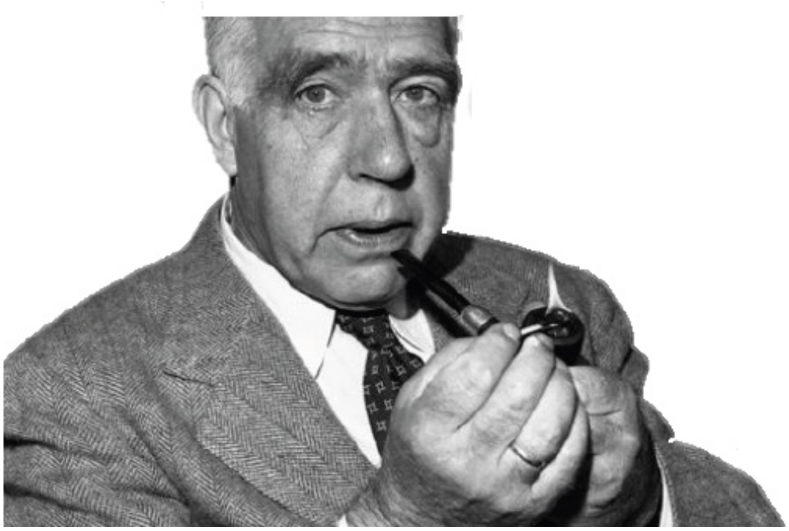
Second Annual Niels Bohr International Academy Workshop on Neutron Science

Copenhagen, June 25-29, 2012

Second Annual Niels Bohr International Academy Workshop on Neutron Science

Bridging Elastic and Inelastic Scattering by Means of Computational Studies and Analysis

<ins>Invited Speakers</ins>:
C. Austen Angell
Dimitri Argyriou
Mauro Boero
Heloisa N.Bordallo
Juergen Eckert
Donald Engelman
Andrew D. Jackson
David Keen
Simon Kimber
Frederica Migliardo
Denis Morineau
Kristine Niss
Neal Skipper
Alan K. Soper
Jernej Stare
Matt Tucker
Tejs Vegge



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Bridging Elastic and Inelastic Scattering by Means of Computational Studies and Analysis

About the workshop:

Where are the atoms and what do they do?
The workshop will focus on the use of theoretical simulations for the detailed, atomic level interpretation of experimental data from X-ray and neutron diffraction. 30 world-leading scientists and 20 students will convene for a week of intense discussions, lectures and student project work.

The meeting is sponsored by the **Niels Bohr International Academy** and by the **Copenhagen University**. A limited number of students travel and accommodation is sponsored by the **European Spallation Source**.

The **Second Annual Niels Bohr International Academy Workshop on Neutron Science** will take place of June 25-29, 2012, in Copenhagen, Denmark.

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SCIENTIFIC PROGRAM

Program for the Second NBIA Meeting on Neutron Science, June 25-29, 2012

(1) All participants can take part on the lectures, however only 20 will take part on the hand on exercises.
(2) "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		
9:00 am – 9:30 am	Registration	
9:30 am – 10:15 am	Welcome	
10:15 am - 11:15 am	Don Engelman (Yale)	Dynamics at the molecular level in biological systems
11:15 am - 11:45 am	Coffee break	
11:45 am - 12:30 pm	David Keen (RAL)	Reverse Monte Carlo (RMC) modelling of amorphous structure
12:45 pm - 2:00 pm	Lunch	
2:00 pm - 2:45 pm	Matt Tucker (RAL)	RMCProfile: The local point of view of crystalline materials
2:45 pm - 3:30 pm	Heloisa N. Bordallo (NBI)	Application of incoherent inelastic neutron scattering in pharmaceutical analysis
3:30 pm - 4:00 pm	Coffee break & Posters	
4:00 pm - 4:45 pm	Jernej Stare (National Institute of Chemistry)	Car-Parrinello simulation of hydrogen bonded solids
5:00 pm-6:00 pm	**Student Working Groups**	
Tuesday, 2nd day		
9:00 am - 10:00 am	Juergen Eckert (USF)	Quantum dynamics of bound hydrogen: Neutron scattering and computational studies
10:00 am - 10:30 am	Coffee break	
10:30 am - 11:15 am	Simon Kimber (ESRF)	Local structure and PDF
11:15 pm - 12:45 pm	**Student Working Groups**	
11:15 pm - 12:45 pm	Guided visit of the NBI	
12:45 pm - 2:00 pm	Lunch	
2:00 pm – 2:45 pm	Mauro Boero (CNRS-University of Strasbourg)	First principles and hybrid QM/MM dynamical simulations: A few basics and contact with experiments
2:45 am - 3:30 pm	Dimitri Argyriou (ESS)	Science at ESS
3:30 pm - 5:00 pm	**Student Working Groups**	
3:30 pm - 5:00 pm	ESS Science: Opportunities & Ideas : Round Table with ESS Scientists	
5:00 pm – 6:00 pm	Poster presentations: 2 minutes clips	
5:00 pm - 7:30 pm	Beer party and posters	
Wednesday, 3rd day		
9:00 am - 10:00 am	**Students Working groups**	
10:00 am – 10:30 am	Coffee Break	
10:30 am - 11:30 am	Neal Skipper (UCL)	The structure of nanocarbons in solution by neutron scattering and computer simulation
11:30am - 12:15am	Andrew D. Jackson (NBIA)	Niels Bohr, CERN, European facilities, bond between cultures
12:15 pm - 2:00 pm	Lunch	

2:30 pm – 9:00pm	*Sponsored by ØMIC*	Visit to Arken Museum (http://www.arken.dk/content/us) & Conference dinner
Thursday, 4th day		
9:00 am -10:00 am	Austen Angell (Arizona State University)	Fundamental aspects of the glass transition in liquids and disordering crystals
10:00 am -10:30am	**Posters** Coffee break	
10:30 am – 11:15 am	Kristine Niss (Roskilde University)	"Simple"- glass-forming liquids
11:15 am -12:00 pm	Tejs Vegge (DTU)	Rotational and translational diffusion in materials for energy storage from quasielastic neutron scattering and density functional theory calculations
12:00pm – 12:30 pm	Guided visit of the NBI – students groups	
12:30 pm - 2:00 pm	Lunch	
2:00-4:00	**Student Working groups**	
2:00-4:00	Guided Tour for the senior scientists: National Gallery of Denmark - Statens Museum for Kunst http://www.smk.dk/en/visit-the-museum/visiting-information/	
4:00-4:30	**Posters** Coffee break	
4:30 pm – 6:00	**3 Groups of Students (30 minutes each group)**	Student presentations on their results
Friday, last day		
9:00 am-9:45 am	Federica Migliardo (University of Messina)	Dynamics of biomolecules by EINS, INS and QENS
9:45 am-10:45 am	Denis Morineau (Université de Rennes 1)	Basics and illustrative cases of fluids confined in nanochannels studied by neutron and simulation methods
10:45 am – 11:15am	**Posters** Coffee break	
11:15 – 12:30	Alan K. Soper (RAL)	Total scattering as a probe of structure in liquids and glasses
12:30 pm-2:00 pm	Lunch and Good bye	

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INVITED TALKS

Fundamental aspects of the glass transition in liquids and disordering crystals

Austen Angell
Dept. of Chemistry and Biochemistry - Arizona State University
Payson, Arizona, USA

The glassy state is a state of frozen-in disorder that is obtained when a cooling process is carried out too quickly for the thermodynamically favored path to be followed. At the glass temperature, the time scale of the ordering process becomes longer than the time scale of the experiment by which the system is observed.

