First Annual Niels Bohr International Academy Meeting on ESS Science

June 27 – July 1, 2011 - Copenhagen

Organizers:
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Niels Bohr International Academy

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Monday 27 June 2011

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Coffee break (10:30-11:15)

Introduction to neutron scattering spectroscopy - Mark Johnson (Institut Laue-Langevin) (11:15-12:30)

Lunch (12:30-14:00)

Neutron scattering and computer simulation studies of aromatic liquids - Neal Skipper (UCL) (14:00-14:45)

Classic Molecular Dynamics and NMR - Michael Vogel (Technische Universität Darmstadt) (14:45-16:00)

Coffee break (16:00-16:30)

Simulation of proton dynamics in a condensed phase: application to hydrated histamine and solid hydrogen-bonded ferroelectric material - Jernej Stare (National Institute of Chemistry) NOTE: This lecture is followed by hands on exercises (16:30-18:00)

Tuesday 28 June 2011

Biomolecular structure refinement by complementing solution NMR spectroscopy with molecular dynamics simulations - Jozica Dolenc (ETH) NOTE: This lecture is followed by hands on exercises (09:00-10:30)

Guided tour of the Niels Bohr Building (28 June 10:00-10:30)

Probing transition states: Insights from NMR, crystal structure determination and simulations - Lynn Kamerlin (Uppsala University) (10:30-11:15)

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Comparison of QENS and PFG NMR techniques to probe diffusion in nanoporous materials - Herve Jobic (IRCELYON) (11:45-13:00)

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Students chose project, hands on data analysis (includes a coffee break) (28 June 14:30-18:30)

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Boat tour & Dinner sponsored by the Oresund Materials Innovation Community (18:30-21:30)

Wednesday 29 June 2011

ESS Science: Opportunities & Ideas - Dimitri Argyriou (ESS Lund) (09:00-09:45)

Inelastic Neutron Scattering: Perpectives - Juergen Eckert (UCSB) (09:45-11:00)

Coffee break (11:00-11:30)

The ever-expanding role of NMR spectroscopies - Beat Meier (ETH) (11:30-12:45)

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Hydration water in biological systems - Jan Swenson (Chalmers University of Technology) (16:00-16:45)

Cold neutrons are cool enough to help us getting home faster - Heloisa N. Bordallo (Niels Bohr Institute) (16:45-17:30)

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Student presentations on their results - 4 Groups of Students (20 minutes each group) (09:00-10:45)

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Structural and dynamic properties of dense particle suspensions: Insight from neutron spin echo and molecular dynamics simulations - Peter Schurtenberger (Lund University) (11:15-12:15)

Molecular Dynamics revealed by Solid State NMR - Gerd Buntkowsky (Technische Universität Darmstadt) (12:15-13:00)

Lunch (13:00-14:15)

Excursion & Conference dinner sponsored by the Helmholtz-Zentrum Berlin. (14:15-20:15)

Friday 01 July 2011

Polymer Dynamics across Tg using QENS - Valeria Arrighi (Heriot-Watt University) (09:00-09:45)

Dynamics in solids studied by NMR spectroscopy - Leo van Wüllen (Universität Münster) (09:45-11:00)

Posters & Coffee break (11:00-11:30)

You never know where it will go: a pathway from bilayers to membranes to targeting tumors - Donald M. Engelman (Yale University) (11:30-12:45)

Lunch and Good bye (12:45-14:00)

Abstract ID : 93

The eternal truths of physics

Primary authors : Prof. HERMAN J.C. BERENDSEN (Emeritus Professor of Physical Chemistry, University of Groningen)

Co-authors :

Presenter :

Track classification :

Contribution type : --not specified--

Submitted by : BORDALLO, Heloisa

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Comments :

Status : SUBMITTED

Track judgments :

Abstract ID : 90

Introduction to neutron scattering spectroscopy

The power of neutron scattering resides in the unique properties of neutrons: they are electrically neutral, have a small magnetic moment, have energies and wavelengths on the scale of condensed matter systems, etc. For applications in spectroscopy, neutron scattering spans the entire energy range (E) from 0 to 500 meV of excitations in condensed matter, with an energy resolution that can be as good as a few micro eV at small energy transfer. In addition, reciprocal space (Q) can be probed allowing the dispersion of excitations to be measured. As a probe of (Q,E) space, neutron scattering spectroscopy is only challenged by inelastic X-ray scattering, for which there are very few instruments in the world. Otherwise these inelastic scattering techniques complement lab-based techniques like infra-red and Raman spectroscopy. The first part of this talk will therefore be used to introduce neutron scattering spectroscopy, including typical instruments and applications.

Analysing inelastic scattering data requires a model of interacting atoms and traditionally experimental data was used to refine inter-atomic force constants. Nowadays there is still a strong synergy between experiment and simulation, with the difference being that lattice and molecular dynamics type simulations, using ab initio methods or classical force fields, are now often the basis for models of ever-more complex systems. In the second part of this talk, I will therefore show a range of examples of how neutrons and numerical methods are giving clear insight into the role of structural excitations in DNA [1], short hydrogen bonds [2], solid oxide fuel cells [3], thermoelectric materials [4], magnetic materials, including iron-pnictide superconductors [5], phase change memory materials [6], etc.

[1] Merzel et al., Phys. Rev. E (2007) 76 31917
[2] Fontaine-Vive et al., J. Chem. Phys. (2006) 124 234503
[3] Koza et al., Nature Mater. (2008) 7 805
[4] Paulus et al., J. Am. Chem. Soc. (2008) 130 16080
[5] Zbiri et al., Phys. Rev. B (2009) 79 64511
[6] Otjacques et al., Phys. Rev. Lett. (2009) 103 245901

Primary authors : Prof. JOHNSON, Mark (Institut Laue Langevin)

Co-authors :

Presenter : Prof. JOHNSON, Mark (Institut Laue Langevin)

Track classification :

Contribution type : --not specified--

Submitted by : Prof. JOHNSON, Mark

Submitted on Wednesday 15 June 2011

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Status : SUBMITTED

Track judgments :

Abstract ID : 41

Neutron scattering and computer simulation studies of aromatic liquids

Aromatic interactions are now known to play a key role in a wide range of important problems, including; the stereochemistry of organic reactions, organic host-guest chemistry and crystal packing, protein folding and structure, DNA and RNA base stacking, protein-nucleic acid recognition, drug design, and asphaltene (heavy crude oil) aggregation and fouling. Neutron scattering used in conjunction with isotope labelling of hydrogen for deuterium is a very powerful method for studying both the structure and dynamics of aromatic molecules, and can be combined with computer modelling to provide new insight into both the fundamental interactions and practical properties. We will discuss studies of pi-pi interactions in liquid benzene, phenol derivatives in clays, and the phase behaviour of asphaltenes.

Primary authors : Prof. SKIPPER, Neal (Universitry College London)

Co-authors : Dr. HEADEN, Tom (Cella Energy) ; Dr. HOWARD, Chris (UCL) ; Dr. DANIEL, Bowron (STFC, ISIS Facility) ; Dr. BOEK, Edo (Imperial College London)

Presenter : Prof. SKIPPER, Neal (Universitry College London)

Track classification :

Contribution type : --not specified--

Submitted by : Prof. SKIPPER, Neal

Submitted on Friday 25 March 2011

Last modified on : Friday 25 March 2011

Comments :

Status : SUBMITTED

Track judgments :

Abstract ID : 63

Classic Molecular Dynamics and NMR

The talk will give an introduction into the use of molecular dynamics (MD) simulations and nuclear magnetic resonancs (NMR) experiments for studies of disordered materials. The priciples of both techniques will be explained and the capabilities will be demonstrated based on examples. In particular, it will be shown that MD simulations and NMR experiments provide interisting insights into the nature of ion transport in solids and of water dynamics in biological and technological confinements.

