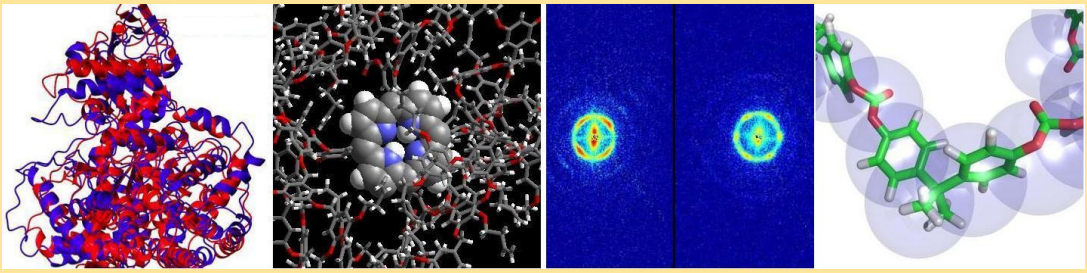

Third Annual Niels Bohr International Academy Workshop on ESS Science: Crossing space and time domains with SAS and QENS

Copenhagen, June 24-28, 2013

The main focus of this workshop-school is the use of SANS/SAXS for structural studies along with that of quasielastic neutron scattering for slow dynamics, and the manner in which molecular dynamics simulations and other types of computational modeling can be utilized for the analysis and interpretation of the experimental data.

Each topic is introduced by a motivational or tutorial talk on a selected scientific achievement, in such a way that all participants can gain a broader sense of the benefits of the various approaches described. Basic information on the complementary properties of the different types of techniques, their data interpretation, as well as information on recent applications and developments are also given.

Organizers

Heloisa N. Bordallo
bordallo@nbi.ku.dk

Juergen Eckert
juergen@usf.edu

Lise Arleth
arleth@nbi.ku.dk

Invited Speakers

Dimitri Argyriou
Lise Arleth
Heloisa N. Bordallo
Juergen Eckert
Emiliano Fratini
Teresa Head-Gordon
Andrew Jackson
Jacob J. K. Kirkensgaard
Margarita Krutyeva
Sandrine Lyonnard
Janez Mavri
Jörg Pieper
Dorthe Posselt
Roger Pynn
Ritva Serimaa
Neal Skipper
Dmitri Svergun
Mark Telling
Tobias Unruh

Access

The main door of Building C will be unlocked from 8 am to 4 pm each day of the workshop. The door to Building A, which is to the right, is also unlocked during the same period.

Lectures & Posters

All lectures will be held in Auditorium A of Building C of the Niels Bohr Institute.

Please try to be respectful and do not use your computers during the lectures.

All posters will be exposed in auditorium C. Afternoon refreshments will be served by the posters.

Work space

Down the hall in the B building, which houses the Niels Bohr International Academy, there is a lounge with a chalkboard and a free espresso machine. If you are looking for a quite place the library is ideal.

Wireless connectivity

The local networks are named:

NBI CC wlan, NBI CA wlan and NBI eduroam

To connect, you need to specify a password. This is "TRia1616Blv17".

Computers have been stolen from the Institute. **Please never leave your computer unattended.**

Lunch

Lunches are provided free of charge to the registered participants at the NBI cantine. On Wednesday and Thursday we will provide delicious homemade sandwiches.

Guided tour at the NBI

A guided tour of the Niels Bohr's Office will take place on Thursday, June 26 from 10:00 to 10:30 for the invited speakers.

Round Table with ESS Scientists

Tuesday, 25 June 14:00 – 16:00

This parallel section is aimed as a brainstorming meeting between the invited speakers and ESS scientists.

Social Program

Wednesday, 26 June 13:30 – 22:00

Guided tour of the Viking Museum in Roskilde followed by the conference dinner at the museum's restaurant.

Thursday, 27 June 13:30 – 16:30

Guided tour of the Statens Naturhistoriske Museum followed by coffee and cake at the museum's café (invited speakers).

Further questions

Feel free to contact the secretary of NBIA, Helle Kiilerich, whose office is on the first floor, in room BA-6.

Third Annual Niels Bohr International Academy

Workshop on ESS Science:

Crossing space and time domains with SAS and QENS

Scientific Program

Preliminary Program for the Third NBIA Meeting on ESS Science, June 24-28, 2013		
Only 20 students will take part on the hand on exercises. "ESS Science: Opportunities & Ideas" session is intended to give the participants an opportunity to discuss on what they think is most important to develop a good neutron facility, including instrumentation, sample preparation laboratories, software, hardware, etc..		
Day/Time	*Lecturer*	*Topic*
Monday, 1st day		
8:00 am - 9:15 am	**Registration & Welcome**	
9:15 am - 10:30 am	Teresa Head-Gordon (UC, Berkeley)	Computing Experimental Observables from Molecular Simulation: Insights and Predictions
10:30 am - 11:00 am	Coffee break	
11:00 am - 11:45 pm	Tobias Unruh (Erlangen University)	Combination of QENS and MD simulation for soft matter research
11:45 am - 12:15 pm	Janez Mavri (National Institute of Chemistry)	Classical Molecular Dynamics Simulations of Hydrated Proteins
12:30 pm - 2:00 pm	Lunch	
2:00 pm - 2:30 pm	Andrew Jackson (ESS)	Nanoscale Structural Analysis with Neutrons
2:30pm - 3:00 pm	Mark Telling (ISIS)	Quasi-Elastic Neutron Scattering: A Tool for the Study of Molecular Dynamics
3:00 pm - 3:30 pm	*Posters* Coffee Break	
3:30 pm - 5:15 pm	Andrew Jackson (ESS)	***SANS Tutorial*** - Students chose project, hands on exercises
Tuesday, 2nd day		
9:00 am - 9:45 am	Roger Pynn (Indiana University)	A Practical Guide to doing a SANS Experiment at a National Neutron Facility
9:45 am - 10:30 am	Dimitri Argyriou (ESS)	ESS Science: Opportunities & Ideas
10:30 am - 11:00 am	Coffee break	
11:00 am - 11:45 am	Lise Arleth (NBI-KU)	Combining SAXS and SANS to investigate biomolecular systems
11:45 am - 12:15 pm	Jörg Pieper (University of Tartu)	QENS and Optical Spectroscopy in Photosynthesis Research
12:30 pm - 2:00 pm	Lunch	
2:00 pm - 3:45 pm	Mark Telling (ISIS)	***QENS Tutorial*** - Students chose project, hands on: Data analysis etc
2:00 pm - 3:45 pm	ESS Scientists	Round Table with ESS Scientists
4:00 pm - 5:00 pm	Students clip presentations: 3 minutes clip to show their research work	
5:00 pm - 6:30 pm	Beer party and posters	

Wednesday, 3rd day		
9:00 am - 10:30 am	**2 Students: Working groups**	
10:30 am - 11:00 am	Coffee Break	
11:00 am - 11:45 am	Dmitri Svergun (EMBL)	Computational methods for the analysis and interpretation of small-angle scattering data
11:45 am -12:15 pm	Ritva Serimaa (University of Helsinki)	X-ray and neutron scattering studies on natural polymer based materials
12:30 pm - 2:00 pm	Lunch	
2:00 pm -	Excursion & Conference dinner Viking Museum in Roskilde sponsored by the ESS	
Thursday, 4th day		
9:00 am - 9:45 am	Neal Skipper (UCL)	SANS and QENS studies of layered clay and graphite materials
9:45 am - 10:30 am	Juergen Eckert (USF)	What are small molecules doing inside large pores?
10:30 am - 11:00 am	Coffee break	
11:00 am - 11:30 pm	Jacob Judas Kain Kirkensgaard (NBI-KU)	Combining SANS and computational modeling for structural determination in star polyphile liquid crystals
11:30 am - 12:00 pm	Margarita Krutyeva (JCNS)	Dynamics of macromolecules - NMR & neutron scattering
12:15 pm - 1:30 pm	Lunch	
1:30 pm - 4:00 pm	**2 Students: Working groups**	
1:30 pm - 4:00 pm	Guided Tour for the senior scientists: Natural History Museum of Denmark http://geologi.snm.ku.dk/english/udstillinger/flora_danica/	
4:00 pm - 4:30 pm	Students coffee break	
4:30 pm - 6:00 pm	**2 Groups of Students** **(30 minutes each group)**	Student presentations on their results
Friday, last day		
9:00 am - 9:45 am	Sandrine Lyonnard (DSM/INAC-CEA)	Looking into fuel cell electrolytes with QENS & SANS
9:45 am - 10:30 am	Dorthe Posselt (RUC)	Structure and dynamics of phospholipid membranes doped with 1-alkanols
10:30 am - 11:00 am	Coffee break	
11:00 am - 11:45 pm	Emiliano Fratini (University of Florence)	Structure and dynamics in concentrated protein solutions
11:45 am - 12:30 pm	Heloisa N. Bordallo (NBI-KU)	Biomaterials, Complexity and Neutrons
12:30 pm - 2:00 pm	**Lunch and Good Bye**	

Third Annual Niels Bohr International Academy

Workshop on ESS Science:

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Invited Talks

Computing Experimental Observables from Molecular Simulation: Insights and Predictions

Teresa Head-Gordon

University of California, Berkeley

My talk will describe a number of research challenges in protein disease aggregation, bulk water structure properties, and de novo enzyme catalysis. I will show that computing relevant experimental observables such as the Nuclear Overhauser Effect for disease peptide amyloid-β and small angle X-ray scattering for bulk water, allows for very high quality interpretations of those experiments. I will also show how molecular simulation is used to rationalize experimental directed evolution when applied to optimization of enzyme catalysis.