Normally one thinks of these events as occurring in viscous liquids, but this a very limiting view, because closely related phenomena occur in rotationally disordered crystals and binary metallic alloys to name just two types of non-liquid "glass forming" systems.

To understand the physics of glass formation one usually needs to know about the motion of particles within the glassformer phase and the competing time scale by which the system can escape from the disordered phase into the thermodynamically preferred state, either a crystal in the first case, or a more ordered crystal in the other cases. In some cases this latter problem is irrelevant, because the glassformer phase is the stable phase.

In this lecture we will present the essence of "the glass problem", highlighting the fact that it is a problem relevant to all types of liquid substances from liquid metals, through polymers to liquids as simple as an elemental form of oxygen (ozone). Some simple rules that predict which molecular liquids will be glass formers and which not, will be presented.

The kinetic properties of liquids that lead, by viscous slow-down, to the vitrification phenomenon, will be used to bring a systematic pattern (now called "fragile" vs "strong") to the behavior of liquids of different types, and it will be shown that the pattern extends to the thermodynamic properties. This will direct our attention to a feature of the disordered crystal cases that belong at the "strong" end the same pattern seen for liquids. It is found to be tied to a well-known type of phase transition (lambda transition) that now occurs far above the glass transition, in the few cases where melting does not preclude its observation (C_{60} is a nice example, because it can't melt).

The remainder of the lecture will be given to trying to show how these insights can be related to the behavior of the "strong" liquids (like the archetypal glassformer SiO_2, and other three dimensionally connected network liquids GeO_2 and BeF_2), the disordering of which only becomes a lambda transition when the external pressure is adjusted to a critical value. This is then related to the behavior of the weak network liquid, H_2O, for which the second critical point is found at temperatures below the melting point (but still far above the glass temperature. For the less ionic liquids this transition can be identifiedwith a metal-semiconductor transition. Water then is seen to occupy a position intermediate between the "strong" covalent network extreme and the "fragile" molecular liquid extreme. The behavior of water is the Rosetta stone of the glass transition problem as will be explained, using an excitations model to predict the extraordinary behavior of fragile liquids near and below the glass transition.

We make an effort to emphasize the points at which neutron scattering techniques can be brought to bear on critical aspects of the glassformer problem.

Science at ESS

Dimitri Argyriou

European Spallation Source

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.

First principles and hybrid QM/MM dynamical simulations: A few basics and contact with experiments

Mauro Boero

IPCMS, CNRS - University of Strasbourg

Strasbourg, France

Fundamental equations of motion for first principles molecular dynamics, their outcome and the extraction of radial distribution functions, IR spectra and chemical reactions pathways will be discussed. A couple of practical applications to NaCl in solution at finite dilution and to proteins (Cytochrome c Oxidase) acting as a proton pump in the cell respiration process will be discussed to show the quality of the agreement with experiments (neutron scattering, X-ray, IR) and the limitations still existing in nowadays approaches.

After a brief overview of the theoretical background and the most advanced algorithms used in computational sciences, a couple selected applications will be presented, at the crossroad between biochemistry and physics. Specifically, applications to salt aqueous solutions (NaCl) and proteins will be discussed in terms of structural and electronic characterization [1-3]. We shall focus mainly on the extraction of pair correlation functions, directly comparable to neutron and X-ray scattering measurements and infra-red (IR) spectra to show possibilities and limitations of this class of approaches. In the case of proteins, where experimental limitations in the atomistic resolution exist [4,5], we shall focus mostly on deviations of a biochemical system from the pristine crystallographic data and how these deviations must be monitored and controlled during a reactive simulations involving structural modifications [6-8].

References:

[1] J. D. Smith et al. Science 306, 851 (2004)
[2] G. E. Walrafen and E. Pugh, J. Sol. Chem. 33, 81 (2004)
[3] D. A. Schmidt et al., J. Phys. Chem. A 113, 7725 (2009)
[4] T. Tsukihara et al., Proc. Nat. Ac. Sci USA 100, 15304 (2003)
[5] R. Fukunaga and S. Yokoyama, Nature Struct. Mol. Biol. 12, 915 (2005)
[6] K. Kamiya et al. , J. Am. Chem. Soc. 129, 9663 (2007)
[7] M. Boero et al. J. Am. Chem. Soc. 128, 16798 (2006)
[8] M. Boero, J. Phys. Chem. B 115, 12276 (2011)

Application of incoherent inelastic neutron scattering in pharmaceutical analysis

Heloisa N. Bordallo
Niels Bohr Institute
Copenhagen, Denmark

In this talk I will discus on the use of inelastic neutron scattering as an alternative tool for a more accurate physical characterization of pharmaceutical drugs. I will focus on the relaxation processes in the pharmaceutical compound phenacetin, (p-ethoxyacetanilide, $C_{10}H_{13}NO_2$), which was studied by means of incoherent inelastic neutron scattering.

By evaluating the mean-square displacement obtained from the elastic fixed window approach, using the neutron backscattering technique, a crossover of the molecular fluctuations between harmonic and non-harmonic dynamical regimes around 75 K was evidenced.

From the temperature dependence of the quasi-elastic line-width, explored by time-of-flight technique, it was possible to attribute the onset of this anharmonicity to the activation of the methyl group rotations. Finally, the use density functional theory-based methods allowed us to calculate the lattice vibrations in the harmonic approximation.

The overall spectral profile of the calculated partial contributions to the dynamical susceptibility, $\chi''(\omega)$, compares satisfactorily to the experimental spectra in the region of the lattice modes where the intermolecular interactions are expected to play an important role.

This study contributes to understanding the relations between intermolecular hydrogen bonds, intramolecular dynamics and conformational flexibility in pharmaceutical drugs destined to be used in solid dosage form.

This work was done in collaboration with Boris A. Zakharov (Novosibirsk State University), Elena V. Boldyreva (Novosibirsk State University), Mark R. Johnson (ILL), Michael Marek Koza (ILL), Tilo Seydel (ILL) and Jennifer Fischer (Forschungszentrum Jülich, Institut of Complex Systems, Jülich, Germany).

Quantum dynamics of bound hydrogen: Neutron scattering and computational studies

Juergen Eckert

University of South Florida

Tampa, Florida, USA

The dynamics of hydrogen in a bound state is of importance in a wide variety of physical and chemical processes. While the experimental observation of a very wide range of hydrogen dynamics is greatly facilitated by the use of neutron scattering methods, accurate computational modeling of the various motions of hydrogen is rather difficult because of their quantum dynamical nature. The large degree of delocalization of hydrogen for low frequency excitations adds additional difficulties in that the relevant potential energy surface is explored over a wide range of coordinates, and hence has to be of very high accuracy.

I will describe a range of hydrogen dynamics from the rotational and translational motions of weakly bound molecular hydrogen in adsorption based hydrogen storage materials to those of activated dihydrogen, the vibrational motions of chemically bound hydrides, including those forming hydrogen bonds, exchange reactions of bound hydrogen with one another or other molecules in catalysis, and finally, the diffusion of these species within its environment. The degree to which the experimental observations of these dynamical processes can be interpreted depends largely on employing high level computational studies, and can in such cases provide a great deal of fundamental insight into the chemistry of hydrogen in materials.

