Biomaterials Plenary Session
Room 307 - Session BP-SuA

Biomaterials Plenary
Moderator: H.J. Griesser, University of South Australia

3:00pm **BP-SuA4 New Perspective on Hydrogen Bonding in Water using X-rays*, A. Nilsson,*** Stanford Synchrotron Radiation Laboratory **INVITED**

Hydrogen bonding (H-bonding) in water and at interfaces provides the mechanism for many processes of great importance for biological system. Recent experiments using x-ray and electron spectroscopy have raised the question whether we really understand the nature of H-bonding and the structure of liquid water. Using x-ray absorption spectroscopy (XAS) together with density functional theory (DFT) calculations we have demonstrated the appearance of specific spectral features that can be related to asymmetric H-bonding configurations. These can be seen at the surface of ice and in the liquid phase showing the existence of broken H-bonded local structures. The surprising result for the liquid phase is the large number of broken H-bonded species compared with the established wisdom based on molecular dynamic (MD) simulations. We find that most molecules in the liquid are in two-hydrogen-bonded configurations with one donor and one acceptor hydrogen bond compared to the four-hydrogen-bonded tetrahedral structure in ice. Measuring XAS spectra through x-ray Raman scattering (XRS), where inelastic scattered x-rays cause a core excitation, different samples can be studied in air using hard x-rays. This provides means to study water at various temperatures and pressures. From x-ray emission spectroscopy (XES) and photoelectron spectroscopy (PES) studies of ice, providing information of the occupied orbitals projected onto the oxygen atoms, a deeper insight into molecular orbital rearrangements upon H-bonding could be obtained. The decrease in repulsive interaction through charge transfer and rehybridization is essential for a strong attractive electrostatic interaction. The new applications of x-ray spectroscopy (both XAS and XES) and PES to water based systems provides a unique opportunity to obtain new information that has not been accessible previously. A perspective of implications to interfaces will be given.

3:40pm **BP-SuA6 Synthetic Receptors for Biosensor Surfaces*, I. Lundstrom,*** Linkoping University, Sweden **INVITED**

Several biosensor principles are based on biomolecular interactions on surfaces or in thin sensing layers. One of the most wellknown techniques for the direct elucidation of biomolecular interactions utilizes optical changes in a thin hydrogel (dextran) sensing layer occurring upon the binding of biomolecules to the ligands in the sensing layer. Labelling one of the molecules in an interaction pair with fluorescent groups leads, however, to a large sensitivity, and forms therefore the basis for several detection schemes. Molecular beacons, for example, utilize changes in fluorescence resonance energy transfer or quenching for the detection of structural changes in a biomolecule upon binding to a ligand or upon hybridisation. We are developing synthetic helix-loop-helix polypeptide scaffolds, which show promise as a vehicle for new biosensor principles. Their interesting property is that (arbitrary) ligands can be site selectively introduced in a predetermined order into the scaffold using simple solution chemistry, based on active esters, and without need of protecting groups. The scaffolds are also easily functionalised for covalent binding of them to different types of surfaces and hydrogels. In the talk the use of these versatile scaffolds for biosensing purposes will be described after a short introduction to their chemistry. The coupling of the scaffolds to gold surfaces and to dextran matrices and their use for non-labelling biospecific interaction analysis are touched upon. It will furthermore be shown how the scaffolds can be provided with a binding ligand for a molecule and a (fluorescent) reporter group, indicating that binding has occurred.. In the example an inhibitor, benzenesulfonamide, is used as the ligand for an enzyme, carbonic anhydrase, and dansyl as the fluorescent reporter group. The use of arrays of scaffolds with ligands with different affinities for different biomolecules to enable "diagnostic chips" will finally be discussed.

4:20pm **BP-SuA8 Polyvalency in Biochemistry*, G.M. Whitesides,*** Harvard University **INVITED**

Polyvalent or multivalent interactions are the simultaneous association of multiple ligands on one entity (a molecule or a surface) to multiple receptors on another entity. Multivalent interactions are ubiquitous in biology - in infectious disease, in processes involving antibodies, in blood clotting, metastasis, platelet activation, inflammation, and in many conditions in which cells interact with surfaces- and have become a focus of study in molecular biochemistry. Multiple simultaneous interactions have unique collective properties that are qualitatively different from the properties of their monovalent constituents. Monovalent interactions- generally small molecules directed towards a single receptor site- are clearly fundamental, but understanding them is not necessarily sufficient to understand multivalency and its importance in biology. Our group is interested in confirming, understanding, and quantifying the importance of multivalency in biological interactions, defining the range of biological systems in which it is important, and moving this fundamental knowledge towards applications in the design of drugs and materials.

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