Combination of QENS and MD simulation for soft matter research

Tobias Unruh

Friedrich-Alexander-Universität Erlangen-Nürnberg – FAU, Germany

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Classical Molecular Dynamics Simulation of Hydrated Proteins

Janez Mavri[1,2]

[1]*Laboratory for Biocomputing and Bioinformatics, National Institute of Chemistry, Slovenia*

[2]*EN-FIST Centre of Excellence, Slovenia*

The description of biological processes at the molecular level is one of the greatest challenges in biomedical research, and the key to understanding how biomolecules, biomolecular systems, cells, and, ultimately, living organisms function [1]. In turn, the description of molecular properties at the quantum level is rooted in the field physics, namely, in the laws of quantum mechanics or of its classical Newtonian approximation, the connection between microscopic and macroscopic levels being provided by statistical mechanics. Molecular dynamics simulation of hydrated proteins provide answers about structure (e.g. NMR and X-ray refinement, radial distribution functions), stability (e.g. free energy of binding) and dynamical quantities (e.g. vibrational spectra or time-correlation functions), including calculation of rate constants for enzymatic reactions [2].

In this lecture I will give an overview of molecular dynamics simulation of hydrated proteins and I will highlight recent research results of my group. The choice of initial state, effectively polarized vs. polarizable force fields, proper treatment of long-range electrostatics, protonation states of ionizable residues and therewith associated pK_a values, inclusion of explicit water molecules and necessity for hierarchical treatment of enzymes will be discussed. We will touch the ideas behind treatment of chemically reactive systems using QM/MM approach and quantization of the nuclear motion allowing for treatment of tunneling.

As a case study I will use monoamine oxidase B (MAO B), an enzyme that catalytically decomposes dopamine and to lesser extent also serotonin. For this enzyme we suggested the mechanism that is consistent with all available experimental data. For this enzyme we performed a series of biomolecular simulation [3,4,5].

[1] H.J.C. Berendsen, Simulating the Physical World, Hierarchical Modeling from Quantum Mechanics to Fluid Dynamics, Cambridge University Press, 2007.

[2] A. Warshel, Computer Modelling of Chemical Reactions in Enzymes and Solutions, John Wiley and Sons, 1991.

[3] R. Borštnar, M. Repič, S.C.L. Kamerlin, R. Vianello and J. Mavri, Computational Study of the pKa Values of Potential Catalytic Residues in the Active Site of Monoamine Oxidase B, J. Chem. Theor. Comput. 8 (2012) 3864–3870.

[4] R. Vianello, M. Repič and J. Mavri, How are biogenic amines metabolized by monoamine oxidases? Eur. J. Org. Chem. (2012) 7057-7065.

[5] M. Repič, F. Duarte, M. Purg, S.C.L. Kamerlin, R. Vianello and J. Mavri, How is Dopamine Metabolized? QM/MM Simulation of the Rate Limiting Step of Monoamine Oxidase B, to be submited (2013).

Nanoscale Structural Analysis with Neutrons

Andrew Jackson

European Spallation Source - ESS, Lund, Sweden

SANS is a technique uniquely suited to the nanoscale analysis of the structure of complex materials. A brief introduction to the technique with reference to examples of applications will be given.

Quasi-Elastic Neutron Scattering:
A Tool for the Study of Molecular Dynamics

Mark Telling

ISIS, Science & Technology Facilities Council

The spatial and temporal ranges accessible using the technique of quasi-elastic neutron scattering (QENS) are ideally matched to the vibrational displacements and diffusive motions encountered in molecular systems. The QENS method has been successfully applied to a diverse range of problems which encompass, for example, the mechanical integrity of concrete, improvements in dental care, spider silk formation and food preservation. In addition, while beyond the immediate scope of this talk, the times and length scales accessible using Molecular Dynamic (MD) simulations can be directly related to those probed experimentally by QENS.
In this introduction, the basic principles of the QENS method pertinent to the study of dynamic processes in soft matter systems will be presented. An overview of the neutron instrumentation required for such studies will be given as will be the experimental methodology; from sample preparation and optimization to data reduction. To conclude, the most common data analysis procedures will also be discussed.

A Practical Guide to doing a SANS Experiment at a National Neutron Facility

Roger Pynn[1,2]

[1]*Indiana University, Bloomington, Indiana, United States of America*

[2]*Neutron Sciences Directorate, Oak Ridge National Laboratory, Oak Ridge, Tennessee*

Small Angle Neutron Scattering (SANS) is one of the most widely used neutron scattering techniques, at least in part because experiments are often relatively simple to perform. Nevertheless, a researcher's first experiment at an unfamiliar facility using a new technique can be daunting. In this talk I will offer some practical tips on how to approach a SANS experiment at a national facility. Since neutron scattering is an expensive technique, it should never be used when another, less expensive method can obtain equivalent information. Some examples will make this clear. I will discuss some of the situations in which SANS can be expected to provide unique information since these are essential ingredients for a successful SANS proposal to a national facility. I will explain how experimenters can use widely available computational tools to calculate the signals (and background) they can expect in a SANS experiment and the steps they should take to identify the most appropriate instrument and experimental conditions. I will offer some suggestions on the elements needed to write a good experiment proposal as well as steps that may help to ensure the success of an experiment once the user arrives at a facility.

ESS Science: Opportunities & Ideas

Dimitri Argyriou

European Spallation Source - ESS, Lund, Sweden

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.

Combining small-angle scattering of neutrons and X-rays to investigate biomolecular systems

Lise Arleth

Niels Bohr Institute – NBI, University of Copenhagen

Many important complex biomolecular systems such as protein-DNA complexes or Membrane Protein – Membrane complexes have significantly different contrast situations for X-rays and Neutrons. This can be exploited to obtain a more detailed structural understanding of the systems by combining the X-ray and Neutron based methods and analyse the obtained data sets simultaneously. A central research activity of my research group at University of Copenhagen consists in developing a general platform for determining the low-resolution structure of membrane proteins based on combined Small-Angle Neutron Scattering (SANS) and Small-Angle X-ray Scattering (SAXS). We use the so-called Nanodisc-system as a nanoscale sample holder for the membrane proteins and by combining SAXS and contrast variation SANS, it becomes possible to determine the structure of a general membrane protein as well as the surrounding lipid membrane environment. In my talk, I will describe the results obtained in the project and discuss the challenges and limitations associated with this experimental strategy.

Elliptical Structure of Phospholipid Bilayer Nanodiscs Encapsulated by Scaffold Proteins: Casting the Roles of the Lipids and the Protein, N. Skar-Gislinge, J.B. Simonsen, K. Mortensen, R. Feidenhans'l, S.G. Sligar, B. Lindberg Møller, T. Bjørnholm and L. Arleth, J. Am. Chem. Soc, 2010, 132(39), 13713-13722.

Small-angle scattering from phospholipid nanodiscs: Derivation and refinement of a molecular constrained analytical model form factor, N. Skar-Gislinge and L. Arleth, Phys. Chem. Chem. Phys, 2011, 13, 3161-3170.

QENS and Optical Spectroscopy in Photosynthesis Research

Jörg Pieper

University of Tartu, Estonia

Photosynthetic antenna complexes can serve as role models for bioinspired artificial solar cells. Light harvesting and excitation energy transfer in photosynthesis is relatively well understood at cryogenic temperatures up to ~100K, where crystal structures of several photosynthetic complexes including the major antenna complex of green plants (LHC II) are available at nearly atomic resolution. The situation is much more complex at higher or even physiological temperatures, because spectroscopic properties typically undergo drastic changes at about 120-150K.

Recently, we have addressed this problem using a combination of quasielastic neutron scattering (QENS) and optical spectroscopy on native LHC II and mutants lacking individual pigment molecules. Absorption difference spectra of mutant LHC II reveal spectroscopic changes at temperatures as low as ~80K for individual chromophores. The complementary QENS data indicate an onset of conformational protein motions at about the same temperature. This finding suggests that excited state positions in LHC II are affected by protein dynamics. In more detail, this would mean that at cryogenic temperatures the antenna system is trapped in a certain protein conformation. At higher temperature, however, a variety of conformational substates with different spectral position may be thermally accessible. This finding implies that protein dynamics “fine-tune” electronic energy-levels of LHC II for efficient excitation energy transfer to the reaction center at physiological temperatures.

Computational methods for the analysis and interpretation of small-angle scattering data

Dmitri Svergun

EMBL, Hamburg, Germany

Small-angle X-ray scattering (SAXS) experiences a renaissance in the studies of macromolecular solutions allowing one to study the structure of native particles and complexes and to rapidly analyze structural changes in response to variations in external conditions. Novel data analysis methods significantly enhanced resolution and reliability of structural models provided by the technique [1]. Emerging automation of the experiment, data processing and interpretation make solution SAXS a streamline tool for large scale structural studies in molecular biology. The method provides low resolution macromolecular shapes ab initio and is readily combined with other structural and biochemical techniques in hybrid approaches. Of special interest is the joint use of SAXS with the high resolution methods like crystallography and NMR, but also with complementary biophysical and biochemical techniques. Rapid validation of predicted or experimentally obtained high resolution models in solution, identification of biologically active oligomers and addition of missing fragments to high resolution models are possible. For macromolecular complexes, quaternary structure is analyzed by rigid body movements/rotations of individual subunits. A combination of SAXS and NMR is an extremely effective tool for quantitative analyses of flexible macromolecules. The basics of SAXS data analysis methods will be presented and illustrated by examples of recent applications to solutions of biological macromolecules.