Dynamics at the molecular level in biological systems

Donald Engelman

Yale University

New Haven, Connecticut, USA

At the most fundamental level, life is dynamic. In fact, one can show that the polymers of life cannot form spontaneously in an equilibrium system, so that living systems require the flow of energy and materials to sustain them, and the dynamics are manifest at all levels of organization.

To understand life at the molecular level, therefore, one cannot rely on time invariant views. In this talk, I will review the thermodynamic argument and present a few examples of dynamics at the macromolecular level, taking as examples cases where the motions have been constructed from a set of static structures and combined using molecular dynamics computational approaches to derive views of functional motions that aid in understanding biology.

Niels Bohr, CERN, European facilities, bond between cultures

Andrew Jackson

Niels Bohr Institute

Copenhagen, Denmark

In my talk I will present a personal view of Niels Bohr’s scientific career.

Niels Bohr's way of looking at the atom gave science a new tool of comprehension that made possible, for the first time, to consider all natural phenomena, from the hottest star to the living cells, as the effect of one fundamental principle. Because of Bohr, we know how light is radiated and absorbed, how atoms are put together into molecules, how electricity produces its effects, and we can even get insight in the secrets of the atomic nucleus.

Niels Bohr influence is felt wherever science is pursued all over the world. This world-renowned physicist is remembered at CERN especially for the leading role he played in its foundation. CERN would not exist if it had not been for his great efforts to bring about in the heart of Europe an international laboratory devoted to the innermost structure of matter. As a visionary and leader, Bohr started the Theoretical Study Group at CERN in the early days before the laboratory at Meyrin was ready. He always looked at science as an endeavour, which goes beyond national boundaries, not only as a means for research but also as a bond between men.

Reverse Monte Carlo (RMC) modelling of amorphous structure

David Keen

ISIS, STFC

Didcot, United Kingdom

The reverse Monte Carlo (RMC) modelling technique [1] is a method for producing atomistic models of disordered structures based on available experimental data. The method mimics a Monte Carlo minimisation except that, rather than minimising the system's energy, the cost function uses the differences between functions calculated from the model and their experimental equivalents. There is therefore a strong link between the modelling and the experimental data with the principal experimental data being the total scattering structure factor (S(Q)) and pair distribution function (PDF), although other functions may also be incorporated.

This talk will introduce the method and its historical development, beginning with the first RMC model of liquid Argon in 1988 [2] and continuing towards more recent RMC studies of (for example) the structures of materials produced via high-pressure and high-temperature amorphization [3]. The advantages and disadvantages of the method will be discussed, paying particular attention to the importance of restraints and their inclusion in the more recent RMC codes.

References:

[1] see www.rmcprofile.org; M G Tucker, D A Keen, M T Dove, A L Goodwin and Q Hui, J. Phys. Condens. Matter 19, 335218 (2007)

[2] R L McGreevy amd L Pusztai, Mol. Simul. 1, 359 (1988)

[3] T D Bennett, A L Goodwin, M T Dove, D A Keen, M G Tucker, E R Barney, A K Soper, E G Bithell, J-C Tan and A K Cheetham, Phys. Rev Lett. 104, 115503 (2010); D A Keen, A L Goodwin, M G Tucker, J A Hriljac, T D Bennett, M T Dove, A K Kleppe, A P Jephcoat and M Brunelli, Phys. Rev. B, 83, 064109 (2011)

Local structure and PDF

Simon Kimber

ESRF

Grenoble, France

Dynamics of biomolecules by EINS, INS and QENS

Federica Migliardo

Institut de Biochimie et Biophysique Moléculaire et Cellulaire

Université de Paris-Sud 11

Paris, France

In this talk, the versatility and the importance of neutron scattering in the study of the dynamics of biological macromolecules will be highlighted.

The basic theories about elastic (EINS), inelastic (INS) and quasi-elastic neutron scattering (QENS) will be introduced and discussed. In the framework of the most topical models used to investigate the low-frequency and high-frequency dynamics of biomolecules, a wide overview of recent results obtained on biological systems, such as bioprotectant (i. e. homologous disaccharides and glycerol) mixtures and biomolecules (i. e. proteins and enzymes) solutions also in presence of cosolutes [1-3], will be presented. The role of hydration in biomolecular dynamics will be also pointed out.

References:

[1] S. Magazù, F. Migliardo, S. F. Parker, J. Phys. Chem B, 115, 11004 (2011).
[2] S. Magazù, F. Migliardo, F. Affouard, M. Descamps, M. T. F. Telling, J. Chem. Phys., 132, 184512 (2010).
[3] S. Magazù, F. Migliardo, A. Benedetto, J. Phys. Chem. B, 114, 9268 (2010).

Basics and illustrative cases of fluids confined in nanochannels studied by neutron and simulation methods

Denis Morineau

Institute of Physics of Rennes - University of Rennes 1

Rennes, France

Manipulating fluids at the nanoscale by geometrical confinement is a major issue of contemporary condensed matter science. It is also an area of research where the complementarity of neutron scattering and molecular simulation is particularly apparent.

In this lecture, we consider different cases from the recent literature, where structural (diffraction) and dynamical (quasielastic scattering) investigations by neutron methods have benefitted from realistic (atomistic) and coarse-grained molecular simulations, and vice-versa. We emphasize the special benefits and the limitations of each type of approach with the ultimate hope to inspire more scientists to join the gap between experiments and simulation.

"Simple"- glass-forming liquids

Kristine Niss
DNRF center "Glass and Time", IMFUFA, NSM, RUC
Roskilde, Denmark

The glass transition is a universal phenomenon which in its essence is independent of the interactions between the atoms or molecules of the liquid forming the glass. The universal character of the transition has led physicists to believe that there is one underlying simple explanation of the phenomenon. More than 15 years ago the Nobel laureate P.W. Anderson stated that understanding the glass-transition is deepest unsolved problem in solid state physics [1], but a satisfactory explanation is still lacking. Understanding the glass-transition implies understanding the dynamics (e.g. diffusion, vibration, relaxation) and the physics in general of the viscous liquid forming the glass. Gasses can to a great extend be understood via the ideal gas model where the interactions between particles are ignored. In crystalline solids the physics can be understood by exploding the periodic nature of the structure. No similar simplification can be made for liquids. Here we need to consider the interaction between the molecules, the kinetic energy and the amorphous structure. This is a challenge to a model systems or a theory explaining the glass transition and the physics of liquids in general.

The "Glass and Time" group on RUC has during the last five years succeeded in identifying a class of simple liquids and a theory for describing these has been developed [2]. This theory, called the isomorph theory, has proven very effective in describing computer simulated liquids with simple interactions (e.g. Lennard Jones liquids). But how useful is the theory when it comes to understanding the physics the liquids we deal with in the laboratory? In 2011 we published the first experimental results supporting the isomorph theory [3]. Here we showed how the relative effect of density and temperature on the glass transition can be understood in terms of the isomorph theory. There are several other predictions of the theory, many of these are directly related to the glass transition. Our current and future experimental work focusses on testing these predictions.

Inelastic neutrons scattering (INS), is a strong tool for probing dynamics in liquids and has played a central role for some of the results leading up to the isomorph theory. INS will also be important for our further work on testing the isomorph theory.

