechnology and biomedical applications. The most outstanding protein resistant properties are exhibited by surfaces containing poly- (PEG) and oligo(ethylene glycols) (OEG), (-O-CH@sub 2@-CH@sub 2@-)@sub n@. For surface-grafted PEG, protein resistance is associated with an unfavorable change in the free energy when a protein approaches the surface and thereby compresses and dehydrates the polymer chains. However, this mechanism cannot explain the inertness of rigid, and thus conformationally restricted, OEG terminated alkanethiolate self-assembled monolayers (SAMs). Proposed models suggest the importance of water/SAM interactions at the surface or relate protein resistance to repulsive electrostatic forces. Due to its capability to characterize biological interfaces in situ, neutron reflectometry provides a unique tool to address fundamental questions of protein repulsion. We have studied the importance of interfacial water layers between inert SAMs and the bulk water phase to repel proteins. Temperature dependent studies on the OEG/water interface reveal, that a previously observed, density reduced water phase in the vicinity of the SAM cannot account for the protein resistant properties of the films. Moreover, neutron reflectometry has been used to investigate protein/surface interactions employing biomolecules in their native state and natural environment. Room temperature measurements on protein resistant films of OEG in contact with bovine serum albumin (BSA) solutions reveal the presence of an extended protein depletion layer between the SAM and the bulk protein solution. The results are compared to the strength and range of repulsive forces measured by AFM.

9:40am **BI-MoM5 Soft Interfaces on the Nanometer Scale - How Neutrons Contribute to a Deeper Understanding on the Supramolecular Level**, ***R. Steitz,*** Hahn-Meitner-Institut, Germany*; C. Czeslik,* Universität Dortmund, Germany*; H. Haas,* MediGene AG, Germany*; P. Riccio,* Università degli Studi della Basilicata, Italy **INVITED**

Current problems in soft matter and biomaterial science often require insight on the nanometer scale. In this contribution we will show how neutron reflectivity contributes to a deeper understanding of systems that are also of biological interest. Topics of increasing complexity and biological relevance will be discussed: Chapter one will focus on the properties of ultrathin polyelectrolyte coatings at a solid-liquid interface.@footnote 1@ Chapter two will show how these polymer coatings can be utilized as soft cushions for lipid membranes that form in situ by vesicle fusion from the liquid phase (under physiological conditions), or as switchable binding sites for proteins that penetrate from the aqueous solution.@footnote 2@ Number three will demonstrate the successful in situ assembly of myelin model membranes at a polymer-liquid interface, while number four will focus on the molecular organization within such membranes@footnote 3@ and their respective degradation upon reduced humidity. @FootnoteText@ @Footnote 1@ R. Steitz, V. Leiner, R. Siebrecht and R. v. Klitzing, Colloids and Surfaces A. 163, 63-70 (2000). @Footnote 2@ C. Czeslik, G. Jackler, R. Steitz and H.-H. von Grünberg, J. Phys. Chem. B 108, 13395 (2004). @Footnote 3@ H. Haas, M. Torielli, R. Steitz, P. Cavatorta, R. Sorbi, P. Riccio, A. Gliozzi, Thin Solid Films, 329, 627 (1998).

10:20am **BI-MoM7 Design & Structural Characterization of Amphiphilic 4-Helix Bundle Peptides Vectorially-Oriented at Soft Interfaces**, ***J.K. Blasie,*** *J. Strzalka, S. Ye, T. Xu, E. Nordgren,* University of Pennsylvania*; S. Satija,* National Institute of Standards and Technology*; I. Kuzmenko, T. Gog,* Argonne National Laboratory **INVITED**

Amphiphilic 4-helix bundle peptides have been designed to incorporate both biological and non-biological cofactors. An ensemble of these peptide-cofactor complexes, vectorially oriented at a soft interface between polar and non-polar media, can provide for the translation of their designed molecular function into a macroscopic material property of the interface. Such amphiphilic 4-helix bundle peptides can also serve as model integral membrane proteins for vectorial incorporation into a lipid bilayer providing a molecular laboratory for the detailed study of structure-function correlations. For example, the mechanism by which anesthetic binding to a designed cavity within its hydrophilic domain modulates the ion channel activity of its hydrophobic domain. Detailed structural studies of these amphiphilic peptides within such non-crystalline ensembles can be performed utilizing an essential combination of x-ray scattering, neutron scattering, and molecular dynamics simulation techniques.

11:00am **BI-MoM9 Structural Analysis of Phospholipid Membranes and Toxin Assault**, ***T.L. Kuhl,*** *C.E. Miller, T. Gog, K. Kjaer, J. Majewski,* University of California, Davis **INVITED**

In nature, membranes perform several functions of the living cell from selective transport and recognition, to simple sequestration. In general, the membrane consists of a single bilayer or in special cases, such as the lung surfactants, a single monolayer. Using powerful new neutron and x-ray

sources, the techniques of reflectivity and grazing incidence diffraction permit us to obtain structural information on single lipid monolayers and supported bilayers in an aqueous environment. Recently, we demonstrated that 18 keV x-rays can be used to study lipid bilayers at the solid-liquid interface by x-ray reflectivity. We establish that this is a powerful technique for investigating biological systems in a previously inaccessible manner. Our measurements enabled the density distribution of single phospholipid bilayer membranes in bulk water to be measured with unprecedented precision enabling subtle variations in leaflet segregation to be resolved. Recent results on membrane perturbation by toxin binding will also be highlighted. In this case, scattering techniques enable us to distinguish binding and subsequent penetration of lipid layers upon toxin activation.

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