[1] Petoukhov MV, Svergun DI. (2013) Applications of small-angle X-ray scattering to biomacromolecular solutions. Int J Biochem Cell Biol. 45, 429-37.

X-ray and neutron scattering studies on natural polymer based materials

Ritva Serimaa

Department of Physics, University of Helsinki, Finland

Plant cell wall may be considered as a nanocomposite of cellulose, hemicelluloses and lignin. In the cell wall cellulose chains are aggregated to form partially crystalline microfibrils which are further agglomerated into bundles [1]. Such structures may be present also in natural polymer based materials like pulp, microcrystalline cellulose [2], and cellulose whiskers [3].

X-ray and neutron scattering and imaging methods are powerful tools for structural characterization of hierarchically organized materials. For instance, inelastic neutron scattering (INS) experiments on various types of cellulose have revealed the universal nature of the disordered regions from the point of view of low-energy dynamics [4]. Results on recent x-ray and neutron scattering and x-ray microtomography studies on wood cell wall and the enzymatic hydrolysis of wood based nanocellulose to fermentable sugars will be discussed [5,6].

[1] Svedström K, Lucenius J, Van den Bulcke J, Van Loo D, Immerzeel P, Suuronen J-P, Brabant L, Van Acker J, Saranpää P, Fagerstedt K, Mellerowicz E, Serimaa R. Hierarchical structure of juvenile hybrid aspen xylem revealed using X-ray scattering and microtomography. Trees - Structure and Function 26, 1793–1804, 2012.

[2] Virtanen T, Svedström K, Andersson S, Tervala L, Torkkeli M, Knaapila M, Kotelnikova N, Maunu SL, Serimaa, R. A physico-chemical characterisation of new raw materials for microcrystalline cellulose manufacturing. Cellulose 19 (1), 219-235, 2012.

[3] Rämänen P, Penttilä PA, Svedström K, Maunu SL, Serimaa R. The effect of drying method on the properties and nanoscale structure of cellulose whiskers. Cellulose 19(3). 901-912, 2012.

[4] Müller M, Czihak C, Schober H, Nishiyama Y, Vogl G. All Disordered Regions of Native Cellulose Show Common Low-Frequency Dynamics. Macromolecules 2000, 33, 1834-1840.

[5] Kent MS, Cheng G, Murton JK. Study of Enzymatic Digestion of Cellulose by Small Angle Neutron Scattering, Biomacromolecules 11 (2), 357-368, 2010.

[6] Penttilä PA, Várnai A, Fernández M, Kontro I, Liljeström V, Lindner P, Siika-aho M, Viikari L, Serimaa R. Small-angle scattering study of structural changes in the microbril network of nanocellulose during enzymatic hydrolysis. Cellulose, in press.

SANS and QENS studies of layered clay and graphite materials

Neal Skipper

University College London – UCL, UK

Layered materials such as clays and graphite intercalation compounds (GICs) play an important role in many natural and industrial processes. These range from environmental issues such as waste confinement and remediation, through oil and gas exploration and recovery, to catalysis and graphene production. It is therefore extremely important for us to be able understand and control the molecular structure and dynamics in these systems. This requires information that covers a wide-range of both length- and time-scales. Both clays and GICS are made up of stacks negatively charged 2-dimensional sheets, held together by charge-balancing counterions such as K^+ and Ca^{2+}. In the presence of polar solvents such as water (clays) and ammonia (GICs) these cations tend to solvate, thereby forcing the layers apart in a series of discrete steps. Further colloidal swelling may then take place, depending on the particular composition and external conditions. For this reason this class of materials provide an ideal environment in which to study 2-dimensional confinement of fluids. In this session we will discuss recent SANS and QENS studies of clays and GICs. These allow us to probe the surface and interfacial structure and dynamics, in systems ranging from those in which the sheets form lamellar crystals to those in which they are fully dispersed. We also show that we are able to obtain detailed information on specific intercalated species, including for example amino acids and aromatic hydrocarbons.

[1] Structure and Morphology of Charged Graphene Platelets in Solution by Small-Angle Neutron Scattering. Milner, E.M.; Skipper, N. T.; Howard, C.A.; Shaffer, M.S.P.; Buckley, D.J.; Rahnejat, K.A.; Cullen; P.A.; Heenan, R.K.; Lindner, P.; Schweins, R. J. Am Chem. Soc. 134, 8302-8305 (2012).
[2] Chiral interactions of histidine in a hydrated vermiculite clay. Fraser, DG; Greenwell, HC; Skipper, NT; Smalley, MV; Wilkinson, MA; Deme, B; Heenan, RK. Phys. Chem. Chem. Phys. 13, 825-830 (2011).

What are small molecules doing inside large pores?

Juergen Eckert

University of South Florida, USA

The advent of metal organic materials (MOM) has provided an extraordinary opportunity to tailor porous materials for specific purposes such as gas storage, separation, and catalysis, and to do this for molecules of various sizes from molecular hydrogen all the way to some macromolecules. This can be accomplished by choosing suitable molecular building blocks, which are functionalized for a specific application. While some MOM's are now being investigated as potential vehicles for drug delivery, for example, it is the utility connected with the facile, selective adsorption of many types of small molecules (e.g. CO, CO_2, CH_4, H_2) in large numbers which has in fact given rise to the dramatic increase in the numbers and types of MOM's synthesized. The systematics of such a building block approach has led to the development of searches for new materials based on computer simulations for new materials of this type. The reliability, or predictability, of such an approach, however, rests with the accuracy of the potential energy surfaces employed. These must be derived by way of molecular level experiments, such as X-ray or neutron diffraction to determine siting of sorbate molecules, various spectroscopic methods for the study of sorbate dynamics including the microscopic diffusion of sorbate molecules by quasielastic neutron scattering. Rapid diffusion inside the pores is critical for many applications, but has not been extensively studied to date. I will describe the use of such experimental observations in conjunction with computational studies, which in turn can then applied to the modeling of adsorption isotherms, i.e. the most common method for characterization of the uptake and binding of sorbates in porous materials. This talk will include a brief account of the building block approach used in materials synthesis by our groups at USF and KAUST, and the properties of the resulting materials for hydrogen storage and CO_2 removal, as well as some recent quasielastic neutron scattering work designed to assess the effect of pore sizes on the all important diffusion of CO_2 and H_2 in MOM's.

Combining SANS and computational modeling for structural determination in star polyphile liquid crystals

Jacob Kirkensgaard

Niels Bohr Institute – NBI, University of Copenhagen

Triphilic star-polyphiles are short-chain oligomeric molecules with a radial arrangement of hydrophilic, hydrocarbon and fluorocarbon chains linked to a common centre [1]. They form a number of liquid crystalline structures when mixed with water. In this tutorial you will see how a combination of computational tools and SANS contrast variation allows the determination of a complicated self-assembly structure in such a system. First, coarse-grained molecular dynamics simulations are used to generate a suite of possible self-assembly structures in such three-phase systems under the constraint of the molecular star topology. Secondly, model independent calculations of the Porod invariant determines that three-phase separation is actually taking place. Finally, simulated scattering patterns from these structures are compared to experimental contrast variation neutron scattering data to establish the structure of the sample.

[1] de Campo, L et al, PCCP 2011, DOI: 10.1039/c0cp01201g.

Dynamics of macromolecules - NMR & neutron scattering

Margarita Krutyeva

Forschungszentrum Jülich – JCNS, Germany

Structure, molecular architecture and size govern the dynamical properties of macromolecules. The dynamics of the most system over broad time and length scales is successfully investigated by neutron spectroscopy. At the same time NMR, in particular PFG NMR, has proven to be an invaluable tool for monitoring molecular displacements in a broad range of length scales, from below 100 nm up to tens of micrometre. In my talk I will focus on the combination of the neutron scattering and NMR techniques to improve our knowledge about dynamics of macromolecule (including bio-macromolecules and proteins).

As an example, the experiments addressing translational diffusion of cyclic macromolecules (ring polymers) and blends of rings and linear chains will be presented. Here the effective combination of high resolution NSE spectroscopy probing molecular dynamics up to hundreds of nanoseconds and exploring intrachain dynamics and PFG NMR operating on the timescales many order of magnitude longer to measure centre-of-mass diffusion will be demonstrated.

Looking into fuel cell electrolytes with QENS & SANS

Sandrine Lyonnard[1]*, Quentin Berrod[1], Govind Prajapati[1], Jacques Ollivier[2], Bernhard Frick[2], Jean-marc Zanotti[1], Lionel Porcar[2], Armel Guillermo[3] and Gerard Gebel[1]

[1]*French Alternative Energies and Atomic Energy Commission – CEA, Grenoble, France*

[2]*Institut Laue-Langevin – ILL, Grenoble, France*

[3]*Centre National de la Recherche Scientifique – CNRS, France*

The synthesis and manufacturing of polymer electrolyte membranes with improved functional properties such as high proton conductivity and chemical stability is an actual challenge to increase the performances of Proton Exchange Membrane Fuel Cells. To achieve this goal, a microscopic understanding of the relation between the primary chemical nature of the electrolyte, the morphology, the proton transfer / water diffusion mechanisms, and the effective properties is essential. Multi-scale experimental strategies need to be developed for studying the structure/transport interplay in these complex charged polymers. In this presentation we will show the suitablility of Neutron Scattering techniques to investigate both structural and dynamical aspects, focusing on two representative polymer electrolytes: the benchmark perfluorinated Nafion membrane and an alternative polyaromatic material, the Sulfonated Polyimide.