Primary authors : Prof. VOGEL, Michael (Institute of Solid State Physics, TU Darmstadt)

Co-authors :

Presenter : Prof. VOGEL, Michael (Institute of Solid State Physics, TU Darmstadt)

Track classification :

Contribution type : --not specified--

Submitted by : Prof. VOGEL, Michael

Submitted on Thursday 12 May 2011

Last modified on : Thursday 12 May 2011

Comments :

Status : SUBMITTED

Track judgments :

Abstract ID : 83

Simulation of proton dynamics in a condensed phase: application to hydrated histamine and solid hydrogen-bonded ferroelectric material

Short hydrogen bonds have proved to be extremely prone to nuclear quantum effects, and proton dynamics may be significantly coupled to the fluctuating environment. We developed a cost-efficient methodology for simulation of these effects, based on snapshot structures taken from a preceeding molecular dynamics simulation. At each snapshot geometry, as generated by MD, the instantaneous proton potential is calculated by stepwise moving the proton in the field of frozen nuclei, and the proton energy levels together with wavefunctions are obtained by solving the vibrational Schrödinger equation in the calculated potential. This allows for the evaluation of envelopes of bands that are otherwise difficult to be characterized in the vibrational spectra, i.e., the OH stretching band, and also for the evaluation of a free energy surface along the selected coordinates. We will demonstrate on two selected model systems that the presented methodology assists the interpretation of experimental infrared spectra and yields good agreement with the observed spectral and structural features of the system. Examples of hydrated histamine and solid sodium hudrogen bis-sulfate have been considered, notably differing in the strength of the hydrogen bond and also in the nature of the condensed phase environment.

Primary authors : Dr. STARE, Jernej (National Institute of Chemistry)

Co-authors :

Presenter : Dr. STARE, Jernej (National Institute of Chemistry)

Track classification :

Contribution type : --not specified--

Submitted by : Dr. STARE, Jernej

Submitted on Monday 06 June 2011

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Comments :

Status : SUBMITTED

Track judgments :

Abstract ID : 51

Biomolecular structure refinement by complementing solution NMR spectroscopy with molecular dynamics simulations

In solution nuclear magnetic resonance (NMR) spectroscopy the primary, measured data are collected as temporal and spatial averages of molecular conformations which often can not be represented by a single conformation. The interpretation of NMR observables therefore requires accounting for the conformational averaging in the NMR structure refinement protocol.

Since molecular dynamics (MD) simulations provide representations of the dynamics of molecules in solution, yielding trajectories appropriate for averaging, they have become a well established tool in NMR structure refinement. However, the utility of unrestrained MD simulations in determining biomolecular structure can be limited by insufficient sampling of conformational space and by the finite accuracy of the force field used.

In order to bias the sampling towards the relevant regions of the configurational space, primary experimental data, such as measured nuclear Overhauser effect (NOE) upper distance bounds and 3J-coupling constants, can be introduced as restraints in MD simulations by adding a penalty function Vrestr to the physical force field Vphys. Utilization of coupling constants and NOEs as restraints in biomolecular structure refinement using different functional forms for Vrestr will be presented and illustrated with MD simulations of the C-terminal peptide of GCN4-p1 for which 172 NOEs and 15 3J(HN-HCα)-coupling constants have been measured.

Primary authors : Dr. DOLENC, Jozica (ETH Zurich)

Co-authors :

Presenter : Dr. DOLENC, Jozica (ETH Zurich)

Track classification :

Contribution type : --not specified--

Submitted by : Dr. DOLENC, Jozica

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Comments :

Status : SUBMITTED

Track judgments :

Abstract ID : 54

Probing transition states: Insights from NMR, X-Ray Crystal Structure Determination and Simulations

Recent years have seen tremendous progress in our understanding of the catalytic power of enzymes. Particularly, it is by now generally accepted that the main contributor to enzyme catalysis is the stabilization of the transition state of the enzyme-catalyzed reaction compared to its counterpart in solution. Clearly, in light of this, it would be of interest to characterize enzymatic transition states in greater detail. However, their high energies and fleeting nature makes them too elusive for direct experimental investigation. Therefore, an alternative has been the use of long-lived transition state analogues (TSAs) that aim to mimic the native transition state in order to attempt to indirectly characterize contacts that are important to catalysis. In contrast to the native transition state, a range of experimental techniques can characterize such TSAs, including NMR and X-ray crystallography. However, while great insight has been obtained into enzyme action in this way, it is important to proceed with caution, as things are not always what they seem. That is, despite great structural similarity, the electrostatic contributions to the binding of TSAs can be very different from the corresponding contributions to catalysis (a fact most clearly highlighted in the recent case of ketosteroid isomerase1,2). Nevertheless, the intermarriage of theory and experiment, which combines experimental exploration with theoretical studies of the relationship between the binding of the TSAs and chemical catalysis, can provide experimental insights into the nature of chemical catalysis that would currently be impossible to obtain by any other means.

Primary authors : Prof. KAMERLIN, Shina Caroline Lynn (Department of Organic Chemistry, Stockholm University)

Co-authors :

Presenter : Prof. KAMERLIN, Shina Caroline Lynn (Department of Organic Chemistry, Stockholm University)

Track classification :

Contribution type : --not specified--

Submitted by : BORDALLO, Heloisa

Submitted on Saturday 30 April 2011

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Status : SUBMITTED

Track judgments :

Abstract ID : 74

Comparison of QENS and PFG NMR techniques to probe diffusion in nanoporous materials

Molecular diffusion in the interior of nanoporous materials can be followed by pulsed-field gradient NMR (PFG NMR) and by quasi-elastic neutron scattering (QENS). The two techniques will be introduced and comparisons analysed for several systems.

The classical instruments to measure QENS are time-of-flight (TOF) and back-scattering (BS) spectrometers. The technique is called quasi-elastic because the spectra are centred around zero energy transfer and small energy transfers are implied, typically   2 meV. Depending upon the instrumental resolution, a broadening of the spectra will be observed if the molecules diffuse over a time scale ranging from 10-8 to 10-12 s. Another neutron technique which has been used recently to derive diffusivities in porous media is the neutron spin-echo (NSE) technique. It has been found that NSE pushes down the lower limits of diffusion coefficients accessible by neutron methods by two orders of magnitude. In leading neutron scattering facilities, one can now cover a very wide range of time scales, from femtoseconds to microseconds.

During QENS experiments, one probes molecular diffusion over space scales ranging from a few Å to several nm. At short distances, jumps between adsorption sites can be observed, so that the characteristic lengths and times of the elementary steps can be determined using jump diffusion models. Such jump processes can be analysed by simulation techniques, which makes comparisons between QENS and simulations very fruitful. Over larger space scales, one approaches Fickian diffusion so that the influence of the jumps becomes less important in deriving diffusion coefficients.

The first QENS measurements were performed on hydrogenated molecules, since the large incoherent cross section of hydrogen gives a good contrast with the signal from the sorbent. From these experiments, one obtained self-diffusivities. However, one can also probe the diffusion of molecules which do not contain hydrogen atoms, e.g. CO2, CF4, deuterated molecules… The scattering of these molecules is coherent and one can extract in this case a transport diffusivity.

Anisotropic diffusion will also be discussed, since 3D porous frameworks can contain only 1D channels. One can differentiate normal 1D diffusion from single-file diffusion (when the molecules cannot cross each other in the channels).

Primary authors : Dr. JOBIC, Herve (IRCELYON)

Co-authors :

Presenter : Dr. JOBIC, Herve (IRCELYON)

Track classification :

Contribution type : --not specified--

Submitted by : Dr. JOBIC, Herve

Submitted on Thursday 26 May 2011

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Comments :

Abstract ID : 89

Looking into the future of neutron scattering with ESS: Current status and scientific opportunities

The European Spallation Source (ESS) is on track to be build in Lund, Sweden and co-hosted by both Denmark and Sweden. The ESS will offer an order of magnitude greater peak neutron flux than what is currently available in the world. These unprecedented bright neutron beams will enable new science and allow us to examine matter with a clarity that is not attainable with current neutron sources. With accelerator and target station currently under detailed design considerations, ESS is focusing on the neutron instrumentation suite. In the talk I will discuss the status of the ESS project and focus on the proposed neutron scattering instrumentation, its capabilities and the processes we have put in place to identify and pursue scientific opportunities.