References:

[1] Science 267, 1609 (1995)
[2] J. Chem. Phys. 131, 234504 (2009)
[3] Nature Physics 7, 816 (2011)

The structure of nanocarbons in solution by neutron scattering and computer simulation

Neal Skipper

University College London

London, United Kingdom

Nanostructured forms of carbon such as the fullerenes, nanotubes and graphene are relatively insoluble in common organic and aqueous solvents. However, these materials can be reversibly reduced by the solvated electrons formed in metal-ammonia solutions, and the resulting nanocarbon salts are then soluble in common aprotic solvents such as THF, DMF and NMP. These solutions then have great practical potential as a means to purify and process nanotubes and graphene in particular. Neutron scattering in conjunction with isotope labelling has proven to be a very powerful method for understanding the structure of both the host metal-ammonia solutions and also the dissolved nanocarbons. We will discuss the methodology and methods of analysis, including the use of small angle scattering, necessary to study these complex fluids. We will also focus on the interplay between experiments and computer simulations.

References:

H Thompson, JC Wasse, NT Skipper, S Hayama, DT Bowron, AK Soper. Structural Studies of Ammonia and Metallic Lithium-Ammonia Solutions. J. Am. Chem. Soc., 2003, 125, 2572–2581.

CA Howard, H Thompson, JC Wasse NT Skipper. Formation of Giant Solvation Shells around Fulleride Anions in Liquid Ammonia. J. Am. Chem. Soc., 2004, 126, 13228–13229.

S Fogden, CA Howard, RK Heenan, NT Skipper, MSP Shaffer. Scalable Method for the Reductive Dissolution, Purification, and Separation of Single-Walled Carbon Nanotubes. ACS Nano, 2012, 6, 54–62

EM Milner, NT Skipper, CA Howard, MSP Shaffer, DJ Buckley, KA Rahnejat, PL Cullen, RK Heenan, P Lindner, R Schweins. Structure and Morphology of Charged Graphene Platelets in Solution by Small-Angle Neutron Scattering. J. Am. Chem. Soc., 2012, 134, 8302–8305.

Total scattering as a probe of structure in liquids and glasses

Alan Soper

ISIS, STFC

Didcot, United Kingdom

Radiation total scattering experiments have been the method of choice of investigating structure at the level of atomic separations for nearly a century. This is because the radiation wavelength can readily be tuned to that appropriate to the length scale of the structure being probed, and because beams of x-rays or neutrons can be highly penetrating, enabling structures at high pressures or over a range of temperatures to be probed. Crucial to the success of these methods is the ability to convert raw scattering data - essentially x-ray or neutron counts in the detectors - to scattering cross sections on an absolute scale. Nowadays these methods are supplemented by powerful modelling strategies that attempt to reconstruct the atomistic structure on a computer in a manner consistent with the scattering data. The various methods will be outlined and some recent results highlighted.

Car-Parrinello simulation of hydrogen bonded solids

Jernej Stare
National Institute of Chemistry
Ljubljana, Slovenia

Hydrogen bond dynamics in the condensed phase has been for long subject of experimental and theoretical studies, since it governs the structure and functionality of a variety of biomolecules and materials. On a simulation level, the use of ab initio molecular dynamics methodology is essential for a reliable prediction of many crucial properties of hydrogen bonds. Furthermore, as hydrogen dynamics can feature notable nuclear quantum effects, it is often necessary to employ advanced techniques for quantization of nuclear motion. A combined treatment featuring both ab initio molecular dynamics according to the Car-Parrinello scheme (CPMD) and assessment of nuclear quantum effects will be presented on the example of sodium hydrogen bis-sulfate, a crystalline ferroelectric material with a very short hydrogen bond; various methodologies for the calculation of vibrational spectra will be discussed.

The students will be given a tutorial on basic techniques of molecular simulation of crystalline solids. The main features of the CPMD program package will be presented, focusing on molecular dynamics simulation and extraction of various properties from the trajectory (e.g., infrared and INS spectra). Project work will include the setup of the model of a crystalline solid, main protocols of molecular simulation (geometry optimization, harmonic vibrational analysis, molecular dynamics), calculation of INS spectra, and critical evaluation of the computed quantities. Familiarity with Unix/Linux OS, the common program packages for molecular simulation (Gaussian, CPMD, VASP, etc.) and molecular visualization tools (VMD, Molden, etc.) is appreciated, but not required.

RMCProfile: The local point of view of crystalline materials

Matt Tucker

ISIS, STFC

Didcot, United Kingdom

Many of the useful materials that make modern life possible are crystalline. Quartz keeps our watches on time, perovskites are widely used in consumer electronics and solid oxide fuel cells may help to power the future.

The importance of local structure and disorder in crystalline materials is being recognised more and more as a key property of many functional materials. From negative thermal expansion to solid state amorphisation and the 'nanoscale' problem to improved fuel cell technology, a clear picture of the local atomic structure is essential to understanding these phenomena and solving the associated problems.

Total scattering, an extension of the powder diffraction method, is increasingly being used to study crystalline materials. The unique combination of Bragg and diffuse scattering can be used to determine both the average structure and the short-range fluctuations from this average within a single experiment. To maximise the structural information from such data, three-dimensional atomic models consistent with all aspects of the data are required.

RMCProfile [1,2] expands the reverse Monte Carlo (RMC) modelling technique [3] to take explicit account of the Bragg intensity profile from crystalline materials. Analysis of the RMCProfile-generated atomic models gives more detailed information than is available directly from the data alone. I will give several examples where RMCProfile has been used to successfully study the structure and disorder of crystalline materials to illustrate its potential.

References:

[1] www.rmcprofile.org

[2] M G Tucker, D A Keen, M T Dove, A l Goodwin and Q Hui, J. Phys. Condens. Matter 19, 335218 (2007)

[3] R L McGreevy amd L Pusztai, Mol. Simul. 1, 359 (1988)

Rotational and translational diffusion in materials for energy storage from quasielastic neutron scattering and density functional theory calculations

Tejs Vegge

Department for Energy Conversion and Storage, Technical University of Denmark

Lyngby, Denmark

Rotational and diffusional kinetics in materials for energy storage is investigated using quasi elastic neutron scattering (QENS) measurements in combination with density functional theory (DFT) calculations. Computational path techniques based on the nudged elastic band (NEB) methods are used to identify transition states and determine the rate of molecular rotations and diffusion. Integrated computational and experimental analysis of the Q-dependence of the elastic incoherent structure factor (EISF) and the quasi elastic broadening is used to separate localized motion from long range diffusion.

Examples will be shown from metal alanates, i.e. $NaAlH_4$ and $Na_3(AlH_6)_3$ with and without $TiCl_3$ additives [1], metal halide ammines like $Mg(NH_3)_6Cl_2$ for reversible ammonia storage [2] and metal borohydrides $Ca(BH_4)_2$ and $Mg(BH_4)_2$ for hydrogen storage [3,4]. Resent results from lithium diffusion in solid electrolytes for lithium-ion batteries will also be shown.

References:

[1] J. Voss, et al., J. Phys. Chem. B 111, 3886 (2007)
[2] A. Tekin, et al., Energy & Environmental Science 3, 448 (2010)
[3] D. Blanchard, et al., J. Phys. Chem. C 114, 20249 (2010)
[4] D. Blanchard et al., J. Phys. Chem. C 116, 2013 (2012)

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POSTERS

High lead oxide glass structure

Oliver Alderman

University of Warwick, Coventry, United Kingdom

Pulsed neutron and high-energy x-ray diffraction data for twenty lead silicate and germanate glasses have been recorded up to high momentum transfers to yield high spatial resolution pair correlation functions. The glasses cover wide compositional ranges from zero to 80 mol% PbO, the latter of which are accessible by means of rapid twin-roller quenching. The diffraction data are analysed by means of peak fitting to the real space pair correlation functions and empirical atomistic modeling driven by the measured structure factors and bulk densities. Results support the notion that PbO is an intermediate oxide in terms of glass formation; although pure PbO glass does not form, Pb2+ cations are coordinated by low numbers of oxygen atoms (about four), and hence contribute to glass network formation. This is evident in the silicate series, where the average O-Si coordination falls below one for glasses with more than 67 mol% PbO. In the germanate series, a maximum Ge-O coordination of 4.14 at 27 mol% PbO is observed, in stark contrast to the case for typical alkali germanate glasses, where Ge-O coordination reaches a much higher maximum. This suppression of the germanate anomaly is a consequence of the observed low Pb-O coordination.