We will present an overview of the SANS studies devoted to polymer microstructure [1]. The kinetics of water sorption obtained on an extended time-range, from subsecond to years, will also be discussed [2]. Then we will show how the water/proton dynamics can be interestingly studied by combining quasi-elastic neutron scattering (QENS [3]) at molecular level and NMR at mesoscopic/micronic scales [4]. By QENS the characteristic times and diffusion coefficients of two types of protons have been obtained: localized non-diffusive slow protons (strongly interacting with acid groups), and diffusive hydration protons confined in ionic channels.

In a third part of the presentation, we will briefly show some results on i) model self-assembled surfactant systems, which are used to tune the confinement geometry and size [5], and in-situ SANS/QENS on operating fuel cells which we are very recently developing.

[1] S. Lyonnard and G. Gebel, Neutrons for Fuel Cells Membranes: structure, sorption and transport properties, European Physical Journal 213 (1) (2012), 195-211.

[2] G. Gebel, S. Lyonnard, H. Mendil-Jakani, A. Morin, Water sorption kinetics in Nafion® membranes: a small-angle neutron scattering study, Journal of Physics Condensed Matter, 23 (23), 234107 (2011).

[3] J-C. Perrin, S. Lyonnard and F. Volino; Quasielastic neutron scattering study of water dynamics in hydrated nafion membranes, Journal of Physical Chemistry C, 111 (2007), 3393-3404.

[4] J-C. Perrin, S. Lyonnard, A. Guillermo and P. Levitz; Water dynamics in ionomer membranes by field-cycling NMR relaxometry, Journal of Physical Chemistry B, 110 (2006), 5439-5444.

[5] S. Lyonnard, Q. Berrod, B-A. Bruning, G. Gebel, A. Guillermo, H. Ftouni, J. Ollivier and B. Frick, Perfluorinated surfactants as model charged systems for understanding the effect of confinement on proton transport and water mobility in fuel cell membranes. A study by QENS., Eur. Phys. Journal Special Topics, 189 (1), 205-216 (2010).

Structure and dynamics of phospholipid membranes doped with 1-alkanols

Dorthe Posselt[1]*, Marcus Trapp[2], Wiebke Lohstroh[3], Christine M. Papadakis[3] and Thomas Gutberlet[2]

[1]*IMFUFA, Department of Science, Systems and Models, Roskilde University, Denmark*

[2]*Helmholtz-Zentrum Berlin, Germany*

[3]*Technische Universität München, Physik-Department, Germany*

An important part of biological plasma cell membranes is the lipid bilayer, functioning as a two-dimensional matrix, into which proteins are embedded, cholesterol is dissolved and the cytoskeleton is anchored. Incorporation of amphiphilic solutes into the bilayer is predicted to increase the lateral pressure near the aqueous interfaces and decrease the lateral pressure toward the center of the bilayer [1]. The presence of lateral stress in the membrane is expected to influence the lipid dynamics. From previous structural work using small-angle x-ray and neutron scattering, it is known that medium chain length 1-alkanols (butanol, hexanol, octanol, decanol, dodecanol) incorporated into 1,2-Dimyristoyl-sn-Glycero-3-Phosphocholine (DMPC) membranes results in a thinning of the membrane for shorter chain alcohols while longer chain alcohols lead to an increasing thickness of the membrane with hexanol a turning point giving the smallest membrane thickness [2]. Also, densitometry data [3] and molecular dynamics simulations [4] confirm a looser packing density of lipids in the core of the membrane when 1-hexanol is incorporated into DMPC membranes. The presence of amphiphilic chains with a mismatch in length is thus expected to influence the dynamics of the lipid matrix. The dynamics of DMPC membranes doped with hexanol and decanol is studied using quasi elastic neutron scattering at the time-of-flight spectrometer TOFTOF at FRMII in Munich. Previous measurements on the time scale of 60 ps revealed no distinct influence on the local chain dynamics when incorporating 1-alkanols [5]. Recently, we performed QENS measurements on a time scale of 300 ps in the q-range 0.3-1.2 $Å^{-1}$ at temperatures above and below the main transition temperature for DMPC with the aim of elucidating whether long range collective motions are affected by the presence in the membrane of 1-alkanols. Our results show that in the lipid fluid phase there is a difference in dynamics on this timescale for membranes organised in a multilamellar vesicle, however for unilamellar vesicles there are no differences in dynamics between doped and non-doped systems

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Structure and dynamics in concentrated protein solutions

Emiliano Fratini

Department of Chemistry "Ugo Schiff" and CSGI, University of Florence, Italy

The comprehension of the phenomenon of protein clustering is of fundamental importance in various diseases and in new promising routes for drug delivery based on storing high concentrated functioning protein.
Neutron spin echo (NSE) and small angle neutron scattering (SANS) were used to investigate the correlation between structure and short-time dynamics of lysozyme solutions. It was found that, upon increasing protein concentration, the self-diffusion coefficient at the short time limit becomes much smaller than that of the corresponding hard-sphere and charged colloidal suspensions at the same volume fraction. Moreover contrary to literature conclusions, at relatively low concentrations, there is evidence that the system consists mostly of monomers or dimers, while, at high concentrations, large dynamic clusters dominate [1,2]. From the estimation of the mean square displacement by using short-time and long-time diffusion coefficient measured by NSE and NMR, we find that these clusters are not permanent but have a finite lifetime longer than the time required to diffuse over a distance of a monomer diameter.
By using statistical mechanics models [3], it is clear that the appearance of a low-Q peak is not a signature of the formation of clusters. Rather, it is due to the formation of an intermediate range order (IRO) structure governed by a short-range attraction and a long-range repulsion.

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Biomaterials, Complexity and Neutrons

Heloisa N. Bordallo[1,2]

[1]*Niels Bohr Institute – NBI, Univeristy of Copenhagen, Denmark*

[2]*European Spallation Source – ESS, Lund, Sweden*

It may be a challenge to define accurately what qualifies as biomaterial, however complexity is what links them together. Therefore, we can consider that a biomaterial is any type of material that has been engineered to, either alone or as part of a complex system, be used to direct, by controlling interactions with components of living systems, the course of any therapeutic or diagnostic procedure.

As neutron scattering is a particularly good technique for investigating the structure and dynamics of complex system, consequently it not surprising that it can play a considerable role in the study and development of a range of bio- and bio-inspired materials. Up to date, the majority of studies have been structural studies of self-assembly behavior in solution or at interfaces using small-angle scattering and reflection. Currently, however, there is a growing interest in using neutron scattering to study the dynamics of these systems.

In this lecture I will give an overview of the recent results on various biomaterials that we have studied using quasielastic neutron scattering and imaging techniques in my group. I will highlight recent research results on the hydration process of dental cements and how this hydration affects the pore structure. I will also show that as complex sample environments can readily be accessed with neutrons, inelastic neutron scattering can help understanding the process of tableting and encapsulation of molecular drugs.

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Posters

First principles study of Al_3Sc and Al_3Li precipitates in an Al matrix

Sónia Costa[1]*, Helena Braga[2], Joaquim Barbosa[1] and Ana Pinto[1]

[1]*CT2M - Centre for Mechanics and Materials Technologies, Universidade do Minho*

[2]*CEMUC, Engineering Physics Department, Engineering Faculty, Porto University, Portugal*

Aluminium alloys are widely used in industrial applications, with particular emphasis to transportation industries, owing to the particular combination of low density, high corrosion resistance and high strength to weight ratio. The strength of aluminium alloys is mainly due to age hardening mechanisms. However, in order to fulfil service's new requirements of structural aircraft and automobile components, alloys with higher resistance at higher temperatures are needed. One of the most promising approaches to improve the mechanical properties of aluminium alloys is based on the addition of alloying elements, either with low solubility or totally insoluble in aluminium, promoting nanoparticles formation, e.g. Al_3Sc. Furthermore, Al_3Li precipitates enhance (Al) mechanical properties. Therefore, it is our goal to study Al_3Li, Al_3Sc and $Al_3(Sc,Li)$ precipitates in an Al matrix.

Density Functional Theory (DFT), as implemented in VASP, was used to optimize Al_3Li and Al3Sc crystal structures and to obtain their mechanical properties. Bulk, Shear, Young modulus and expansion coefficients were obtained. Gibbs energies for each compound were calculated as well as lattice dynamics spectra using PHONON after ab initio optimization. These results allow us to define precipitates' stability range in composition and temperature and to characterize them to further enhancement within an Al matrix.

In order to control and optimize precipitation processes and alloys subsequent properties (mechanical strength, ductility, corrosion resistance etc), and in order to validate ab initio simulations, it is mandatory to understand and quantify precipitates chemistry, structure, morphology and distribution.

Small-Angle Scattering techniques carried out with X-rays (SAXS) or with neutrons (SANS) can be used as a tool to characterize precipitates' microstructures.