Primary authors : Dr. ARGYRIOU, Dimitri N. (European Spallation Source ESS AB)

Co-authors :

Presenter : Dr. ARGYRIOU, Dimitri N. (European Spallation Source ESS AB)

Track classification :

Contribution type : --not specified--

Submitted by : BORDALLO, Heloisa

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Track judgments :

Abstract ID : 87

Neutrons, Computation and the Dynamics of Molecules: Current Status and Prospects

An enormous range of time scales, and hence types of molecular dynamics, is in principle accessible to various neutron scattering methods, from reptation in polymers to the stretching mode of the hydrogen molecule. Detailed analysis and definitive interpretation of such neutron scattering experiments is, however, increasingly dependent on parallel computational studies, particularly in complex systems. The latter include crystalline materials with very large unit cells, or with partial disorder, non-crystalline or amorphous materials, including, for example, reactants, intermediates or products of a chemical reaction on dispersed metal catalysts, or for that matter, many materials of technological importance. While improvements in neutron source intensities (ESS) and associated advances in instrumentation will no doubt substantially increase the use of neutron scattering methods for studies of the dynamics of molecules, these will have to be accompanied by advances in computational studies. For example, computations that are now lengthy and complex need to become (almost) routine for interpretation of the neutron scattering experiments. I will describe a number of current neutron scattering and computational studies with depend on the synergy of these methods, but delineate how such improvements would widen the scope of this type of an investigation. These will include the dynamics of adsorbed hydrogen in MOF’s, reactions on high surface area catalysts, and the dynamics of hydrogen bonded systems.

Primary authors : Dr. ECKERT, Juergen (University of South Florida)

Co-authors :

Presenter : Dr. ECKERT, Juergen (University of South Florida)

Track classification :

Contribution type : --not specified--

Submitted by : Dr. ECKERT, Juergen

Submitted on Friday 10 June 2011

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Comments :

Invited Talk

Status : SUBMITTED

Track judgments :

Abstract ID : 88

Structure and Dynamics of Biomolecules by NMR

The talk will introduce the principles for structure determination in noncrystalline solids, e.g. amyloids and prions. The present state of the art in the authors labs will be described and first results for the characterization of the dynamics in prion fibrils will be presented.

Primary authors : Prof. MEIER, Beat (ETH Zurich)

Co-authors : Prof. ERNST, Matthias (ETH Zurich) ; Dr. BöCKMANN, Anja (IBCP Lyon) ; Dr. SCHANDA, Paul (ETH Zurich) ; Dr. MELKI, Ronald (Laboratoire d’Enzymologie et Biochimie Structurales, Paris) ; Dr. BOUSSET, Luc (Laboratoire d’Enzymologie et Biochimie Structurales, Paris) ; Dr. WASMER, Christian (ETH Zurich) ; Mrs. HABENSTEIN, Birgit (IBCP Lyon)

Presenter : Prof. MEIER, Beat (ETH Zurich)

Track classification :

Contribution type : --not specified--

Submitted by : Prof. MEIER, Beat

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Comments :

Status : SUBMITTED

Track judgments :

Abstract ID : 61

Hydration water in biological systems

In this presentation the dynamical behaviour of hydration water in biological systems, such as hydrated proteins, lipid membranes and food materials, will be compared. Of particular biological interest is also to elucidate how the dynamics of the hydration water influences the dynamical properties of the biomolecules and vice versa. From quasi-elastic neutron scattering (QENS) experiments and dielectric relaxation measurements we can conclude that there is generally a interplay between the water dynamics and the biomolecular dynamics, although the water affects the biomolecules more than the other way around.

The power of combining QENS and dielectric spectroscopy is also discussed, as well as the limitations and difficulties of analysing QENS data on dynamically heterogeneous systems exhibiting anharmonic motions in a energy range that considerably exceeds the accessible energy window of the spectrometer. Furthermore, we discuss the usefulness of molecular dynamics (MD) simulations for the interpretation of the experimental data and for providing a detailed site-specific atomistic understanding of the structure and dynamics.

Primary authors : Prof. SWENSON, Jan (Chalmers University of Technology)

Co-authors :

Presenter : Prof. SWENSON, Jan (Chalmers University of Technology)

Track classification :

Contribution type : --not specified--

Submitted by : Prof. SWENSON, Jan

Submitted on Wednesday 11 May 2011

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Status : SUBMITTED

Track judgments :

Abstract ID : 92

Cold neutrons are cool enough to help us getting home faster

Concrete, the most abundant of the man-made materials, also predates both pottery and metal as the first industrially produced material. Over 8000 years ago it was produced in half ton from fired limestone giving a concrete with compressive strength similar to that of conventional construction concrete produced in ready mix plants today. About 5000 years ago the Egyptians heated gypsum to use as a cementitious material, and later the Greeks developed a calcium silicate system, which was used by the Romans to produce concrete that has proven to be durable for over 2000 years. Today, Portland cement, is normally used for concrete production.

In a time where the effects of climate change on weather patterns is accepted as real and serious, and where the cement industry produces 5-7% of the world’s carbon dioxide emission, decreasing the production of carbon dioxide is perceived crucial. Thus, improvements in the production of concrete are critical ; more durable concrete that requires less carbon dioxide per unit of manufacture has to be made. To reach such a goal the knowledge of the physical chemistry of the water-cement paste interactions, that are fundamental in understanding and predicting the service life of concrete infrastructure, must be expanded. The durability of concrete is related to its ability to limit fluid transmission and knowledge of how to reduce the rate at which water will be transmitted through cement paste is critical to achieve durability.

Our motivation is to use incoherent inelastic neutron scattering to differentiate between the capillary pore water and gel water, focusing is on the mobility of water in hydrated cement paste. While the onset of the water dynamics, which is modified by the local environment, could be investigated with elastic temperature scans using high-resolution neutron backscattering, neutron spin echo spectroscopy was used to measure the water diffusion over the pore network.

In summary, different motions of water in capillary or gel pores were monitored ; by using a combination of cement pastes ; cured at different times and RH, and examined by neutron scattering spectroscopy at different time (space) scales allowing for the understanding of the water-cement paste interaction at the molecular level. Such interactions control some of the most important macro properties of concrete. Moreover to extend our understanding the mobility of interlayer water in clays will be considered.

To conclude neutron scattering may eventually prove to be as valuable as the nitrogen adsorption techniques to understand this amorphous, complex and extremely valuable material.

Primary authors : Prof. BORDALLO, Heloisa (NBI, Danmark)

Co-authors : Dr. ALDRIDGE, Laurence (ANSTO, Australia)

Presenter :

Track classification :

Contribution type : --not specified--

Submitted by : BORDALLO, Heloisa

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Comments :

Abstract ID : 69

Structural and dynamic properties of dense particle suspensions: Insight from neutron spin echo and molecular dynamics simulations

Dense particle suspensions often exhibit a so-called arrest transition, where the dynamics of the particles suddenly arrests and the sample exhibits solid-like properties. The gels and glasses that form in this arrest transition represent classes of non-equilibrium solids that play an important role in various food and materials science applications. Colloids or proteins with short-range attractions can exhibit different liquid-solid transitions as a function of the strength of the attraction and the volume fraction. The possibility to modify the solution properties by playing with interparticle interaction strength and range lead to interesting phenomena and provide a tool kit to produce cluster phases, gels and glasses with tailored structural and mechanical properties.
However, the resulting systems often pose enormous problems to experimentalists and theoreticians due to the existing very large range of length and time scales. Here I will demonstrate how we can use small-angle neutron scattering and neutron spin echo experiments combined with rheology experiments, molecular dynamics and Brownian dynamics computer simulations to obtain a wealth of information from these complex systems.

Primary authors : Prof. SCHURTENBERGER, Peter (Lund University)

Co-authors :

Presenter : Prof. SCHURTENBERGER, Peter (Lund University)

Track classification :

Contribution type : --not specified--

Submitted by : Prof. SCHURTENBERGER, Peter

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Comments :

Status : SUBMITTED

Track judgments :

Abstract ID : 48

Molecular Dynamics revealed by Solid State NMR

Solid state NMR spectroscopy allows structural and dynamical studies of molecular conformations in solid environments. As far as the dynamic properties of solid systems are concerned, NMR can cover a very large dynamical range: It is possible to study processes on a time scale of 10-12 sec (indirect detection of a reaction kinetics) to processes on a time scale of 107 sec (slow dynamic processes like conformational changes of a molecule or slow chemical reactions) and observe directly or indirectly molecular structures and their transformations on these time scales. These effects are studied by combinations of several NMR techniques, like 15N- and 2H-solid state NMR line shape analysis, MAS NMR and others. This combination does not require crystalline samples or special clean and well defined surfaces like conventional surface science techniques, but can work with typical ill-defined real world systems. The talk discusses after a short introduction the salient features of these NMR experiments to give the reader a basic knowledge of the systems and the experiments. The rest of the talk then focuses on the structural and dynamical properties of small molecules confined in mesoporous silica and of hydrogen interacting with transition metal nanoparticles. It is shown that solid state NMR is able to reveal fascinating new features of the guests, which are often not known for their bulk phases. These features depend strongly on the interplay of the their interactions with the silica surface and their mutual interactions.

