Complexity and Structure at Interfaces Involving Aqueous Solutions: Results of Neutron Reflectometry

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Neutron reflectometry is now a relatively mature technique for exploring composition and structure at interfaces between air and water and between solids and water. Wet interfaces was an area where there was a general dearth of suitable techniques and hence there has been much to find out and many surprises. Most of the surprises have been either to do with the very wide deviations of the nature of adsorption from mixtures away from the bulk composition and/or with the formation of structures that are more extended away from the surface than had been suspected. Both these features are seen in both commercial formulations and in biosystems.

The main topic of the talk will be ordering beyond a single monolayer at wet interfaces. While this occurs for single solutes of both synthetic and biosurfactants it is much more likely in mixtures and the various factors influencing the composition of mixtures at air/water and solid water will be discussed and illustrated with examples.

Exploring Novel Quantum Order and Dynamics: Neutron Scattering under Extreme Conditions

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Neutron scattering is playing a preeminent role in detailed studies of a variety of exciting phase transitions in condensed matter. Related phenomena with strong link to magnetism and spin fluctuations include superconductivity, strangely ‘hidden’ order parameters, quantum criticality in heavy-fermion intermetallics and magnetic insulators, and the effects of frustration and low-dimensionality in quantum spin systems. In such studies, it is the combination of high-quality single crystals of sufficient mass, state-of-the-art neutron instrumentation, powerful and reliable sources, and sophisticated sample environment, which provides access to crucial microscopic information about the involved phases and mechanisms behind the transitions. As an example, spin-dimer based magnetic insulators are model systems for the investigation of quantum criticality and, in particular, the ground states of strongly interacting hardcore bosons, for which there are increasing parallels to ultra-cold atoms in optical lattices. Quantum fluctuations in such magnets can efficiently be controlled by hydrostatic pressure, magnetic field, or chemical composition, leading to complex novel states of matter. We have investigated corresponding quantum phase transitions by neutron scattering and bulk experimental techniques in a series of model compounds [$ACuCl_3$ (A=K, Tl, NH_4), $SrCu_2(BO_3)_2$, $Sr_2Cu(BO_3)_2$, $BaCuSi_2O_6$, and $(C_5H_{12}N)_2CuBr_4$], which cover both the effect of dimensionality and the degree of quasi-particle mobility. The different materials all show distinct spin dynamics associated with the boson system, which they represent, and promote characteristic quantum phases including BEC of magnons, Bose-glasses, valence-bond phases, Luttinger-spin liquids, and potentially even supersolids. The results are discussed in the context of recent developments in high-pressure neutron spectroscopy, quantum many-body theory, and crystal-growth of novel custom-build inorganic materials.

Dynamic Miscibility and Confinement Effects in Multi-component Soft Materials

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For the wide range of substances categorised as “soft matter”, neutron scattering is the technique par excellence to unveil both the structural and dynamical properties at the relevant length scales. This rests mainly on two unique advantages: the suitability of the length and time scales accessed by neutrons, and the capability to manipulate the contrast by specific deuteration of any constituent of the system. On the other hand, the envisaged trends in the field of "soft matter" move towards the study of increasingly complex, often multi-component materials tailor made for industrial applications. Of course, the understanding of features at a molecular level is the key for advancing in this direction. The combination of neutron scattering with other experimental techniques and especially with molecular dynamics simulations provides a very powerful tool for this purpose. In this talk, we will address the question of dynamic miscibility in multi-component systems, in particular in the case of thermodynamically miscible polymer blends. How does the neighbouring presence of chains of another kind modify the different dynamical processes taking place in a glass-forming polymer? We will see that strong dynamic asymmetry in the system leads to the emergence of a newly identified phenomenon, the dynamic confinement. This concept might be ubiquitous in soft materials, especially in complex systems. Seeking for possible universal features of confinement in "soft matter" is an exciting and stimulating exercise.

Materials for Hydrogen Storage : the Role of Neutron Diffraction

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Solid-state metal hydrides display hydrogen densities close to that of liquid hydrogen and thus provide a safe and efficient way of storing hydrogen (energy). A fundamental aspect that needs to be better understood are the metal-hydrogen interactions and their influence on physical properties such as maximum hydrogen content, thermal stability, magnetism and hydrogen induced metal-insulator transitions. In this talk some metallic, covalent and ionic metal hydrides are presented for which structural and physical properties (electric, thermodynamic, spectroscopic, magnetic, optic) change strongly as a function of external parameters such as composition, temperature and pressure. The role of neutron diffraction to structurally characterize these systems will be highlighted. Among metallic systems some show hydrogen induced valence changes ($CeMn_{1.8}Al_{0.2}$-H), antiisostructural phase transitions (Ce_2Ni_7-H), and metal-insulator transitions ($LaMg_2Pd$-H, La_2MgNi_2-H). $La_2MgNi_2H_8$ displays the first dinuclear $[Ni_2H_7]^{7-}$ and tetranuclear $[Ni_4H_{12}]^{12-}$ complexes, is non-metallic and conforms to the 18-electron rule. Other systems display networks of closely spaced hydrogen sites ($ZrTi_2$-H) whose energy difference can be determined by *in-situ* measurements of H site occupancies as a function of temperature. Among covalent systems, various boro-hydrides are investigated in order to better understand the dynamics and decomposition of the complex $[BH_4]^-$ anions. $Mg(BH_4)_2$ has a theoretical hydrogen storage capacity of >10 wt.%. Its structure displays ten symmetry independent $[BH_4]^-$ anions totalling 330 atoms per unit cell. It is one of the most complex crystal structures ever solved from powder diffraction data. Among ionic systems, members of the cubic RH_{3-x} series (*R*=La, Nd, Pr) continue to be investigated in order to shed new light on their metal-insulator transitions. *Ab-initio* calculations on nearly stoichiometric $La_{32}H_{94}$ (=$LaH_{2.94}$) suggest that hydrogen forms vacancies pairs. Their existence needs to be confirmed experimentally which represents a considerable challenge. Finally, the highly absorbing ternary deuteride $^{nat}SmMg_2D_7$ is characterized by high-flux neutron diffraction. Its structure displays strong magnesium-hydrogen interactions and orders magnetically. Taken together, these results lead to a better understanding of the metal-hydrogen interactions in, and the properties of, metal hydrides. The structural features responsible for the changes in their properties are often very subtle and at the limit of experimental resolution. Considering the ever increasing need for *in-situ* studies, this underlines the importance of constantly improving both diffraction equipment and methodology.