Spherically grooved moderators - simulation and experiment

Mads Bertelsen and Pia Jensen

Niels Bohr Institute, Copenhagen, Denmark

Home grown simulations on improving neutron moderator geometry in order to control flux distribution. Some simple experiments have been conducted to test the simulation, and agreement is as good as can be expected with the used model.

We have produced a light-weight simulation in order to investigate neutron moderation in a grooved moderator. The simulation uses neutron scattering and absorption data from NNDC[1] and classical mechanics for scattering. Grooves significantly improved the beam intensity compared to similar flat moderator surfaces, as expected from previous works[2-4]. It is found that absorption is an important effect when investigating the flux distribution.

To confirm the results from the simulation, an experiment was conducted using a small radioactive Ra-Be neutron source, paraffin-wax moderator blocks and a He-3 counter. Measurements were done with a flat and a spherically grooved moderator. The relative intensities matched the simulation output within reason, confirming the viability of the lightweight simulation approach.

The simulation was further used to optimize moderator shape by varying the moderator thickness and the depth and width of a single groove. Such optimizations, and the effect in it self, should be considered when building new neutron moderator systems, where our results can be used as a starting point for analysis with more complex simulation packages.

In order to give other people the opportunity to do moderator simulations, the simulation will be rewritten as a McStas[5] component. This will emphasize the connection between moderator geometry and neutron instruments, which should be investigated further.

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Functionality from flexibility: dynamics in crystalline and amorphous frameworks

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There is often thought there to be a void between fully ordered, crystalline, and disordered, or amorphous, materials. Whilst the challenges involved in measuring and refining structural data of materials with disorder, computational modelling methods give the opportunity to understand better the connectivity, properties and functionality of these materials. Through the use of total scattering and Bragg diffraction, and Rietveld and reverse Monte Carlo (RMC) analysis we explore the structure-property relationships in several framework materials.

The structure of amorphous calcium carbonate

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A poster detailing a synthesis method for making large quantities (ca. 3g) 'stable' amorphous calcium carbonate (ACC) and experimental neutron scattering data of deuterated ACC coupled with a computational model of the structure of ACC.

Amorphous calcium carbonate (ACC) is thought to play a key role in many biomineralisation processes that occur in various sea organisms.[1] This work is part of a project aimed at understanding the structure of ACC utilising both experimental and computational techniques. Very few structural investigations have been performed on ACC, mainly due to its instability and tendency to transform to the more stable crystalline form calcite within about 1 hour after synthesis. However, a model structure for ACC has been proposed by Goodwin et al. in 2010.[2] Presented here will be a synthesis method used to obtain stabilised ACC with experimental neutron diffraction data. Also presented alongside this data will be the initial computational modelling results fitting experimental neutron data to a computer model of ACC using the Empirical Potential Structure Refinement (EPSR) fitting program.

Structure-Property Relations of Nanostructured Materials for Heterogeneous Catalysis Towards Energy Conversion

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Transition metals in the d^8 family such as Ni, Pd, and Pt have been synthe- sized with great control in size and shape in using a high-temperature chemical synthetic method. Spherical nanocrystals were produced ranging from 4-12 nm for heterogeneous catalysis testing. The tunability in nanocrystal size allows us to perform controlled catalytic studies of model energy conversion reactions such as CO oxidation, Fischer-Tropsch synthesis, and alkane oxidation. The monodispersity of the particles allow for a systematic and correlation between size and catalytic activity. Preliminary catalytic studies in ambient conditions have been done for bimetallic nanoparticles supported on CeO_2.

My work at the European Synchrotron Radiation Facility (ESRF) aims to use X-Ray diffraction and pair distribution function analysis techniques to perform structural characterization on the catalysts to complement the techniques of transmission electron microscopy and CO chemisorption for identification of size and shape of the cat- alysts. With the library of characterization techniques, we can rigorously resolve structure of the as-synthesized nanocrystals and describe structure-property relations of these materials as they pertain to heterogeneous catalysis.

Exploring phonons without a single:
The MAX phase ceramic dilemma

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Mn+1AXn phase ceramics are a relative new group of materials where M is anearly transitional metal, A is from the A elements (usually IIIA and IVA),and, X is either carbon or nitrogen. These materials are a nanolaminate where the MX or ceramic layer is interleaved with a metallic or A layer element on an atomic scale. This composition has resulted in MAX phase ceramics having highly desirable properties of both metals and ceramics. These conductive, easily machined, light weight, stiff, corrosion resistant materials which maintain integrity at high temperatures, are by their very highly desirable for engineers and scientists alike. The inability to perform large scale production of MAX phases has halted their entry into everyday life akin to the inability of growing a measurable single crystal has hindered research into the basic atomic properties of the material. Lacking a sizable single crystal simulation has hypothesized many of the properties of specifically Ti_3SiC_2 and $TiAlC_2$. Initial evidence that the computer simulations were not yielding an accurate model of these materials was discovered by Kisi et al when measured values of the single crystal elastic tensor C44=410GPa where simulations predicted C44=120GPa for Ti_3SiC_2.

Using an oriented polycrystal sample and a method developed by Buchenau the measurements done by Kisi et al was verified using inelastic coherent neutron scattering on Taipan, ANSTO. Looking further into the computer model a phonon DOS was obtained over a range of temperatures for both samples using Pharos, Los Alamos. The range of temperatures allowed the simulated DOS for DFT and DFT-MD to overlay on experimental data. The comparison between the experiment and the simulated highlighted that at higher energies the simulation was a good match but at lower energies many features were missing. Delving deeper into the computer model to discover the source of error it was found all the elements in the model had varying degrees of anharmonicity. Furthermore by looking at the individual vibrations of the atoms some of the previously unexplained features of the experimental data could be traced to motion eliminated when querying the model because of the underlying assumptions when doing so.

This research has its main value in highlighting the potential reasons why simulations do not match the experimental reality, and by increasing the very small body of evidence that measures atomic level phenomena.

Field-induced magnetism in super-oxygenated $(La,Sr)_2CuO_{4+y}$

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The super-oxygenated $(La,Sr)_2CuO_{4+y}$ (LSCO+O) may be a key to understanding the complex interplay between superconducting and magnetic phases in the cuprate high-Tc super- conductors [1]. Earlier studies of LSCO+O suggests that the system performs an electronic phase separation into a) a magnetically ordered phase, resembling the "1/8" phase of the oxygen-stoichiometric $(La,Sr)_2CuO_4$ (LSCO), and b) a near-optimally doped superconductor [2].

e have produced a new, large single crystal sample of LSCO+O, with a Tc of 38.5 K, similar to optimally doped LSCO. In contrast to all other LSCO+O samples investigated to date, muon spin rotation shows no signature of static magnetic order. Neutron diffraction, however, shows a field-induced signal from magnetic long-range 1/8 order, as seen in LSCO [3], but this signal vanishes in the limit of zero field. In near-optimally doped LSCO samples, similar behavior has been found, but with a field-offset before appearance of the static magnetic signal [4,5]. This could suggest that our system is right at the quantum critical point in the phase diagram of field-induced magnetism [6], and that this new "hyper-oxygenated" system does not show the electronic phase separation, seen in most other LSCO+O samples.