Primary authors : Prof. BUNTKOWSKY, Gerd (TU Darmstadt)

Co-authors :

Presenter : Prof. BUNTKOWSKY, Gerd (TU Darmstadt)

Track classification :

Contribution type : --not specified--

Submitted by : Prof. BUNTKOWSKY, Gerd

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Comments :

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Track judgments :

Abstract ID : 81

Polymer Dynamics across Tg using QENS

Molecular motion in polymeric materials reaches a high degree of complexity, far beyond that observed in small molecules. Chain connectivity plays a major role and the dynamic behaviour of polymers encompasses a widespread length scale. As a consequence, a complete, accurate picture of polymeric behaviour can only be achieved through combined use of experimental techniques which sample complementary frequency (or time) ranges.

A choice of instrumental techniques is available to polymer scientists for studying sub-Tg relaxations in bulk or solutions, as well as polymer motion above the glass transition temperature, Tg. These studies have great potential for improving our understanding of the mechanical behaviour and the rheological properties of polymers in bulk.

Over many years, the technique of quasi-elastic neutron scattering (QENS) has proven to be unique in providing simultaneous frequency and spatial information on high frequency (107 to 1014 Hz) molecular motion at local length scales. This high frequency range has been exploited to investigate side group rotations, and to test theoretical descriptions of the glass transition as well as the Rouse model.

QENS experiments usually suffer from a limited energy range and to overcome these limitations, it is often necessary to combine data from a number of instruments, differing in both resolution and energy range. By overlapping the intermediate scattering functions, it has been possible to separate molecular processes and extract reliable information on the distribution of relaxation times (DRT).

Recent years have seen not only advances in polymer synthetic chemistry, but also in molecular modelling and neutron scattering has afforded a way to compare computer simulations and experimental data and. This has further improved our understanding of polymeric behaviour and stimulated work on increasingly complex systems such as polymer blends and nanocomposites.

Primary authors : Dr. ARRIGHI, Valeria (Heriot-Watt University)

Co-authors :

Presenter : Dr. ARRIGHI, Valeria (Heriot-Watt University)

Track classification :

Contribution type : --not specified--

Submitted by : Dr. ARRIGHI, Valeria

Submitted on Wednesday 01 June 2011

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Status : SUBMITTED

Track judgments :

Abstract ID : 91

Dynamics in solids studied by NMR spectroscopy

Solid State Nuclear Magnetic Resonance spectroscopy has long evolved as one of the most powerful analytical techniques for the characterization of the structure of and the dynamics in solids. Employing the orientational dependence of the internal interactions such as chemical shift interaction (CS), homo- and heteronuclear dipolar interaction (DIP) or quadrupolar interaction (QUAD) enables the analysis of structural motifs on short length scales (1 – 2 Å, CSA and QUAD); the r-3 dependence of the dipolar interactions offers a handle to study structural motifs on intermediate length scales (2 – 10 Å). Utilizing the modulation of the orientational dependence of the interactions due to the dynamic processes offers the opportunity to analyse dynamic processes over an extremely wide range of correlation times ranging from 10-9 s to 100 s, applying T1, T2 and T1 .relaxation times measurements, line shape analysis and two dimensional exchange experiments.

The presentation will give a detailed introduction into the various solid state NMR methodologies to study motional processes with correlation times from nano-seconds to seconds. Examples from our group (and others) – mainly from the field of solid electrolytes – will illustrate the enormous wealth of information which can be obtained from this approach.

Primary authors : Dr. VAN WüLLEN, Leo (Institute for Physical Chemistry; University of Münster)

Co-authors :

Presenter : Dr. VAN WüLLEN, Leo (Institute for Physical Chemistry; University of Münster)

Track classification :

Contribution type : --not specified--

Submitted by : Dr. VAN WüLLEN, Leo

Submitted on Thursday 16 June 2011

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Comments :

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Track judgments :

Abstract ID : 52

You never know where it will go: a pathway from bilayers to membranes to targeting tumors

The 1960's confusion about membrane lipid structure was resolved with solution x-ray scattering observations, and the relevance of bilayer structure is now unquestioned. Neutron studies of Cytochrome b5 showed that a peptide can spontaneously insert across a bilayer, and ideas of membrane protein folding were examined using fragments of Bacteriorhodopsin. A surprising result was the observation that the C helix of Bacteriorhodopsin exhibits spontaneous, pH-dependent insertion from solution to form a helix across lipid bilayers.

We are using a related peptide family, the pH (Low) Insertion Peptides (pHLIP), to study the insertion process, to selectively image acidic tissues in vivo and to translocate cargo molecules across the plasma membranes of living cells. The peptide has three kinds of states: soluble in water, bound to the surface of a membrane, and inserted across the membrane as an alpha-helix. At physiological pH, the equilibrium is toward water and the membrane surface, which explains its lower affinity for cells in healthy tissue; at acidic pH, titration of Asp residues shifts the equilibrium toward membrane insertion and tissue accumulation. Using a thermodynamic analysis, we have defined energies and inferred lipid involvement in these states. We have begun to define the parameters of molecules that can be translocated, and have also explored variations of the pHLIP sequence.

Because pHLIP is unfolded on the surface of a bilayer and folding is pH-triggered, we are able to apply kinetic analysis. When the pH is dropped, it is found that a helix forms rapidly on the surface of a bilayer, followed by a slow insertion across it in several kinetically distinct steps. Exit when the pH is jumped is more rapid, and includes partial unfolding of the helix while still in the bilayer.

Translocation is selective for low pH, and various types of cargo molecules attached by disulfides can be released by reduction in the cytoplasm, including peptide nucleic acids, a polar cyclic peptide (phalloidin), and organic compounds. Because a high extracellular acidity is characteristic of a variety of pathological conditions (such as tumors, infarcts, stroke-afflicted tissue, atherosclerotic lesions, sites of inflammation or infection, or damaged tissue resulting from trauma), the pH (low) insertion peptide may prove a useful tool for selective delivery of agents for drug therapy, diagnostic imaging, genetic control, or cell regulation. Two cases will be discussed in this area: use of phalloidin to immobilize cells, and delivery of Peptide Nucleic acids to control gene expression.

Finally, application of the technology to image tumors in mice and inhibit cancer cell proliferation will be discussed.

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Track classification :

Contribution type : --not specified--

Submitted by : BORDALLO, Heloisa

Abstract ID : 50

NEUTRON AND RAMAN SCATTERING IN SELECTED ALIPHATIC AMINO ACID CRYSTALS

The search to understand basic molecular systems, in particular, related to the stability of hydrogen bonds in proteins and enzymes, induced a great number of researches in the last years. In the solid state, amino acid assumes the zwitterions form, RHC(NH3+)(CO2-), where R is a radical. For L-alanine, where R is equivalent to CH3, an analysis of the structural parameters shows that deuteration induces significant geometric changes as a function of temperature, and this can be related to the observation of new lattice vibration modes in the Raman spectra. The particular study on fully deuterated L-alanine shows the occurrence of a structural rearrangement at about 170 K. The study of partially deuterated L-alanine shows that between 80 and 100 K, a subtle modification related to ND3+ deformation can be related to a conformational modification of amino acid molecule in the unit cell. Additionally we have observed that by decreasing the temperature, one of the hydrogen bond increases its length below 100 K while another hydrogen bond length presents anomaly between 160 and 250 K. The second part of the work deals with studies of inelastic neutron scattering on L-valine between 270 and 320 K in both partially deuterated and fully hydrogenated L-valine. The research gives a description of the low frequency modes of the material. At low temperature, it was possible to understand that a phase transition occurs related to the activation of an infrared mode in the Raman spectra. On the other hand, results show that between 295 and 423 K the structure of L-valine is stable. The band associated to torsional vibration of CO2 on heating suggests that the hydrogen bonds among the molecules in the unit cell are softened due to the increasing of the distance between adjacent molecules. Finally, we present results on L-leucine where a relationship between the local dynamics of NH3, CH3, CO2 and CH2 moieties and the molecular structure of the amino acid is presented. Also, the investigation shows that pronounced changes between 190 and 250 K is present for many modes of L-leucine crystal, including lattice modes as well as a re-distribution of the intensity of the dynamic susceptibility function down to 130 K.