Solute-solvent interface area effect on SANS: saturated fatty acids in decalin solutions

R. Eremin[1], K. Kholmurodov[1], V. Petrenko[1], L. Rosta[2] and M. Avdeev[1]

[1]*Joint Institute for Nuclear Research, Dubna, Russia*

[2]*Wigner Research Centre for Physics, Institute for Solid State Physics and Optics, Hungary*

Solute-solute and solute-solvent interaction in the solutions of mono-carboxylic acids in organic solvents are great interest to study. As an example, different acids have different stabilization ability within ferrofluids synthesis, which should be predicted in order to prepare target ferrofluid with predetermined properties (e.g. magnetite particle size distribution). Furthermore, such kind interactions for acids solutions can be responsible for their properties and determine critical effects, as an example, transition to nematic phase. The method of small-angle neutron scattering (SANS) can be used for solute-solute and solute-solvent interaction studying. It was shown in [1] that simple Guinier analysis takes into account residual incoherent background can be successfully applied for investigation of acid-acid interaction for mono-carboxylic acid in benzene solutions in term of Guinier parameters. Nevertheless, in case of decalin-based solutions the approach mentioned above predicts overestimates values of background [2] at the same acid concentrations. Assuming the influence of the specific solvent organization the combination of the classical molecular dynamics simulations (MDS) method and consequent SANS experimental curves modeling was employed for investigation of the solute-solvent interface area. The experimental data on monocarboxylic acids in decalin were got at the SANS spectrometers at the steady-state reactor of the Budapest Neutron Center (Hungary). The deuterated solvent is chosen to get better signal to noise ratio. MD The characteristic size of the acid molecules (2 nm) is close to the resolution limit of the SANS method. It should be noted that decalin has two types of stereoisomers (cis and trans) and it arouses interest to study the influence of this effect on the structural properties. For this purpose we apply the DL_POLY general-purpose code as one of the basic MD simulation tools. Before we started SANS curve modeling the series of the MD simulation to elucidate the effect of different stereoisomers of decalin on the macroscopic properties of the pure solvents [3] was performed in order to provide correct determination of the Lennard-Jones potential (corresponding to van der Waals interaction). Model predictions for the mixtures of decalin stereoisomers are in a good agreement with experimental data at the same conditions, and limiting solutions of monocarboxylic acids (namely, myristic, stearic, oleic acids) in protonated decalin were modeled in order to study the influence of stereoisomers effect and to determine their partial volumes [4]. Next, we initialized the modeling on deuterated decalin-based solutions of the acids mentioned above. As a result profiles of the scattering length density (SLD) were plotted in cylindrical coordinates (for myristic and stearic acid). It should be noted that the sufficient effect of the influence of acid molecule can be observed up to 1.5 nm in the direction perpendicular to the axis of the cylinder. This fact can be explained in [2] by the relative large size of the decalin molecules (approximately, 1 nm). Using the cylinder-cylindrical shells model we simulated SANS curves. Taking into account of the solute-solvent interface area on SANS influence calculated from MD leads to good fit of experimental curves and background values are almost similar to predicted for benzene-based solutions ones obtained in the scope of Guinier approach [2].

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The structure and dynamics of intrinsically unfolded proteins

Jennifer Fischer[1]*, Ralf Biehl[1], Bernd Hoffmann[2] and Dieter Richter[1]

[1]*Forschungszentrum Jülich, Institut of Complex Systems ICS-1*

[2]*Forschungszentrum Jülich, Institut of Complex Systems ICS-7*

Up to know structure and dynamics are believed to play the key role in protein function. Now it is evident that roughly 30% of eukaryotic proteins are partially or even completely unfolded [1]. Nevertheless, intrinsically unfolded proteins are functional and involved in several biological processes. To get further insight into disordered structures and their dynamics, we use Ribonuclease A (RNase A) as a model system, as it is a well known protein denaturing reversibly upon heating. Additionally, by varying the buffer conditions such as pH values several states can be prepared.

First results of the structure and dynamics using Small Angle Neutron and X-ray Scattering (SANS, SAXS) as well as Neutron Spin Echo Spechtroscopy (NSE) and Circular Dichroism Spectroscopy are presented. The combination of these techniques allows us to observe large-scale internal dynamics of subdomains or of unfolded protein strands that operate on the same length scale as rotational diffusion. However, the timescale can be different and depends on the protein structure and internal interactions.

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Hidration Transitions: high order analysis by syncrotron x-ray scattering

Giovanni Grassi[1]*, Leander Michels[2]*, Roosevelt Droppa JR.[3], Jon Otto Fossum[2], Geraldo José da Silva[1]

[1]*University of Brasília – UNB, Brazil*

[2]*Norwegian University of Science and Technology, Norway*

[3]*Federal University of ABC, Brazil*

The sample studied in the present work is Lithium-Fluorohectorite (Li-Fh) prepared at the Department of Physics of Norwegian University of Science and Technology (NTNU), which was made by a cation exchange dialysis process. The main focus of this work is related to the study of the structural properties of the sample in the presence of water, regarding the hydration states transitions [1]. It is essentially an experimental study using the technique of x-ray scattering performed at Brazilian Synchrotron Light Source (LNLS).A previous paper [2] encouraged us to do measurements in high-order peaks, i.e., peaks of higher reflections: 002, 003, 004, 005 and 006 in order to identify the Hendricks-Teller type peaks [3] isolated, not overlapping with pure Bragg peaks. Verified its existence for higher-order reflections values, we plan to conduct further experiments focusing only on these regions in order to be able to make fittings with the HT model.

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Excitation energy transfer, electron-vibrational coupling and structure of phycobiliproteins of the cyanobacterium Acaryochloris marina

G. Gryluk[1]*, M. Rätsep[1], S. Combet[2], D. Lairez[2], H.-J. Eckert[3] and J. Pieper[1]

[1]*Institute of Physics, University of Tartu, Tartu, Estonia*

[2]*Laboratoire Leon Brillouin, CEA-Saclay, Gif-sur-Yvette, France*

[3]*Max-Volmer-Laboratories for Biophysical Chemistry, Technical University Berlin, Germany*

In adaption to its specific environmental conditions, the cyanobacterium *Acaryochloris marina* developed two different types of light-harvesting complexes: chlorophyll-d-containing membrane-intrinsic complexes and bilin-containing phycobiliproteins (PBPs). The latter complexes are believed to form a rod-shaped structure comprising three homo-hexamers of phycocyanin, one hetero-hexamer of phycocyanin and allophycocyanin as well as a linker protein connecting the PBPs to the reaction center. Shape and size of PBPs have been verified by small angle neutron scattering of PBPs in phosphate- and non-phosphate-containing buffer solutions at the PACE instrument at the Laboratoire Leon Brillouin Saclay, France.

Excitation energy transfer and electron-vibrational coupling in PBPs have been investigated by selectively excited fluorescence spectra. The data reveal a rich spectral substructure with a total of five low-energy electronic states including a terminal emitter at about 673 nm. Furthermore, a large number of vibrational features can be identified for each electronic state with intense phonon sidebands peaking at about 30 cm^{-1} and e.g. two characteristic vibronic lines at about 1590 and 1634 cm^{-1}, which appear to correspond to C-NH+ and C-C stretching modes of the bilin chromophore, respectively. The exact phonon and vibrational frequencies vary with electronic state implying that the respective chromophores are bound to different protein environments. A possible structural assignment of the electronic states will be discussed.

Chemically-driven protein evolution in the alkaline phosphatase superfamily

Alexandre Barrozo*, Paul Bauer, Fernanda Duarte, Christopher Maxwell and Shina Caroline Lynn Kamerlin

Department of Cell and Molecular Biology, Uppsala University and Uppsala Biomedical Center, Sweden

In the past 30 years, scientists have demonstrated that most enzymes are capable of promiscuous catalytic activity (one enzymes catalysing the turnover of more than one substrate). It has been suggested that such promiscuity can play an important role in the evolution of enzyme function [1,2]. The alkaline phosphatase superfamily members are examples that possess a pronounced promiscuous activity. The native reaction for one member of the superfamily is often a promiscuous side reaction for another [3]. Moreover, the reactions catalysed by these enzymes (cleavage of P-O and S-O bonds), despite the deceptive similarity of the substrates involved, proceed with very different solvation and protonation requirements [4]. We present here a detailed study of the promiscuous catalytic activity of two evolutionarily related but structurally different members of this superfamily (*Pseudonomas aeruginosa arylsulphatase*, PAS, and phosphonate monoester hydrolase, PMH). We demonstrate that, although subtle changes in the electrostatic environment of the active site can have significant effects on the specificity, the promiscuity arises out of the ability of the non-native substrates to exploit the pre-existing electrostatic pre-organization of the active site towards the native substrate. We believe this provides an example of chemically-driven protein evolution within an enzyme superfamily.

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Model-Independent Decomposition of SAXS Data from Heterogeneous Samples yield Solution Structure of the Intrinsically Oligomeric Protein PICK1

Morten Karlsen*, Thor Thorsen, Jens Simonsen, Ina Ammendrup-johnsen, Mette Rathje, Simon Erlandsson, Kenneth Madsen, Lise Arleth and Ulrik Gether

Copenhagen University

PICK1 is a 46 kDa cytosolic protein that plays an important role in regulation of excitatory neurotransmission in the brain through its involvement in AMPA receptor trafficking. It is proposed to form a homodimer, and the quaternary structure may play an important role in the function and regulation of PICK1.
Lacking a crystal structure, we have used solution based Small Angle X-ray Scattering (SAXS) to determine the low-resolution quaternary structure.
In contrast to other BAR domain proteins, PICK1, in addition to the dimeric fraction, has a significant tetrameric fraction. Since the samples were polydisperse, we developed a method to decompose the scattering data into dimeric and tetrameric components. By combining data from different samples it was possible to decompose the data without a priori assumptions about protein structure, other than the molecular mass.
Through rigid body modeling, based on the BAR domain of the homologous protein Arfaptin and the crystallized PDZ domain of PICK1, a quaternary structure was determined. The domain arrangement is very similar to previously published structures of other BAR domain containing proteins, including SnX9 and Endophilin.
Our data provide the first direct insight into the tertiary and quaternary structure of full-length PICK1, and we conclude that PICK1 is not in a configuration that fits previously published hypotheses explaining the auto inhibition as a mechanism in which the BAR domain is sterically hindered by the PDZ domains binding to the concave surface of the BAR domain.