At the conference, we will present the latest data from this ongoing work.

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Work done in collaboration with: L. Udby, J. Larsen, N.B. Christensen, S.B. Emery, Y.F. Nie, N.H. Andersen, J.-G. Grivel, Ch. Niedermayer, B.O. Wells, and K. Lefmann

Work at Univ. Conn. (SBE, YFN and BOW) supported by USDOE-BES under grant DE-FG02-00ER45801.

Low temperature studies of β-polymorph of chlorpropamide

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Studies of polymorphism of organic crystals at variable conditions have a wide range of theoretical, as well as practical applications. Firstly, such investigations provide detailed information about dynamics of intermolecular interactions and possible phase transitions. Molecular crystals are used as model objects for prediction of behavior of more complex biological systems. Secondly, studies of molecular crystals of pharmaceutical compounds can be helpful for modeling processes which take place at production stages of solid drug forms.

An antidiabetic drug chlorpropamide is a well known model system for investigation of polymorphism in pharmaceuticals. Diversity of polymorphic modifications of chlorpropamide is due to flexibility of molecules of this compound in combination with different types of packing in a crystal structure. Five polymorphs of chlorpropamide (α, β, γ, δ and ε) can be obtained without any transformations at ambient conditions. Low temperature forms (ε/, β// and β///) also have been described.

In contrast to all other polymorphs with z-type packing a metastable β-form is the only one which has a unique π-type of hydrogen-bonded ribbon. This accounts for a very long shelf life of this polymorph at ambient conditions. The aim of the present work was to follow the effect of low temperature on the crystal structure of β-polymorph by Raman spectroscopy and single-crystal X-ray diffraction and to compare the results with the effect of cooling on α- and ε-polymorphs.

Samples of α- and β-polymorphs of chlorpropamide were prepared by slow cooling crystallization and characterized by X-ray powder diffraction (D8 GADDS of Bruker AXS) and differential scanning calorimetry (DSC-204 Netzsch), in order to identify the corresponding crystalline form. The morphology of grown crystals was studied by scanning electron microscopy (TM-1000 HITACHI). Single crystals of α- and β-polymorphs suitable for X-ray and Raman-spectroscopy experiments were selected from the grown batches and had no visible imperfections when observed using polarized optical microscope.

A low temperature single-crystal X-ray diffraction study was carried out using an Oxford Diffraction KM-4 diffractometer and a low temperature Oxford Instruments Cryojet device. The crystal was cooled from ambient temperature down to 20 K.

The polarized single-crystal Raman spectra were collected using a LabRAM Horiba single spectrometer with a charge-coupled device (CCD) detector (Symphony). A liquid helium ST-500 Microscopy Cryostat was used for recording the low-temperature spectra. The crystals of α- and β-polymorphs were wrapped in indium foil for better thermal contact, keeping an open field at the upper surface accessible for light, and were fixed on a cold finger of the cryostat.

A low-temperature phase transition was observed in different temperature ranges by Raman-spectroscopy (60 - 80 K) and by single-crystal X-ray diffraction (125 - 150 K), probably because of kinetic effects. The structure of the low-temperature polymorph was refined at several temperatures down to 20 K.

Spin dynamics of hematite

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It has been proven through experiments, theoretical work and simulations, that superparamagnetic (SPM) relaxation occurs in ferromagnetic nanoparticle systems, and that the relaxation time follows the Arrhenius-like Néel-Brown law. Nanoparticles of hematite, which has a canted anti-ferromagnetic (AFM) structure, have been investigated through several experiments, indicating, but giving no conclusive proof, that the Néel-Brown law is also valid for AFM systems.

In this work we have shown by simulation of Langevin dynamics that hematite nanoparticles perform antiferromagnetic SPM relaxation and that it follows the Néel-Brown law.

Inelastic time-of-flight and backscattering neutron measurements on hematite nanoparticles are analyzed, and, making use of the good energy resolution of the backscattering method, the SPM broadening of the elastic line is shown with great precision to follow the Néel--Brown law, in accordance with our simulations. Values for the energy barrier, KV/k_B, are found for both 8 nm and 15 nm diameter particles.

Mesoporous hematite has been analyzed and compared to the nanoparticles. In the backscattering experiment, little to no sign of SPM behavior has been found in these particles. However, in the time-of-flight experiment, a considerable broadening of the elastic line is shown to be well described by a SPM broadening and a quantized low frequency mode as seen in the nanoparticles.

Finally, detailed information about the incoherent signal seen in previous work is obtained, leading to the discovery of a new broad Lorentzian shaped signal that is related to the magnetism of the samples.

Investigating water mobility in ash-modified concrete using neutrons

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In recent years, the research related to agricultural wastes, aiming to evaluate their potential for recycling as well as the elimination of the landfills, increased dramatically.

This project focuses on the use of quasi-elastic neutron scattering (QENS) experiments to determine the role of water in mature concrete produced using different Brazilian sugar cane bagasse ashes from the co-generation industry. These ashes are recognized as having pozzolanic properties, and can therefore be used as alternative supplementary cementitious materials for concrete production. The durability of concrete is related to its ability to limit fluid transmission and knowledge of how to reduce the water mobility is critical to improving durability. QENS is a unique technique for such investigation as it probes both dynamic and geometric aspects of the protons motions in very short time scale.

In this talk I will present results obtained from our experiments at the IRIS facility in England. These results clearly show differences in the water hydration states observed in concrete made using standard Oregon Portland Cement (OPC) and concrete made using ash-modified cement.

Peak broadening effects from nanocrystallite material: modeling of average shape

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Crystallite shape in powder samples has a pronounced effect on X-Ray diffraction maxima. Broadening of diffraction peaks is inversely proportional to crystallite size, and materials with nanoparticle size cause substantial broadening of the maxima [1]. In the case of anisotropic crystallite shape the broadening is diffraction-vector dependent. In order to correct for this effect in Rietveld refinement, the quadratic formalism can be used. When applied correctly this formalism results in more reliable crystal structure parameters and at the same time physically realistic average dimensions of crystallites and their crystallographic orientation [2]. The method has been demonstrated on patterns of nanosized materials by full pattern fitting and confirmed by electron microscopy [3].

Here we will show that the formalism also works very well in combination with LeBail fitting. This turns out to be important in cases where the precise atomic structure of the material is not known. Determination of crystallite size and morphology of industrially important materials such as boehmite and zeolites will be presented.

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Revealing the dynamics leading to molecular self-diffusion by neutron scattering and MD simulations

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It is obvious that different dynamics in a molecular system occur at different time scales. Eventually all short-time motions lead to molecular self-diffusion. The understanding of the processes leading to molecular self-diffusion is essential for the description of transport mechanism in molecular liquids.

In order to probe the motions on a molecular length scale and in the pico- to nanosecond time regime, time-of-flight quasielastic neutron scattering (TOF-QENS) experiments were performed on various n-alkanes. As a second method, Molecular Dynamics (MD) simulations were carried out, allowing to identify the motions which were observed by TOF-QENS. The simulated dynamics perfectly agree with the measured spectra.