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Track judgments :

Abstract ID : 65

Energy-density fluctuations in a molten salt

We measured the density fuctuations spectrum of a prototype liquid ionic binary mixture (RbF) through inelastic neutron scattering as a function of the momentum transfer in the 2-12 nm^-1 range. Data show the existence of two distinct collective excitations above 4 nm^-1 : a high-frequency mode, associated to density-fluctuations, and a low-frequency one, which can be related to energy fuctuations. We associate the latter mode to a propagating heat wave. So far, this kind of excitation was never observed in ordinary liquids. This result points out how thermal fluctuations may have a prominent role in describing the microscopic collective dynamics in liquids outside the hydrodynamic limit.

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Track classification :

Contribution type : --not specified--

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poster presentation

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Abstract ID : 66

Interpretation of NOESY Cross-relaxation Rates from NMR and MD simulations for simple surfactant systems

Comparison between measured nuclear magnetic resonance (NMR) parameters to the ones calculated from atomistic molecular dynamics simulations (MD) for lipid bilayer systems has always been essential part of validating the MD force fields. The most common parameters to compare has been the order parameters and spin lattice relaxation times for acyl chains.
In addition to these also nuclear Overhauser enchancement spectroscopy (NOESY) cross relaxation rates have been calculated from MD simulations and compared to the experiments. The cross relaxation rates depend on both, orientation and distance correlation between proton pairs in the system.
However, the interpretation of cross relaxation rates measured by NMR in tedious. Our goal is to use molecular dynamics simulations to ease this task. As an example system we use simple surfactant mixture of cetyltrimethylammonium (CTA+) and succinate ions. For this system we determine NOESY cross relaxation rates from both, NMR experiment and MD simulations. Then we use this data to validate the simulation model and interpret the NMR results.

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Track classification :

Contribution type : --not specified--

Submitted by : Dr. OLLILA, Samuli

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Track judgments :

Abstract ID : 47

Exploration of the long chain n-alkanes adsorption and diffusion in the MOF-type MIL-47 (V) material by combining experimental and molecular simulation tools

The adsorption properties of linear alkanes (from n-pentane to n-nonane) single vapor within the rigid MOF MIL-47 (V) have been explored by combining gravimetric measurements and molecular simulations. Both experimental absolute isotherms and enthalpies of adsorption for all alkanes were contrasted to those obtained by Configurational Bias Monte Carlo simulations based on two different force fields. From a fair agreement between experimental and simulated data, a further step consisted of investigating the microscopic adsorption mechanism in play in order to shed some light into the preferential orientations and conformations of all investigated alkanes. While the trans conformation is predominantly observed for all alkanes, the proportion of the alkane conformations lying parallel to the direction of the tunnel significantly increases with the chain length, emphasizing that the confinement effect is stronger for the longer chain alkanes. Finally, Molecular Dynamics simulations allowed us to emphasize that all alkanes are mainly gliding along the direction of the tunnel, leading to a 1D type diffusion mechanism, the motions being mainly centred around the middle of the pores at low loading, while they are significantly shifted towards the pore wall when the alkane concentration increases.

We have also recently performed MD simulations of the diffusion of n-alkanes from C5 to C21 in this MIL-47(V) for a given loading. We have pointed out a spectacular behavior with the self-diffusivity decreasing up to C12 and further increasing with a maximum for C18 prior to decreasing again for the longer chain length. We have further evidenced that the trend of the self-diffusivity as a function of the chain length can be explained in light of the evolution of the fraction of the "gauche" conformations when the alkane becomes longer.

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Track classification :

Contribution type : --not specified--

Submitted by : Dr. RIVES, Sebastien

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Comments :

Abstract ID : 49

Sassena - X-ray and Neutron Scattering Calculated from Molecular Dynamics Trajectories using Massively Parallel Computers

Massively parallel computers now permit the molecular dynamics (MD) simulation of multi-million atom systems on time scales up to the microsecond. However, the subsequent analysis of the resulting simulation trajectories has now become a high-performance computing problem in itself. Here, we present software for calculating X-ray and neutron scattering intensities from MD simulation data that scales well on massively parallel supercomputers. The calculation and data staging schemes used maximize the degree of parallelism and minimize the IO bandwidth requirements. The strong scaling tested on the Jaguar Petaflop Cray XT5 at Oak Ridge National Laboratory exhibits virtually linear scaling up to 7000 cores for most benchmark systems. Since both MPI and thread parallelism is supported, the software is flexible enough to cover scaling demands for different types of scattering calculations. The result is a high performance tool capable of unifying large-scale supercomputing and a wide variety of neutron/synchrotron technology.

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Track classification :

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paper submitted. The software will be available as soon as the paper is accepted.

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Track judgments :

Abstract ID : 53

INTERACTION MECHANISM OF INORGANIC CATION IN THE INTERALMINAR SPACE OF HIGH CHARGE EXPANDABLE SILICATES.

The study of the interaction mechanisms between exchangeable cations and layered silicates is of interest from the basic and applied point of view. On one hand, it is crucial to the evaluation of the physicochemical properties of these materials. On the other hand, the hydration of interlayer cations and the clay surface control the swelling, dispersion and ion exchange properties of these layered silicates, and it is an important part of the clays' usability in catalysts, waste disposal, and other applications.

Although the swelling 2:1 layered silicates have been traditionally recognised as those containing a total layer charge between 0.4 and 1.8 units (smectite and vermiculite groups), a new family of synthetic swelling 2:1 phyllosilicates with tuned layer charge values, ranging between 2.0 and 4.0, have been recently synthesized and a general synthesis method have been reported by us (Chem. Mater. 2006, 18, 2867).

In this work the sorption capacity of a set of inorganic cations with the same electronic configuration by expandable high charge micas have been explored. The short and long range structural order of the samples have been analyzed. Their hydration and swelling capacity have been determined by termogravimetric analysis and XRD. The hydration/dehydration processes have been studied using a diffractometer with a reaction chamber and variable temperature. Finally, the interactions between the interlayer cations and the silica network have been explored by MAS-NMR.

The results have shown that cation exchange is effectively achieved and the hydration state of the interlayer space not only depends on the cation charge but also on the silicate surface. Short order structural studies have revealed the existence of a complex between the interlaminar cation and the oxygen of pseudohexagonal cavity of the structure, which may affect the hydration/dehydration of the phylosilicates.

By a combination of neutron diffraction, computer modelling and more complex experiments of MAS-NMR, we will be able to answer key questions, about the orientation and dynamics of different inorganic cations at the clay interlayer space under non ambient conditions.

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Track classification :

Contribution type : --not specified--

Abstract ID : 55

Effects of confinement on polymer dynamics.

Effects of a confinement, e.g. solid surface, on the structure and dynamics of polymers are a much studied subject nowadays [1]. Understanding the structure and dynamics of polymers close to the confining surface (interface) and in the intermediate phase between the interface and a bulk phase (interphase) is important for applications in nanotechnology such as coatings for electrical devices, lubricants, and polymer nanocomposite materials. Confinement effects in polymer melts may lead to unusual properties. This concerns both the chain conformation, which may be distorted in particular if the chain dimensions are significantly larger than the confinement size, as well as chain dynamics, which may be altered due to surface interactions and changes of topology and chain self-density [1–4]. Today microscopic studies on the chain dynamics under confinement are mainly available through simulations. Only a few experiments have addressed this problem on the chain level, e. g the flow of polymers through nanopores, the extensional rheology of nano-sized polymer films or NMR relaxometry. Basically all simulations of polymer chains under confinement available indicate reduced chain mobility independent of the interaction potential of the wall. E. g. the MD analysis of the Rouse modes of unentangled chains under confinement reveals a uniform slowing down of all modes that was interpreted by an effective increase of monomeric friction [5].

The aim of this work is to study the influence of the solid surfaces (confinement) and their interaction with polymers on the dynamics of polymer melt by neutron scattering methods. The confining systems are presented by well-ordered cylindrical nanopores (2D confinement) of anodic aluminum oxide (AAO). We focus on the segmental dynamics on the local time scale measured by quasielastic neutron scattering (QENS) up to a few nanoseconds and on the large scale dynamics measured by high resolved neutron spin-echo (NSE) spectroscopy extending the time scale to a few hundred of nanoseconds. The main goal is investigation of the influence of the confining surfaces and geometrical confinement on the structure and dynamics of polymer chains at the interface and their extent into a possible interphase for different types of interaction between solid walls and the melt.