Molecular dynamic study of carboxylic acids at the water/oil interface: determination of area per molecule and second surface virial coefficient

K. Kovalchuk*, E. Riccardi and B.A. Grimes

Ugelstad Laboratory, Department of Chemical Engineering, Norwegian University of Science and Technology, Sem Sælands vei 4, 7491 Trondheim, Norway

The present study addresses the naphthenate deposition problem that is encountered during pressure reduction, where degassing of the carbon dioxide from the production water results in an increased pH and dissociation of naphthenic acids at the water/oil interface followed by reaction with the salt ions in the aqueous phase leading to a precipitation.

Goal of present study: Understanding the factors influencing the interfacial organization and composition of tetra-naphthenic acids at the interface as well as understanding the nature of interactions between surfactants in mixed interfacial systems.

Methods and results: Molecular dynamic simulations were used to study the adsorption dynamics and interfacial structure (positioning at the interface and interfacial arrangement) of a model compound (BP10) that mimics an indigenous tetra-naphthenic acid, a fatty mono-acid, and mixture of these two surfactants. The present work is focused on determining the molecular parameters such as the area per molecule (A) and the second virial coefficient (B_2) of the molecules at the interface. The value of B_2 is related to the strength and nature of molecular interactions at the interface which is important when considering complex mixed interfaces. The MD results will be employed to predict the multi-component equilibrium concentration and composition of the interfacial adsorbed compounds through the use of a molecular-thermodynamic equation of state.

Segmental dynamics and nanostructure of functionalized dimethylsiloxane oligomers

Gerardo Martinez

Centro de Física de Materiales (CSIC-UPV/EHU) and Materials Physics Centre (MPC), Spain

Most of advanced materials used now days by state of the art technological applications are multi-component or/and nanostructured systems [1-2]. In such arrangements, "confinement effects" at molecular level (topological constrains, interface interactions, etc.) emerge in a natural way, giving rise to changes that will affect both the structure and dynamics of the system as well as the macroscopic properties. The ability of many soft materials like block copolymers to self-assemble in well-ordered nanostructures provides an elegant route to induce confinement effects. These systems usually exhibit dynamic heterogeneities at the molecular level, i.e., different mobility's associated to the diverse components. On the other hand, various results found in literature report confinement-related effects on the component dynamics of block copolymers [3-11]. In general, all these studies report a relatively minor effect of the nanostructure on the component segmental dynamics. This is the case even when the size of the segregated phase is reduced to about 10 nanometre. In fact, most of the results have been interpreted as originated at the interface of a few nanometres thick [8,9]. Therefore, in nanostructured materials of a few nanometres length these effects are expected to be large, leading to a bigger variation on the components dynamical properties. Usual confinement lengths in block copolymers are about a few tens nanometres. In order to investigate the variation of the dynamical properties of the confined phase at lower scales we would need to work in systems that present phases with even smaller confinement length. One way to obtain such systems is by making use of functionalized oligomers. In this work we will investigate how the mobility of functionalized dimethylsiloxane oligomer is modified due to changes in the nanostructure. The systems under investigation were fabricated by functionalizing oligodimethylsiloxane with both, either dodecanoic acid or methyl dodecanoate. Also the unfunctionalized oligodimethylsiloxane (ODMS) is characterized for comparison. Making use of dielectric relaxation techniques we investigate the effect of confinement on the segmental dynamics of the ODMS nanosegregated phase, similarly, to get insight of the thermodynamic properties of the system differential scanning calorimetry was used. Scattering methods (X-ray) are also used to access the structural features. The results obtained by DSC exhibit thermodynamic differences between the two functionalized oligomers. This outcome is related with the different structures obtained by X-ray diffraction. One interesting feature is that although both functionalizations are chemically similar the resulting structures are quite different. In the first case, where well-ordered lamellae about 5 nm thick are formed, the ODMS crystallization is inhibited, whereas in the latter it is not possible to avoid this crystallization. Concerning BDS measurements, we observe that the dynamics of the ODMS segments in the nanostructures resembles the behaviour of the bulk ODMS, and that the structural rearrangements mainly slow- down the segmental ODMS motions.

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Influence of the surface treatment on the local structure of magnetic nanoparticles

Fernando Henrique Martins da Silva[1]*, Fabio Luis Oliveira Paula[1], Juliano Gomes[1], Francisco Tourinho[1], Renata Aquino[1], Jerome Depeyrot[1], José Mestinik[2] and Regine Perzynski[3]

[1]*University of Brasília – UNB, Brazil*

[2]*IPEN/USP, São Paulo, Brazil*

[3]*Physicochimie des Electrolytes, Colloïdes et Sciences Analytiques - PECSA/UPMC, France*

Magnetic fluids are colloidal dispersions in a liquid carrier of magnetic nanoparticles based on composites of metal oxides (ferrites). To disperse properly these nanoparticles, it is necessary during the synthesis process to avoid their dissolution in acidic media. Thus a core-shell strategy has been developed and consists in protecting the ferrite nanocore with a thin coat enriched with iron obtained after a hydrothermal surface treatment with $Fe(NO_3)_3$. Recently we have studied this composition heterogeneity and proposed a chemical core-shell model based on a core of stoichiometric ferrite and a shell of maghemite. In this work, we explore the modifications of the local nanocrystal structure induced by the duration of the hydrothermal treatment using X-ray diffraction and absorption techniques. X-ray diffraction results show that the structure of both kinds of nanocrystals is spinel type and remains the same during the surface treatment. Nevertheless, for manganese ferrite particles, as the duration of the treatment increases, the diffraction peaks are shifted towards larger diffraction angles. This shift is associated to a reduction of the cell size, from 8,46Å in non-treated particles, to 8,34Å in surface treated ones (under 120 minutes of hydrothermal treatment). For cobalt ferrite nanoparticles, the peaks position of the diffraction pattern remains the same. Moreover, in both kinds of nanomaterials, the oxidation state of the metallic cations is deduced from the absorption edge of the XANES spectra. Only in the case of manganese ferrite nanoparticles, the oxidation state of the divalent metal changes from +2 to +4 as the duration of the surface treatment increases. This is associated to a decrease of the ionic radius which varies between 0,83Å for Mn^{+2} to 0,53Å for Mn^{+4}. The observed reduction of the cell size is therefore due to the oxidation of manganese ions induced by the hydrothermal surface treatment.

Study with Inelastic Neutron Scattering of the anti-tumor drug Paclitaxel encapsulated into a nanocomposite based on iron oxides, hydroxyapatite and chitosan

Murillo Martins[1]*, Margarida Saeki[2], Anders Madsen[1] and Heloisa Nunes-Bordallo[1]

[1]*Niels Bohr Institute – NBI, University of Copenhagen*

[2]*Universidade Estadual Paulista, Brazil*

Paclitaxel is a diterpene with high antitumor activity and very unique action mechanism that is effective against ovarian and breast cancers. However, this drug also has disadvantages such as low water solubility and the fact that it can also damage healthy cells. Indeed, the effects of these disadvantages can be reduced by encapsulating the drug with a polymer modified by a material with high affinity to cancer cells. On the other hand, this encapsulation can modify the structural conformation of the drug leading to changes on its effectiveness. In this project, nanocomposites based on iron oxide nanoparticles (maghemite (g-Fe_2O_3) and/or magnetite (Fe_3O_4) and also manganese and zinc ferrites $Mn_{(1-x)}Zn_xFe_2O_4$), hydroxyapatite and chitosan, containing encapsulated paclitaxel for drug delivery systems for breast cancer treatment, are synthesized.

Since the drug loses its translation symmetry after the encapsulation, its structure cannot be analyzed by direct structural techniques. Thus, we cannot establish a relation between drug's effectiveness and data collected by neutron and X ray diffraction. In this sense, we propose the study of the dynamic of these materials with inelastic neutron scattering. This is a rarely used approach and can indicate modifications in encapsulated molecules.

Water Intercalation and Dynamics of humidity uptake by meso-, and nano-porous clay

Leander Michels[1]*, Giovanni Grassi[2], Henrik Hemmen[1], Zbigniew Rozynek[1], Roosevelt Droppa[3], Geraldo José da Silva[2] and Jon Otto Fossum[1]

[1]*Norwegian University of Science and Technology – NTNU, Norway*

[2]*University of Brasília - UnB, Brazil*

[3]*Federal Universtity of ABC - UFABC, São Paulo, Brazil*

The swelling of layered smectite clay particles consists of a change in the interlayer repetition distance (d-spacing) as a function of temperature and humidity. In this work, a fine scan of the relative humidity under room temperature was done for the synthetic clay Lithium Fluorohectorite (Li-Fh), Iron Fluorohectorite, Nickel Fluorohectorite, Sodium Fluorohectorite. For the Li-Fh the hydrodynamically stable hydration states are zero, one, one and a half, two and three intercalated monolayers of water which are described in a similar work for the Sodium Fluorohectorite with discrete jumps in d-spacing at the transitions between the hydration states. The reproducibility and reliability of this relative humidity controlled d-shift enables us to use the interlayer repetition distance d as a measure of the local humidity surrounding the clay particles. We provide an example of application of this observation: imposing a humidity gradient over a quasi-one-dimensional temperature-controlled sample and using x-ray diffraction to record the d-spacing, we are able to extract profiles of the relative humidity along the sample length. Their time evolution describes the transport of water through the mesoporous space inside the clay.