By these methods we were able to show that for the short molecule hexadecane all major processes leading to molecular self-diffusion are already taking place at times up to 1 ns. Here mainly rotations of the bonds and rotation of the entire molecules characterize the observed dynamics. For longer chains the global dynamics of the molecules emerge from the time window accessible by TOF-QENS. This allows to get an deeper insight on the short-time intra-molecular dynamics, which are responsible for any large-scale global motions.

Neutron Scattering characterization of the polymer network and hydration water in pHEMA hydrogels

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Poly(2-hydroxyethyl methacrylate) (PHEMA) hydrogels are biocompatible systems widely used in biomedical applications such as contact lenses, drug delivery, burned patients treatments, artificial tissues, ect.

Understanding the dynamics of the hydrogel components at the molecular level is fundamental for controlled release technology.
In this work, we have studied chemical and physical hydrogels in the hydration range 20-40% w/w and in the temperature range 270-300K.

Quasi Elastic Neutron Scattering (QENS) and Small Angle Neutron Scattering (SANS) techniques have been used on deuterated hydrogels to investigate the dynamical and structural properties of the polymer network. Moreover, QENS on fully hydrogenated systems and Differential Scanning Calorimetry have been preformed to highlight the confining effect of the hydrogel matrix on the water molecules. The effect of the cross-linker nature on the hydrogel properties will be detailed.

Heterogeneous and anysotropic dynamics of a 2D gel

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We report X-ray Photon Correlation Spectroscopy (XPCS) results on bi-dimensional (2D) gels formed by a Langmuir monolayer of gold nanoparticles.

We report X-ray Photon Correlation Spectroscopy (XPCS) results on bi-dimensional (2D) gels formed by a Langmuir monolayer of gold nanoparticles. The system allows an experimental determination of the fourth order time correlation function which is compared to the usual second order correlation functions and to the mechanical response measured on macroscopic scale. The observed dynamics is anisotropic, heterogeneous and super-diffusive on the nanoscale. Different time scales, associated with fast heterogeneous dynamics inside 2D cages and slower motion of larger parts of the film, can be identified from the correlation functions. The results are discussed in view of other experimental results and models of three-dimensional gel dynamics.

Dynamic motions and phase transitions of perovskite formate frameworks $[(CH_3)_2NH_2][M(HCOO)_3]$

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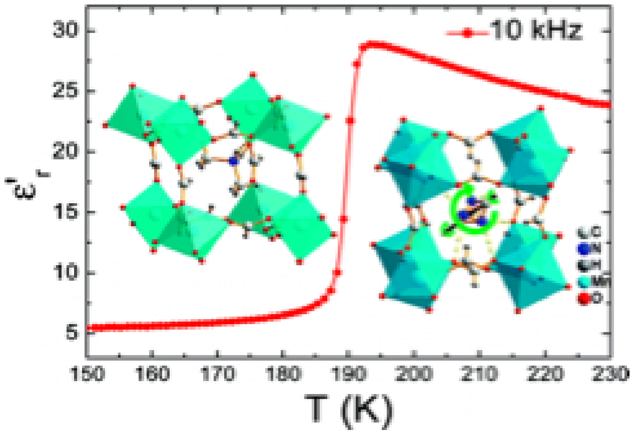
The nanoporous metal-organic frameworks (MOFs), crystalline hybrid materials which combine inorganic and organic components and that contain cavities and channels, have been extensively studied in the past decade in view of their interesting applications, for example, in catalysis and gas storage[1]. The dense hybrid frameworks, a subgroup inside the MOFs family, are receiving increasing attention as they can display a rising number of functional properties[2].



An example is the recently discovered family of MOFs $[(CH_3)_2NH_2][M(HCOO)_3]$ which crystallize in the perovskite architecture (ABX_3) (Fig.) and display weak ferromagnetism [3], dielectric properties [4] and even multiferroic behavior [5]. In that structure the formate ion $HCOO^-$ occupies the X site, the dimethylammonium cation $(CH_3)_2NH_2^+$ the A site, while different divalent cations can occupy the B site. These compounds show a dielectric transition, associated with a structural phase transition, in the 160-190 K temperature range for M = Mn^{2+}, Fe^{2+}, Co^{2+}, Ni^{2+} and Zn^{2+} [4-5], and at 270 K for M = Mg^{2+} [6].

This dielectric transition seems to imply the freezing of the $(CH_3)_2NH_2^+$ cation inside the cavity (fig.) in an order-disorder mechanism [7-8]. The dynamic behaviour of the $(CH_3)_2NH_2^+$ cation has been characterized by NMR spectroscopy (M=Zn) [7], DSC measurements (M=Co) [9] and Raman spectroscopy (M = Mn and Mg) [6,8]. However, the role of the hydrogen bond ordering between the $((CH_3)_2NH_2^+$ and the $HCOO^-$ and how it affects its dielectric properties remains to be solved. The low temperature structure of one member of the family (M=Zn), is also unknown. Neutron diffraction and molecular dynamics simulations will bring light to these questions.

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Data management and software centre: catering for science at ess

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The European Spallation Source's Data Management and Software Centre (DMSC) will be responsible for all IT used by scientists performing experiments at ESS. The DMSC will therefore have a pivotal role in how efficient these experiments are performed and considering the cost of ESS, we perceive the mission of DMSC to be to: *maximise the scientific outcome from ESS, through IT.*

To fulfil the mission, the DMSC needs to support the scientist, not only during the experiment but also prior to and after the experiment. This will ensure that allocated beam time is used on valuable data acquisition and will optimize the scientific impact from acquired data. Thus, we need to cater for the scientist from *idea* to *publication* with proper software and face-to-face support as illustrated in Figure 1 below.

Figure 1. The steps faced by a scientist at ESS from obtaining an idea to making a publication. The right hand column lists software involved for each step and the owls illustrate local support from DMSC and other ESS staff.

We propose that DMSC engages in cooperation with other neutron facilities, synchrotrons, and on-going software projects to avoid duplicating existing development efforts unnecessarily. This will not only save cost but also promote standardised software solutions as well as a common *look & feel* across different facilities for the benefit of their users. Some cross-facility frameworks that we are considering are MANTID (www.mantidproject.org) and ICAT (www.icatproject.org).

While excellent control software and data reduction tools are indispensible, the user community has also shown a strong interest for post-experiment support in the form of theory and scientific computing such as atomic-scale simulations. This support will help increase the likelihood of scientists using ESS producing high-impact publications. We therefore feel that it is important for DMSC to investigate how it can best provide such post-experiment support.

With this presentation we encourage the neutron community and future users of ESS to provide comments, suggestions, requirements and ideas with regard to DMSC, and to share good and bad experiences with respect to software related to neutron scattering.

Study of dynamic properties of water methanol solutions with quasielastic neutron scattering experiment and molecular dynamics calculations

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Water plays a fundamental role in life and in many technological applications. The water molecule has a rather simple structure, which translate in many chemical and physical peculiar properties though. We focus our attention on the hydrofobic effect, i.e. the characteristic repulsive behaviour of water molecules when in contact with apolar groups, e.g. from hydrophobic or amphiphilic molecules.

Within this framework, we investigated how the presence of solute moieties in aqueous solutions affect the picoseconds time scale of molecule self-diffusion. To better understand this phenomenon, we studied the mixture of water and a simple amphiphilic system, the methanol, by means of a combined experimental and computational efforts.