In our previous work performed with poly(ethylene oxide) (PEO) confined in AAO templates we observed a slowing down of the dynamics at intermediate time scale (>1 ns). On the other side, the dynamics at shorter time scale (<1 ns) remained indistinguishable from the Rouse dynamics as observed in the bulk. (fig.1) This finding indicates a nonuniform change of the normal modes governing the relaxation dynamics of polymer chains. In this case the nature of the confinement implies an attractive interaction between polymer and pore walls. The observed effect has been attributed to slowing down of long-wave Rouse modes as a result of a (transient) adsorption of polymer segments at the surface. This is in contradiction to simulations that were interpreted in terms of an overall slowing down of all Rouse modes [5]. In a first approximation the adsorption effect was modelled by a Rouse chain with pinned segments, such that on average all segments “touching” the surface are (transiently) pinned.

In our recent experiments with polyethylene-alt-propylene (PEP) confined in AAO templates we did not observe any pronounced confinement effect on the local dynamics at the time scale of order of nanoseconds.

The neutron scattering results will be supplemented by NMR, broadband dielectric spectroscopy (BDS), bulk rheological studies and computer simulations. This work is part of the Priority Program SPP1369 financed by Deutsche Forschungsgemeinshaft.

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Track classification :

Contribution type : --not specified--

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Comments :

Status : SUBMITTED

Track judgments :

Abstract ID : 57

Conformational motions in hydrated myoglobin by dielectric relaxation spectroscopy

Protein function requires conformational motions; conformational protein dynamics are coupled to the dynamics in the bulk solvent and the hydration shell. In this study we investigated the protein-hydration shell interactions by measuring the dielectric response of myoglobin embedded in solid poly(vinyl) alcohol and hydrated at different levels. The hydration-shell relaxations depended sensitively on hydration. We found that the internal motions of myoglobin can be predicted from the hydration-shell relaxations using a simple model. Here we report two examples: the temperature dependence of the Mössbauer elastic fraction in myoglobin and the msd of all the non-methyl hydrogen atoms in myoglobin measured by neutron scattering. The rapid decrease in the elastic fraction and the rapid increase in the msd at ~200 K are both predicted from the dielectric data. This quantitative connection of dynamics between myoglobin and its hydration shell manifests the essential role of water for the functions of proteins.

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Track classification :

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Submitted by : Dr. CHEN, Guo

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Track judgments :

Abstract ID : 58

The role of total scattering and multiscale modeling in the technological development of geopolymer concrete

‘Geopolymer’ concrete which is derived from coal fly ash and blast furnace slag activated by an alkali source has recently become an emerging area of research due to application as a sustainable alternative to traditional concrete (ordinary Portland cement-based concrete). The success of this material in the industrial setting is in large part due to the increasing pressure to use environmentally friendly materials, and with Portland cement accounting for 5-8% of global man-made CO2 emissions, geopolymer concrete is a viable alternative.

In order to attain a practical alkali-activated geopolymer concrete there has been extensive research into both the real-world material and a variety of associated model systems. In this paper, we outline how molecular research on these model systems using neutron and X-ray total scattering analysis and simulation techniques has contributed to understanding the structural mechanisms occurring during formation of the model systems. Techniques utilized include reciprocal-space and local structure analysis from total scattering, density functional modeling, and coarse-grained Monte Carlo simulations. Hence, by understanding the mechanisms responsible for the behavior of model systems, and therefore various aspects of the chemistry of the industrial counterpart especially at the nanoscale, there exists new evidence regarding the performance and durability of this new material.

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Abstract ID : 59

Relaxation Behaviour of Xylitol-Water Mixtures

Dielectric spectroscopy, differential scanning calorimetry (DSC) and photon correlation spectroscopy (PCS) were employed to study supercooled xylitol mixed with water in wide frequency and temperature ranges. The presence of water clearly has an effect on both the viscosity related and cooperative α-relaxation and the secondary β-relaxation, as observed in the dielectric data. The α-relaxation, which shows non-Arrhenius temperature dependence, becomes faster with increasing concentration of water. The secondary β-relaxation shows Arrhenius temperature dependence and the intensity increases dramatically with increasing water concentration. We find one calorimetric glass transition over the whole concentration range. It decreases from 247 K for pure xylitol to about 181 K at a water concentration of about 37 wt%. At higher water concentrations ice is formed and the glass transition temperature increases to a steady value of about 200 K for all higher water concentrations. This Tg corresponds to an unfrozen xylitol-water solution containing 20 wt% water. In addition to the true glass transition we observed a glass transition-like feature at 220 K for all the ice containing samples. However, this feature is more likely due ice dissolution [1]. In the temperature range of the PCS measurements we do not observe the α-relaxation, which is too fast, but only the relaxation of concentration fluctuations in the polarized light scattering data. The relaxation time of this process shows a 1/q2-dependence and it decreases with increasing water content. Furthermore, from the dielectric relaxation data, where this process is also observed, it is clear that the concentration fluctuations exhibit an Arrhenius temperature dependence with an activation energy that decreases with increasing water concentration. At high temperatures the process is considerably slower than the structural α-relaxation, but around the glass transition temperature the two relaxation processes seem to merge. In the near future the structural nature of the concentration fluctuations will be explored by small-angle neutron scattering measurements on LOQ at ISIS, UK.

Reference:

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Contribution type : --not specified--

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Status : SUBMITTED

Abstract ID : 60

The role of small-angle scattering in the investigation of nanoscaled hydrides in carbon scaffolds for hydrogen storage applications

One of the most promising routes towards a hydrogen economy is the use of hydrogen as energy vector for vehicular and stationary applications in the form of solid storage material based on nanoscaffold hydrides. When dealing with nanoporous materials, small-angle scattering gives invaluable information that can help to develop the most suitable solid material. The successful wet or melt infiltration of hydrides into carbon scaffolds has been demonstrated by small-angle neutron scattering (SANS) performed at the JEEP II reactor at IFE.(*) Depending on the hydride and/or the scaffold used, the particle sizes range from 1 to 6 nm. Using in situ small-angle X-ray scattering (SAXS), it was possible to underline important differences in the morphology and surface area of the hydride particles during heating when they are nanoconfined in the porous scaffolds, compared to their values in the bulk state. The demonstrated changes in hydrogenation/dehydrogenation properties of these nanoconfined systems could be related to the differences mentioned above. SANS and SAXS, combined with wide-angle X-ray scattering, were used to investigate $Mg(BH4)2$, $NaAlH4$ and $MgH2$ infiltrated in carbon scaffolds. The main results will be presented.

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(*) A) Sartori, S.; et al. Nanotechnology 2009, 20, 505702. B) Sartori, S.; et al. J. Phys. Chem. C 2010, 114, 18785. C) Sartori, S.; et al. Nanosci. Nanotechnol. Lett., in press. D) Vajeeston, P.; Sartori, S.; et al., to be submitted.

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Contribution type : --not specified--

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Abstract ID : 62

LITHIUM ION DYNAMICS IN LITHIUM METAPHOSPHATE BASED SOLID ELECTROLYTE SYSTEMS

A common lithium ion conductor, lithium metaphosphate has been taken up for transport studies. The choice of material is unique in the sense that it has enabled for investigations of the Li+ ion transport in (i) the crystalline form of LiPO3, (ii) the glassy form of LiPO3 and (iii) a newly identified polymer-metal salt complex (PEO)6:LiPO3. Although the best Li+ ion conduction has been observed in the glassy phase of LiPO3, also the new polymer-metal salt complex, (PEO)6:LiPO3, exhibited good conduction characteristics at relatively lower temperature [1].

The LiPO3 glass exhibits a high ionic conductivity with a value of σdc=4.5 x 10-4 Scm-1 at 280 oC. However, the technical application of this glass is not practically possible because of its hygroscopic nature and lower glass transition temperature. Incorporation of a second glass former, B2O3, in the lithium metaphosphate glass enhances the chemical and thermal stability and also exhibits appreciable ionic conductivity even below the glass-transition temperature. The enhanced conductivity is attributed to the high mobility of Li+ ions, due to the "mixed glass former" effect. The optical absorption spectra of these glasses suggest a transition between octa- and tetrahedral coordination of Li+ ions, as the second glass former B2O3 replaces P2O5. FTIR and Raman spectroscopy indicate the presence of BO4 and boron-phosphate units, as well as various other phosphate and borate structural units. The structural investigation, particularly in the regime of short range order (SRO), can be helped tremendously by NMR techniques. Fortunately, B, Li and O all possesses nuclear magnetic moment, thus it is possible to obtain information about coordination and bonding of these resonating species.