Electric field nematic alignment of fluorohectorite clay particles in oligomeric matrices

Alexander Mikkelsen[1]*, Zbigniew Rozynek[1], René Castberg[2] and Jon Otto Fossum[1,3]

[1]*Norwegian University of Science and Technology – NTNU, Norway*

[2]*Physics Department, University of Oslo, Norway*

[3]*The Centre for Advanced Study – CAS, Norwegian Academy of Science and Letters, Norway*

We study the behavior of fluorohectorite synthetic clay particles dispersed in paraffin wax. We report wide-angle x-ray scattering related to electric-field-induced alignment of the embedded clay particles. The development of anisotropic arrangement of the particles is measured during melting and crystallization of the composites. The degree of anisotropy is quantified by fitting azimuthal changes of the clay diffraction peak intensity to the Maier-Saupe function. This parametric function is then used to extract both the full width at half maximum (FWHM) and the amplitude of the anisotropic scattering and eventually to estimate a nematic order parameter for this system. Finally, the time evolution of the one-to-zero and zero-to-one water layer transition in paraffin embedded fluorohectorite clay galleries is presented, and we demonstrate that such particles can be used as "meso-detectors" for monitoring the local water content in bulk carrier matrices, such as paraffin wax.

Potential of quasi-elastic neutron scattering techniques to investigate the influence of penetration enhancers on Stratum corneum lipid model membranes on a dynamic scale

Josefin Mueller* and Annett Schroeter

Institute of Pharmacy, Martin-Luther-University Halle-Wittenberg, Germany

Being the outermost layer of the human skin, the stratum corneum (SC) plays a key role in its barrier function. During the last decades many investigations were based on the examination of the SC lipid organization, whose main components are ceramides as the most relevant constituent, free fatty acids, cholesterol and its derivatives. Amongst others, the SC is responsible for reduced drug penetration across skin barrier due to its highly ordered lipid matrix structure. Elucidating the organization of lipids in the SC lipid layer as well as possibilities to influence this lipid structure in a reversible way are of high interest, because there are many advantages using the transdermal application route. Therefore, so-called penetration enhancers were implemented to increase the amount of available drug at its site of action. Such modulators are thought to reversibly loosen the highly ordered lipid structure in SC lipid matrix. Since the exact mechanisms on a molecular scale of these penetration enhancers are not completely understood, it is necessary to gain more information about their special influences and interactions with the SC lipid organization. Researches on synthetically derived SC lipid mixtures, using different neutron-based techniques, would contribute to understand the mode of action of these enhancers. For example the use of neutron scattering allows to probe molecular dynamics in the range from ns to ps, thereby enabling the investigation of weak forces and thermal motions in biological systems. In order to gain comprehensive insights into the studied biological systems, the use of different techniques is necessary as each of them offers a unique and characteristic information. While neutron diffraction studies give structural information about the probe and inelastic scattering about periodical movements, quasi-elastic scattering delivers insight into non-periodical movements. With the use of quasi-elastic neutron scattering (QENS) it is possible to study nanoscale dynamics and diffusion processes on a nanometer length scale. This could help us to comprehend the dynamical interactions of the SC-lipids with regard to the transport of drugs through the SC and further on, to manipulate this process. Up to now, dynamical properties of SC-lipid mixtures are less well understood and we are looking forward to improve this knowledge.

Using X-ray imaging to study thermal-induced changes in food

Mikkel Schou Nielsen[1]*, Robert Feidenhans'l[1], Rikke Miklos[2], René Lametsch[2] and Hildur Einarsdottir[3]

[1]*Niels Bohr Institute - NBI, Copenhagen*

[2]*Department of Food Science/Food Chemistry, Faculty of Science, University of Copenhagen*

[3]*DTU Compute, Technical University of Denmark*

When talking about food products, the effect of temperature inevitably comes up. Either when freesing the product for storage or heating when cooking. In food science, structural changes of the food product due to temperature have been investigated extensively [1] but so far these studies have been limited to indirect and/or destructive measurements.

Recently, X-ray imaging techniques for non-destructive investigation have been introduced in food science [2] but the conventional absorption modality does not give sufficient contrast when trying to study temperature-induced changes in soft tissue materials. We therefore propose to apply novel X-ray imaging modalities - i.e. phase-contrast and dark-field imaging - that have emerged within the last decade and give an improved contrast for soft tissue materials [3]. We here present preliminary results for visualising heating of meat using phase-contrast CT and freesing of berries using dark-field radiography. In the former, we are able to detect heat-induced changes in myofibrils and connective tissue as well as the cooking loss of water, and in the latter, we demonstrate structural changes in berries due to freesing and thawing processes.

The results show great promise for using novel X-ray imaging modalities in food science and for industrial processes such as monitoring freesing of food products.

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Structural Studies of Self-assembled 18A-Peptide: DMPC-particles

Martin Cramer Pedersen[1]*, Søren Roi Midtgaard[2], Jacob Judas Kain Kirkensgaard[1], Kasper K. Sørensen[2], Knud J. Jensen[2], Kell Mortensen[1] and Lise Arleth[1]

[1]*Niels Bohr Institute – NBI, University of Copenhagen*

[2]*Department of Chemistry, University of Copenhagen*

Using a combination of small-angle neutron scattering, small-angle x-ray scattering, coarse-grain molecular dynamics simulations and several other techniques, we present a structural study of a peptide-lipid-structure formed by self-assembly of synthetic 18A-peptides and the phospholipid DMPC.

Our analysis shows that a quasi-stable disc-shaped structure is formed, in which the peptides align themselves along the rim of the disc, shielding the hydrophobic part of the phosholipids from the solvent - and thus maintaining an intact bilayer encircled by the peptides.

The molecular dynamics simulations and light scattering experiments independently indicate that the system is quite dynamic, which is supported by the models refined of the scattering data.

The study showcases the importance of rigorous and cross-disciplinary data collection and analysis when investigating complicated systems with multiple scattering contrasts.

Currently, we are investigating the use of these structures in the handling of membrane proteins as well as further expanding our understanding of the dynamics governing the self-assembly of the peptides and the lipids.

Thermal conductivity measurements of a glacial state in a plastic molecular crystal

Daria Szewczyk

Institute of Low Temperatures and Structure Research, Polish Academy of Sciences – PAS, Poland

The transition between polyamorphic states has been one of the most interesting focus during the last decades. This transition could be observed in some materials from a first-order transition between the supercooled liquid state and a new amorphous phase, the "glacial state". The nature of this new state remains still controversial and different explanations have been given from different theories. At present the glacial state is seen as a consequence of a liquid-liquid transition between two liquid states or as an interrupted crystallization due to the low crystal growth rate from the glass state. In this work, the first glacial state obtained from a plastic crystal (adamantanone) will be described. It will also be shown that the features of the thermal conductivity temperature dependence at low-temperature is independent of the origin of the glass state and that the long range translational order does not modify the general properties known till present. Accordingly, the explanation of the phenomenon will be based on the low crystal growth rate of the low temperature ordered phase, given rise to a strongly defective crystal immersed into a glassy state.

Human serum albumin, Bevacizumab and their interaction examined by Small-angle X-ray scattering

Pernille Sønderby[1]*, Pernille Harris[1] and Jens Bukrinski[2]

[1]*Department of chemistry, Technical university of Denmark*

[2]*Novozymes Biopharma Industrial Biotechnology, Denmark*

Human serum albumin (HSA) is used as a functional protein in many different applications where HSAs ability to increase the solution stability of other proteins is utilized. The mechanism of action for this well-known stabilization is largely unknown. The focus of the present study is thus to utilize SAXSs unique ability to study such dense samples in relevant environment.

HSA is a well characterized protein. It is the most abundant plasma protein and is present in concentrations 40-60 g/L in blood. HSA acts naturally as a carrier of fatty acids, and other small hydrophobic molecules and even other proteins. Its stabilizing effects are today also used in the formulation of medicine where it serves as both a stabilizing agent and a potential carrier.

In recent years monoclonal antibodies have been used for the treatment of cancer and autoimmune diseases such as rheumatoid arthritis and Chron's disease2. Bevacizumab (BEV), Avastin®, is a humanized anti-vascular endothelial growth factor (VEGF) monoclonal antibody, which belongs to the subclass IgG1 of the immunoglobulins.

There are several concerns when formulating antibodies. A relatively large concentration is normally necessary to achieve the wanted pharmacological response. These levels of concentration can result in aggregation or unspecific interaction leading to new epitopes which can induce an immunological response when injected. Stabilizing the protein solution is therefore extremely important.

In order to evaluate the interaction of HSA and BEV a series of concentrations of the individual proteins were measured and mixtures of BEV and HSA for two different BEV concentrations at different ratios.