The quasielastic neutron scattering experimental data were collect at the ILL-IN5 beam-line, in a time of flight (TOF) geometry at 300K, at different concentration $(CH_3OH)_x:(H_2O)_{1-x}$, $(0<x<1)$. The molecular dynamic simulations were performed at the ILL-IT facility using the OPLS-AA force field [1] for methanol and the TIP4P/2005 [2] for water. The simulations lasted 200 ps and included 1000 molecules at all concentrations.

We present a preliminary elaboration of our data, using a model free analysis to understand the dynamic behavior of water solution. We focus our attention on the diffusion quantities from a microscopic point of view, following the procedure already discussed for pure water [3].

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Remanent magnetisation in natural nano-structured hemo-ilmenite

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Rocks of ilmenite ($FeTiO_3$) with nano sized hematite (Fe_2O_3) exsolution lamellae (hemo-ilmenite) are responsible for strong magnetic anomalies[1] caused by natural remanent magnetization (NRM) even though hematite is antiferromagnetic and ilmenite is paramagnetic (above ~60 K). The magnetic properties of hemo-ilmenite have been investigated with the use of polarised neutron diffraction experiments performed at the IN12 instrument at ILL, Grenoble.

Previous experiments (2) suggest that the NRM cannot be explained entirely by canting of the antiferromagnetic (CAFM) moments, and that spins in the contact layer between lamellae and bulk may also contribute.

Our main result comes from the measurements of the (003) magnetic hematite peak. At close to zero external field, the spins start out an an average angle of 45 degrees with respect an applied external field. We show that as the field strength is increased the spins turns away from the field. Within our measured field strength range, the spin direction seem to saturate at an angle of approximately 55 degrees and the magnitude of the field necessary for this saturation is around 2 T to 2.5 T. Since the spins align neither parallel nor perpendicular to the external field, the explanation for the NRM is seemingly a combinations of several contributions.

This work was done in collaboration with:
Brok, Erik (Department of Physics, Technical University of Denmark, Center for Electron Nanoscopy, Technical University of Denmark); Lefmann, Kim (NBI, European Spallation Source, Lund, Sweden); Kuhn, Luise Theil (Risø National Laboratory for Sustainable Energy, Technical University of Denmark); Harrison, Richard J (Department of Earth Science, University of Cambridge, United Kingdom); Dewhurst, Charles (Institut Laue-Langevin, Grenoble, France); Schmidt, Wolfgang F (Institut Laue-Langevin, Grenoble, France, JCNS, Forschungszentrum Jülich, Germany); Robinson, Peter (Geological Survey of Norway); McEnroe, Suzanne (Geological Survey of Norway).

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Ripening of ZnO nanoparticles

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ZnO semiconductor nanoparticles (NPs) exhibit promising electro-optical properties for applications in e.g. solar cells or light emitting devices due to the quantum size effect. Thus, the preparation of well-defined, stable ZnO-NPs is of high interest and therefore knowledge about the nucleation and growth processes is crucial.

The synthesis is carried out in ethanol using equimolar solutions of zincacetate and lithiumhydroxide which are simply mixed. The nucleation of the NP occurs instantly, while a further ripening of the ZnO-NPs starting from about 2 nm as a function of temperature can be observed using UV/Vis measurements or transmission electron microscopy (TEM). Cooling to -10°C immediately after the synthesis results in stable particle sizes for months, while at a temperature of 40°C ripening to sizes of 6 nm was observed at a timescale of several hours.

This ripening process is investigated using temperature and time-dependent SAXS measurements. Using a core-shell model including an acetate-layer around the ZnO-NPs the X-ray data could be well described. The acetate-layer obviously acts as stabilizer for the NPs, which was confirmed by experiments in which the NPs were washed. With increasing number of washing steps the stability of the dispersion is decreased. To further investigate the influence of the acetate on the NP growth and ripening time-resolved SANS measurements will be carried out.

The role of functional groups in understanding tunneling effects in paracetamol polymorphs

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The elucidation of the structure-property relation is particularly important for pharmaceuticals, which are prone to polymorphism – i.e. the same molecule can crystallise in different 3D-structures. Paracetamol, widely used as an analgesic and antipyretic drug, is one of the most extensively studied examples. It is a typical representative of organic drug substances composed of aromatic functional molecules.

The marketed phase crystallises in the monoclinic form (form I) space group $P2_1/a$ [1]. In form I the molecular layers are corrugated and thus do not slip easily over each other. On the other hand, in the orthorhombic phase (form II), space group Pcab [2], the layers are relatively planar and can thus slip over each other relatively easy.

Tunnelling and librational excitations for the methyl group was reported for monoclinic paracetamol using backscattering neutron scattering [3]. However, very little is known about paracetamol crystallizing in the orthorhombic phase and methacetine.

Here we report on tunneling results in both paracetamol forms obtained using using the backscattering spectrometer IN16 located at the ILL.

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Where do we need virtual experiments in neutron scattering?

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The use of Monte-Carlo raytracing simulations in neutron scattering has exploded within the last decade and an emerging science of virtual experiments has surfaced. The accuracy of the virtual experiments however relies heavily on the sample description wherefore accurate modelling of a wide range of sample systems with parameters that can be used in neutron raytracing Monte Carlo code is called for.

Simulation is in general an agile and solid tool to visualise theory and connect it to experimental observations. The use of Monte-Carlo raytracing simulations in neutron scattering has exploded within the last decade and an emerging science of virtual experiments has surfaced [1].

Virtual experiments (VE) of neutron scattering can be used for a multitude of purposes including teaching, experimental planning and data analysis. In teaching the VE prepare the students for practicals both in terms of instrumentation, sample scattering characteristics and data analysis [2]. In experimental planning the optimal instrument setting can be investigated and measuring time estimated [3]. In data analysis VE can be used test analysis algorithms for data from instruments that are not yet built. Detailed VE can also be used in connection with analysis of measured data to identify e.g. finite size broadening via resolution and sample parameter analysis [3] and to analyse scattering contributions from sample and environment [4]. The accuracy of the VE however relies on the accuracy of the sample description wherefore precise modelling of a wide range of virtual samples is called for. The models should be decribed by parameters which are useful in neutron raytracing Monte Carlo codes, such as McStas [5].

We envision the use of VE as a key tool for large scale neutron facilities, such as the ESS. An online VE suite of instruments and samples could both be used as an integrated part of beam-time application and planning for instrument scientist and users as well as training of users and data analysis of their results.

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Apical oxygen bonding in YBCO investigated by RMC refinement

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YBa_2Cu3O_{7-x} (YBCO) is arguably the canonical high temperature superconductor, and has been extensively studied since it was first reported in 1987 [1]. Despite this, a consensus has not been reached on the mechanism of superconductivity in the cuprates, though many theories have been proposed. The possible role of structural inhomogeneities remains contentious. You would expect local structure probes such as EXAFS and PDF techniques to be sensitive to any lattice distortions, however previous results have sometimes appeared irreconcilable with average structure models.

In this study neutron total scattering data from a powder sample collected at 50K on the GEM diffractometer at ISIS have been used to perform reverse Monte Carlo (RMC) refinements using the program RMCProfile [2]. These refinements produce large box atomic configurations consistent with both local and average structure data. Our results focus on the Cu-apical oxygen bond length, implicated in charge transfer mechanisms. We find a bimodal distribution, in agreement with previous EXAFS [3] and PDF [4] studies. We show how this can be reconciled with the standard average structure model. The effects of data resolution are also discussed.

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Second Annual Niels Bohr International Academy Workshop on Neutron Science

Bridging Elastic and Inelastic Scattering by Means of Computational Studies and Analysis

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