The polymeric phase i.e. (PEO)6:LiPO3 exhibited a conductivity value of 3.1×10-7 Scm-1 at 78 °C with activation energies of 0.21 eV and 0.88 eV for Li+ ion migration above and below the softening point of the polymer, respectively. However, the actual mechanisms of ion migration and polymer relaxations are yet to be fully understood in this polymer-metal salt complex. Techniques like NMR, neutron scattering and molecular dynamic simulations are likely to provide better understanding and information on the chemical nature as well as on the molecular and collective mobility and diffusivity within this system.

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Abstract ID : 64

Biocatalysis in self-assembled reaction media

Nowadays, one of the problems in biotechnology is performing enzymatic catalysis applying non-natural substrates. In this catalysis, the enzyme is soluble in the hydrophilic medium and the substrate is soluble in the hydrophobic medium. Bicontinuous microemulsions are the perfect environment to carry out this kind of enzymatic reactions. They provide a structure where the interpenetrating water and oil domains provide a high interfacial connected area between these two media. One of the aims of the project is to study where the enzyme and the substrate are located at the bicontinuous microemulsion interface and the distribution and the interaction of all the components which are present in the system. In order to improve the stability and the activity of the enzyme, phospholipids, which are the natural amphiphiles to interact with enzymes, will be introduced in the system. The first part of the project will be focused on the interactions and distributions of all the components that will be present in the bicontinuous microemulsion. Pulsed field gradient (pfg)-NMR and fluorescence correlation spectroscopy (FCS) will determine enzyme and phospholipids self-diffusion coefficients, so a probe about their location in the bicontinuous microemulsion phases and the enzyme distribution at the interface will be obtained. Furthermore, to study how the phospholipid and the non-ionic surfactant are interacting at the interface, two experiments will be performed, a combination of Langmuir-Blodgett experiments and fluorescence microscopy. The interaction between enzyme and the components at the interface will be determined by fluorescence resonance electron transfer (FRET). And neutron spin-echo spectroscopy (NSE) studies will be important to support PFG-NMR and FRET experiments and to determine elastic properties of the interface.

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Structural Biology of Transcription Factor CI by Crystallography and Small Angle Scattering

The molecular mechanisms that determine the expression of one or another set of genes resulting in different development pathways have been studied intensively in bacteriophages. Temperate phages, as opposed to virulent virus, may choose to enter either a lytic or a lysogenic lifestyle following infection of a sensitive host. In the lytic infection cycle, new phages are produced, followed by lysis of the host cell and liberation of phage progeny into the surroundings. Whereas in the lysogenic infection cycle, the phages genome typically integrates into the bacterial chromosomal DNA, resulting in a dormant prophage, mainly expressing genes required for maintenance of the lysogenic state. The decision to enter either the lytic or the lysogenic life cycle is controlled by a bistable genetic switch consisting of phage promoters responsible for transcription of genes required for either the lytic or lysogenic growth, including phage-encoded protein regulating these promoters. In the temperate lactococcal phage TP901-1 one of the main players involved in the regulation of the lytic and lysogenic promoters is a phage-encoded repressor protein, CI, which represses transcription from the lytic promoter PL by binding to multiple operator sites on the DNA1,2. In this project we aim to characterize CI, various truncated versions of CI, and CI-DNA complexs using crystallography and small-angle scattering techniques, to obtain further understanding of the mechanism of repression.

Various truncations of CI were cloned, expressed in E.coli and purified. Subsequently, crystals were obtained for two of the constructs namely the C-Terminal Domain of CI (CTD-CI; residues 91-180) and the N-Terminal Domain (NTD-CI: residues 1-73). The crystals grown from CTD-CI belonged to space group P3121 with unit cell parameters a=30.2 Å, b=30.2 Å and c=177.7 Å. CTD-CI is responsible for the oligomerization of the presumed CI hexamer3. Because of low sequence homology with known structures SAD/MAD techniques have been applied to overcome the phase-problem. The crystals were initially soaked in NaBr and CsI solutions and data were recorded. However, because of the unspecific binding of the HA we were not able to solve the phase problem, and we ended up producing a selenomethonine derivative.

We have furthermore succeeded in crystallizing the NTD-CI, which contains the DNA-binding domain of CI. The NTD-CI fold up in a putative Helix Turn Helix (HTH) domain. The crystal diffracted to 1.6 Å and belongs to the space group P212121 with cell parameters a= 23.68 Å b=43.84 Å and c=72.58 Å. Also here only low sequence identity is found with known HTH structures which complicates structure determination by molecular replacement technique, thus experimental phases will also be sought for this domain.

Δ58CI, a truncated variant of the CI wild type protein,3 was also expressed and purified. The Δ58CI in contrast to the CI protein only forms dimers and therefore only binds to only one operator site consisting of inverted repeated sequences. Parallel with crystallization studies Δ58CI was used to perform small angle scattering studies with or without DNA. DLS and SAXS results showed a change in particle size when decreasing salt concentration in a solution of DNA and delta58. This preliminary indicates DNA-protein complex formation, and will be investigated further by SANS (small angle neutron scattering).

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Short time dynamics of alkanes as seen by neutron scattering and MD simulations

The description of transport mechanisms in molecular liquids is a challenging task. Especially the mechanism of molecular self-diffusion in liquids of organic medium-chain molecules is not yet completely understood. With time-of-flight quasielastic neutron scattering (TOF-QENS), it is possible to get experimental access to the motions on a molecular length scale in the pico- to nanosecond time regime. In this regime one has to assume a superposition of several (intra)molecular motions ranging from methyl group rotation to long-range diffusion.

It could be shown previously that the diffusion coefficients of short- and medium-chain n-alkanes measured by TOF-QENS deviate increasingly from the long-time long-range values determined by pulsed-field gradient nuclear magnetic resonance (PFG-NMR) with increasing chain length of the molecules and decreasing temperature [Smuda et al. JCP 129, 014513 (2008)].

In order to identify the motions which occur at time scales faster than long range diffusion, detailed MD simulations were performed. The simulated dynamics perfectly agree with the QENS-spectra. The trajectories of the atoms contain many information, which together with the neutron scattering results allow to get an deeper insight on molecular self-diffusion.

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Abstract ID : 70

Investigation of Water management in PEM Fuel Cells using Neutron Tomography and Radiography

The application of fuel cells is expected to play an important role in a future sustainable energy strategy. Water management is a key issue for polymer electrolyte membrane fuel cells (PEMFCc) since efficiency, cell performance and long term stability rely crucially on the hydration level of the membrane. If the membrane is too dry the ionic conductivity drops causing irreversible damage of the membrane and a permanent reduction of the cell performance. Otherwise, flooding of the gas diffusion layer (GDL) leads to the blockage of gas transport paths entailing an undersupply of the membrane with reactant gases.
A deep understanding of macroscopic as well as microscopic water dynamics are needed for the improvement of existing and the development of new fuel cell materials. Neutron imaging methods (tomography and radiography) were applied for localization of macroscopic water agglomeration in operating PEM fuel cells providing an informative basis for components and materials optimization.
A promising future direction of these investigations is the identification of molecular water nucleation effects and their microscopic dynamics at the ps-ns scale which is accessible easily by inelastic neutron scattering.

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Abstract ID : 71

New insights on the collective dynamics of lipid membranes

Knowledge of collective density fluctuation of hydrocarbon chains in lipid bilayers is essential for the understanding of some aspects of biological functions of natural membranes. In the last decade important steps in the comprehension of the collective excitations of lipid membranes have been done by means of several techniques. All the presented studies agree on the existence of a highly dispersive sound mode, whose frequency depends on the lipid phase and whose origin has to be mainly related to the in-plane motion of hydrocarbon chains. Here we present a combined molecular dynamics (MD) simulations and Brillouin neutron spectroscopy (BNS) study of the short wavelength collective dynamics in a phospholipid membrane (dimyristoylphosphatidylcholine, DMPC) in both the fluid and gel phase. The longitudinal current spectra derived by MD simulation give evidence for an unexpected elaborate spectrum of excitations. Transverse dynamics have been also investigated. The nature and the possible assignment of the excitations identified have been discussed. In particular it is found that the collective modes in this system have large mixing of longitudinal and transverse symmetry. Neutron measurements support the existence of a complex dispersion relation. Most importantly the original analyzes we have performed allow us to uncover a new and complete scenario to describe the short wavelength collective dynamics of phospholipid bilayers.