The Influence of Extension on Ordering

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Restriction of extension in one or more dimensions can cause strong effects with respect to ordering. Changes in the critical temperature as well as order parameters are often observed, ultimately reflecting the presence of a dimensional crossover. The relevant length scales are linked to the wavelength of excitations close to the critical temperature. Knowledge of the implications of spatial extension on the excitation energies is therefore essential to understand the influence of extension on ordering.

We have used magnetic materials to highlight these effects. First, we dwell on the influence of the thickness of a single layer on magnetic ordering. Then, the effect of stacking magnetic layers with interlayer exchange coupling (IEC) is addressed. The IEC between the layers can be adjusted and its influence on ordering can thus be explored. The criteria for dimensional crossover will be discussed, using results from neutron reflectivity experiments as well as magneto-optical measurements.

The limits will be addressed with respect to the dimensionality of the building blocks, the interactions and the number of repeats. All these length scales will be shown to influence the overall ordering, reflecting a collective behavior of the building blocks. The results will be discussed within the framework of phase transitions and the implications of limited extent on other types such as structural transitions, will be discussed.

Reflections on Biomembranes

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Lipid membranes are widely used as models to investigate the physics and biochemistry of cell membranes but their properties are still relatively poorly characterized in comparison to other soft, thin film materials such as surfactants and polyelectrolytes. Although neutron reflection is now recognized as a very powerful tool in interface research, it's applications to bio-membranes are still limited. Detailed understanding of the structure and composition of model membranes is essential for the interpretation of the interactions between lipids and proteins. This is particularly important for the development of multi-component model membranes that can support membrane proteins and receptors in a functionally relevant environment. There also remain several questions about the nature of lipid-based model systems, including how well they can represent relevant properties of cell membranes, as well as how comparable the properties of different model systems are to each other.

Neutron reflection is one of the few techniques that can provide direct, in-situ compositional and structural information about membranes in an aqueous environment. Examples that will be used to illustrate the insights that neutron reflection can give into model membrane biophysics will include i) lipid self-assembly at solid-liquid interfaces, ii) interfacial enzyme catalysis and iii) model membrane platforms for studying cell adhesion proteins.

High Resolution Spectroscopy at TRISP (FRM II): Technique and Application to Superconductivity and Magnetism

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The triple-axis spin-echo spectrometer TRISP at the FRM II was designed to measure linewidths of phonons and spin excitations with an energy resolution down to 1μeV for excitation energies up to 50meV. The spectrometer is based on the resonance spin echo technique (NRSE) invented by Golub and Gähler and applies the spin echo phonon focusing proposed by F. Mezei. We discuss the basic principles and limits of the technique. Results of typical experiments at TRISP are presented, including a momentum-resolved determination of the electron-phonon interaction in elemental superconductors [1] and measurements of the lifetimes of antiferromagnetic spin waves at low temperatures [2].

[1] T. Keller, P. Aynajian, K. Habicht, L. Boeri, S:K: Bose, B. Keimer, Phys. Rev. Lett. 96, 225501 (2006)

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Nanoscience for the Conservation of Cultural Heritage

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Innovative systems for restoration and conservation of Cultural Heritage are mostly based on soft and hard nanomaterials[1]. Humble nanoparticles of calcium or magnesium hydroxide, microemulsions and magnetic gels embedded with microemulsions have been used to restore frescoes, to remove polymers or clean frescoes and oil paints or to de-acidify paper, wood and canvas. These systems constitute a new platform for conservation and are characterized by scale lengths below 100 nm in one or more dimensions. Scattering techniques are, therefore, the elective tools to tailor the nano-system for the specific conservation or restoration process. With illustrative examples, this presentation will report on some recent restoration workshops. Highlighted examples include the restored masterpieces of Beato Angelico, Taddeo Gaddi, Piero della Francesca, Santi di Tito, Maya wall paints (Calakmul, Mexico), the deacidification of wood from Vasa warship (Stockholm), and the conservation of Organs pipes.

Piero Baglioni and Rodorico Giorgi - Soft and hard nanomaterials for restoration and conservation of cultural heritage. Soft Matter, 2006, 2, 293–303.

Rodorico Giorgi, David Chelazzi, and Piero Baglioni - Nanoparticles of Calcium Hydroxide for Wood Conservation. The Deacidification of the Vasa Warship. *Langmuir* 2005, *21,* 10743-10748.

Emiliano Carretti, Luigi Dei, and Piero Baglioni - Solubilization of Acrylic and Vinyl Polymers in Nanocontainer Solutions. Application of Microemulsions and Micelles to Cultural Heritage Conservation. *Langmuir* 2003, *19*, 7867-7872.

Rodorico Giorgi, Luigi Dei, Massimo Ceccato, Claudius-Vinicius Schettino, and Piero Baglioni - Nanotechnologies for conservation of cultural heritage: paper and canvas deacidification. *Langmuir* 2002, *18*, 8198-8203

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