Hydrogen bond flexibility in paracetamol polymorphs: Insights from quasielastic neutron scattering

Nikolaos Tsapatsaris[1]*, Boris A. Kolesov[2,3], Jennifer Fischer[4], Boris A. Zakharov[2,3], Sven Landsgesell[5], Elena V. Boldyreva[2,3], Tilo Seydel[6], Luke Daemon[7], Juergen Eckert[8] and Heloisa N. Bordallo[1,9]

[1]*European Spallation Source – ESS, Lund, Sweden*

[2]*Novosibirsk State University, Russia*

[3]*Institute of Solid State Chemistry and Mechanochemistry, Russia*

[4]*Forschungszentrum Jülich, Germany*

[5]*Helmholtz-Zentrun Berlin – HZB, Germany*

[6]*Institut Laue Langevin – ILL, Grenoble, France*

[7]*Los Alamos National Laboratory, USA*

[8]*University of South Florida, Department of Chemistry, USA*

[9]*Niels Bohr Institute – NBI, Copenhagen, Denmark*

The well known analgesic paracetamol is found in several polymorphic forms each owning to different physical properties in the solid state. We report on inelastic and quasielastic neutron scattering investigations and density functional theory calculations elucidating the dramatically different dynamical behavior of the molecular structure of paracetamol polymorphs I and II. Differences in the slow and fast proton dynamics in both polymorphs are seen in the temperature dependent onset of stochastic methyl reorientation, which is primarily due to changes in the strength of the hydrogen bond environment for each polymorph and reinforce earlier indications on the anisotropy of the potential surface in the vicinity of the methyl rotor. The findings help advance the understanding of conformational flexibility and stability of molecular pharmaceuticals.

Magnesium borohydride as hydrogen storage material

Olena Zavorotynska*, Stefano Deledda and Bjørn Hauback

Institutt for Energiteknikk, Kjeller, Norway

Magnesium borohydride $Mg(BH_4)_2$ is a particularly interesting material for hydrogen storage applications due to its lightweight and favorable gravimetric density (14.9 wt% of hydrogen), which is exceptionally high for hydrides. Hydrogen sorption reversibility and cycling stability in $Mg(BH_4)_2$, however, still present a challenge. The material releases hydrogen in the 200-450ºC temperature range through a complex reaction pathway, which is not completely understood [1]. Some of the decomposition products are amorphous and thus are not possible to characterize with in-situ diffraction techniques, applied conventionally to study these types of hydrides. Another challenge is the rehydrogenation, which requires extreme conditions [2]. In order to improve hydrogen sorption performance of $Mg(BH_4)_2$ (and other borohydrides) a wide range of approaches has been tried, including high energy reactive ball-milling, preparation of composite materials, dispersion in porous matrix, and introduction of catalysts or catalytic precursors [3]. In all cases, understanding of the structure and the decomposition/rehydrogenation pathway of the resulting material is crucial.

In this contribution we present the results of our studies on the characterization of $Mg(BH_4)_2$, its decomposition products, and the feasibility for rehydrogenation. The hydrogen sorption was studied with differential scanning calorimetry combined with termogravimetric analysis (DSC-TG), volumetric measurements, mass spectrometry (MS), powder X-ray diffraction (PXD) and infrared spectroscopy (IR). Particular attention is devoted to the effect of some additives on the reaction pathways, formation of byproducts, and reversibility of hydrogen sorption.

The results presented in this contribution are obtained within the EU project BOR4STORE [4].

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Third Annual Niels Bohr International Academy

Workshop on ESS Science:

Crossing space and time domains with SAS and QENS

Participants List

Name	Email	Institution	Country
Prof. Argyriou, Dimitri	imitri.argyriou@esss.se	European Spallation Source - ESS	SWEDEN
Prof. Arleth, Lise	arleth@nbi.ku.dk	Niels Bohr Institute - NBI	DENMARK
Dr. Benetti, Ana	arbe@sund.ku.dk	University of Copenhagen	DENMARK
Ms. Bjergskov, Dorthe	dorthe.bjergskov@nbi.ku.dk	Niels Bohr Institute - NBI	DENMARK
Prof. Bordallo, Heloisa	bordallo@nbi.ku.dk	Niels Bohr Institute - NBI	DENMARK
Ms. Costa, Sónia	s.costa@live.com.pt	Universidade do Minho	PORTUGAL
Dr. Da Silva, Geraldo José	geraldo@fis.unb.br	University of Brasília - UnB	BRAZIL
Dr. Eckert, Juergen	juergen@mrl.ucsb.edu	University of South Florida	USA
Mr. Eremin, Roman	era@jinr.ru	Joint Institute for Nuclear Research, Dubna	RUSSIA
Ms. Fischer, Jennifer	j.fischer@fz-juelich.de	Forschungszentrum Jülich	GERMANY
Dr. Fratini, Emiliano	fratini@csgi.unifi.it	Department of Chemistry "Ugo Schiff" and CSGI, University of Florence	ITALY
Mr. Grassi, Giovanni	gigrassi@gmail.com	Universidade de Brasília, UnB	BRAZIL
Ms. Gryliuk, Galyna	gallygriluk@yahoo.com	University of Tartu	ESTONIA
Prof. Head-Gordon, Teresa	thg@berkeley.edu	University of California, Berkeley	USA
Mr. Hernandes Barrozo, Alexandre	alexandre.barrozo@icm.uu.se	Uppsala Universitet	SWEDEN
Dr. Jackson, Andrew	andrew.jackson@esss.se	European Spallation Source - ESS	SWEDEN
Mr. Karlsen, Morten	mkarlsen@sund.ku.dk	Copenhagen University	DENMARK
Dr. Kirkensgaard, Jacob	kirkensgaard@life.ku.dk	Niels Bohr Institute - NBI	DENMARK
Ms. Kovalchuk, Karina	karina.kovalchuk@ntnu.no	Norwegian University of Science and Technology - NTNU	NORWAY
Dr. Krutyeva, Margarita	m.krutyeva@fz-juelich.de	Forschungszentrum Jülich	GERMANY
Dr. Lyonnard, Sandrine	sandrine.lyonnard@cea.fr	French Alternative Energies and Atomic Energy Commission - CEA	FRANCE
Mr. Martinez, Gerardo	gerardo.mtz.rugerio@gmail.com	Material Physics Centre, UPV/EHU	SPAIN
Mr. Martins Da Silva, Fernando Henrique	nandofisunb@gmail.com	Université Pierre et Marie Curie - UPMC	FRANCE
Mr. Martins, Murillo	murillolongo@gmail.com	Niels Bohr Institute - NBI	DENMARK
Dr. Mavri, Janez	janez.mavri@ki.si	Laboratory for Biocomputing and Bioinformatics, National Insitute of Chemistry	SLOVENIA
Ms. Michelsen, Gitte	gittem@fys.ku.dk	Niels Bohr Institute - NBI	DENMARK
Mr. Michels, Leander	leander.michels@ntnu.no	Norwegian University of Science and Technology - NTNU	NORWAY
Mr. Midtgaard, Soren	soromi@life.ku.dk	University og Copenhagen	DENMARK
Mr. Mikkelsen, Alexander	almikkelsen87@gmail.com	Norwegian University of Science and Technology - NTNU	NORWAY
Ms. Mueller, Josefin	josefin.mueller@pharmazie.uni-halle.de	Institute of Pharmacy, Martin-Luther-University Halle-Wittenberg	GERMANY
Mr. Nielsen, Mikkel Schou	schou@fys.ku.dk	Niels Bohr Institute - NBI	DENMARK
Prof. Niss, Kristine	kniss@ruc.dk	Roskilde University	DENMARK
Mr. Pedersen, Martin Cramer	mcpe@nbi.dk	Niels Bohr Institute - NBI	DENMARK
Dr. PETERSSON Årsköld, Sindra	sindra.petersson@esss.se	European Spallation Source - ESS	SWEDEN
Prof. Pieper, Jörg	pieper@ut.ee	University of Tartu	ESTONIA
Prof. Posselt, Dorthe	dorthe@ruc.dk	IMFUFA, Department of Science, Systems and Models, Roskilde University	DENMARK
Prof. Pynn, Roger	rpynn@indiana.edu	Indiana University	USA
Prof. Serimaa, Ritva	ritva.serimaa@helsinki.fi	Department of Physics, University of Helsinki	FINLAND
Prof. Schrøder, Thomas	tbs@ruc.dk	Roskilde University	DENMARK
Prof. Skipper, Neal	n.skipper@ucl.ac.uk	Universitry College London	UK
Dr. Svergun , Dmitri	svergun@embl-hamburg.de	European Molecular Biology Laboratory - EMBL	GERMANY
Ms. Szewczyk, Daria	d.szewczyk@int.pan.wroc.pl	Institute of Low Temperature and Structure Research, PAS	POLAND
Ms. Sønderby, Pernille	perso@kemi.dtu.dk	Department of chemistry, Technical university of Denmark	DENMARK
Mr. Tedesco, Julio	tedesco.jcg@gmail.com	Niels Bohr Institute - NBI	DENMARK
Dr. Telling, Mark	mark.telling@stfc.ac.uk	ISIS, Science & Technology Facilities Council	UK
Dr. Tsapatsaris, Nikolaos	nikolaos.tsapatsaris@esss.se	European Spallation Source - ESS	SWEDEN
Prof. Unruh, Tobias	tobias.unruh@fau.de	Friedrich-Alexander-Universität Erlangen-Nürnberg - FAU	GERMANY
Dr. Zavorotynska, Olena	olena.zavorotynska@ife.no	Institutt for Energiteknikk	NORWAY
Mr. Øhrberg Schreiber, Anders	wsl980@alumni.ku.dk	Niels Bohr Institute - NBI	DENMARK

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Crossing space and time domains with SAS and QENS

Organizers

Heloisa N. Bordallo: bordallo@nbi.ku.dk

Juergen Eckert: juergen@usf.edu

Lise Arleth: arleth@nbi.ku.dk

Local Support

Gitte Michelsen: gittem@fys.ku.dk

Anders Øhrberg Schreiber: wsl980@alumni.ku.dk

Julio Tedesco: tedesco.jcg@gmail.com

Helle Kiilerich: helle@nbi.dk