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Abstract ID : 72

Incoherent Neutron Scattering and Molecular Dynamics simulation on Biomimetic Membranes systems

In this work we have investigated molecular motions on picoseconds time scale and on angstrom space scale for the 1-palmitoyl-2-oleoyl-sn-glycero-3-phosphocholine (POPC) and 1,2-dimyristoyl-sn-glycero-3-phosphocholine (DMPC) pure model membranes, both in full hydration conditions and with a high level of alignment.
To investigate these systems we used Quasi-Elastic Neutron Scattering (QENS) and Molecular Dynamics simulation (MD).
In particular, the incoherent elastic and quasi-elastic region of the neutron spectrum was analyzed so obtaining information about single particle dynamics, that can be interpreted and attributed to particular components of the system. Information about dynamics, both perpendicular and parallel with respect to the normal plane of the bilayer, was derived through a proper orientation of the membrane plane with respect to the exchanged momentum.
In addition to Incoherent Quasi-Elastic Neutron Scattering experiments, we performed 4 nanoseconds Molecular Dynamics simulations of fully hydrated pure POPC and DMPC bilayers. Information about hydrogens single particle dynamics in the direction perpendicular and parallel to the phospholipid membrane plane was obtained. Simulation results were compared with experimental data and with values found in literature. Moreover we have proposed a model for data interpretation.

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Neutron Compton scattering study of the co-solvancy effect

Polymers such as poly-N-isopropyl acrylamide (pNIPAAm) display unusual solvation properties in mixed solvent systems. pNIPAAm shows good solubility in alcohols (i.e. methanol) at all temperatures, but in aqueous solutions a lower critical solution temperature (LCST) is observed. Below this LCST the polymer is well solvated, but at higher temperatures it is believed hydrogen bonding interactions with the solvent become less favourable than internal hydrogen bonding, causing the polymer chain to collapse and precipitate out of solution. The LCST for pNIPAAm in mixed water/methanol is seen to be depressed relative to either pure solvent, with a minimum value of -7°C at a methanol volume fraction of 0.35. This behaviour has been examined through Neutron Compton Scattering using the VESUVIO spectrometer at ISIS, UK, observing changes in time-of-flight distribution widths for neutrons scattered from each element, the first experiment of this kind with a liquid state sample. For a preliminary investigation, we have used samples made with deuterium in those positions expected to undergo hydrogen bonding interactions in both the polymer and solvents. We show that the Compton scattering peak widths observed for the different elements are in agreement with the changes in molecular interactions, both hydrophilic and hydrophobic, expected for the character of the samples and their physical properties.

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Structural studies of the RNA-chaperone Hfq

Over the past decade, RNA has been established as the most dynamic and versatile biomolecule. Unique in its ability to encode, regulate and catalyze cellular processes, RNA is placed in center of the classical dogma of molecular biology, in between DNA and protein. Only a ~2% of the human genome encodes protein, the remaining 98% being a source of potential RNA-genes, clearly augmenting the potential for RNA-mediated processes in the cell.

We have taken an integrative approach to study the structure and function of the RNA-binding protein Hfq[1] – a small phylogenetically conserved protein, crucial to bacterial RNA-mediated regulation. Acting as an RNA-chaperone, the protein binds to a wide variety of RNAs, and mediates interactions between regulatory non-coding RNA (ncRNA) and their target mRNAs in a process known as riboregulation.

Crystallographic studies have shown Hfq to adopt an Sm-like fold, forming a doughnut-shaped homo-hexamer[2][3]. Several structures have shown specific RNA binding sites to reside on opposite faces of the doughnut, explaining the preference of Hfq for binding of uridine- or adenine-rich RNA-sequences[3][4]. In gram-negative pathogens (ie. E.coli, Salmonella, Legionella, ao.) the C-terminus of Hfq is highly conserved, accounting for ~30% of the protein sequence, and is predicted to be intrinsically disordered[5][6]. The comparatively short N-terminal of Hfq comprises less than 5% of the sequence, and is also implicated in the function of Hfq[7]. The N-terminal is even more universally conserved, and also predicted to be intrinsically disordered. The dogma is that the termini of the protein becomes structured upon RNA-binding.

To study the behavior of this promiscuous – yet specific protein in E.coli, we have combined low-resolution small angle scattering methods, with high-resolution protein-crystallography, NMR and additional biophysical methods (VUV-CD, FRET). Our data is integrated with biochemical and functional data, to establish a model for the chaperone-role of Hfq in riboregulatory RNA-annealing[6][8].

Functional studies demonstrated the activity of Hfq in E.coli to be related to the length of the C-terminus[5]. The requirement of the C-terminus for Hfq to simultaneously bind multiple RNA and functional aspects hereof was shown by FRET, and related to biophysical properties by VUV-CD combined with biochemical data[6]. Structural studies by SAXS further demonstrated properties of the termini of the Hfq hexamer, which explain complications in obtaining high-resolution crystallographic data for this molecule, and its possible complexes with RNA[8]. To study the proteins interaction with RNA, a combination of SAXS, SANS and NMR was employed.

Bacterial riboregulatory events mediated by Hfq, must occur at minimum in a three-step process. Hfq binds the ncRNA and the mRNA target, the two partners bind to each other, and Hfq is finally released. Above all, Hfq shows preference for binding uridine-rich sequence stretches. This can be implicated in a process of partially unfolding the first RNA, allowing the primary sequence hereof to be presented on the surface of Hfq, conferring a degree of specificity in the overall particle. The C-termini, by virtue of entropy/enthalpy-compensation, will continuously unfold and bind reversibly to multiple possible RNA-targets, presenting them to the bound ncRNA. On encounter of a matching RNA, the complementary sequence in the two RNAs will anneal, and the complex will subsequently be released from Hfq in a zipper-like fashion.

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Thin-film thermoresistor for measuring frequency dependent heat capacity

This poster presents a setup in which a thermoresistive thin film is used both as heater and thermometer. The objective is to measure the frequency-dependent specific heat of a sample in contact with the film.

The technique is known as the 3-ω method: Sending a harmonic electric current through the film at frequency ω, generates a heat current into the sample at twice that frequency. The amplitude of the resulting temperature variation enters linearly in the third harmonic of the voltage across the film and can be extracted by a fast Fourier transform of the latter.

In supercooled liquids, the time-scales of relaxation processes, such as molecular rearrangement, are highly temperature dependent. Measuring the response of a supercooled liquid to harmonically varying, e.g. electrical field, strain, pressure or temperature at different frequencies and temperatures is used to determine the timescales of the liquid's response to such external fields. Measuring the frequency dependent specific heat is the focus of calorimetric techniques such as the 3-ω method.

When the temperature of a surface in contact with some material is oscillating harmonically at some frequency, ω, the penetration depth of the resulting heat wave inside the material depends on the frequency via the heat diffusion length, l = \sqrt{λ / cω}, where c and λ are the specific heat and the thermal conductivity of the material, respectively. The frequency range of calorimetric techniques is generally much smaller than that of dielectric or mechanical techniques because it is limited by the size of the thermometers and heaters used: Calorimetry gets complicated at high frequencies when the wavelength or penetration depth of the thermal waves become comparable to the size of the heater and/or thermometer used. In a spherical setup build at Glass and Time, frequencies from mHz to some Hz are applicable. With a film thickness around 100 nm, we anticipate to significantly raise the upper frequency limit in a planar plate setup.

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Investigation of the coupling of protein and hydration water dynamics by NMR and MD simulations

Although the molecular processes on which protein function is based, are not known in detail yet, all authors agree that there is a mutual influence, a coupling, of the dynamics of hydration water and protein. In order to gain new insights in this coupling, dry and hydrated samples of elastin, collagen and myoglobin were investigated in a series of nuclear magnetic resonance (NMR) experiments and molecular dynamics (MD) simulations at different temperatures. We find that the temperature dependence and the hydration-level dependence of the protein-water couplings are similar for the proteins in question. Both applied techniques revealed a change of mechanism for the motion of hydration water upon cooling. The protein backbone dynamics were analyzed e.g. by means of intermediate scattering functions calculated from MD simulations. The proteins exhibit a strongly non-exponential relaxation over several orders of magnitude in time, resembling a power-law or logarithmic decay. Possible origins of this behavior are critically discussed.

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