





UNIVERSITY OF
COPENHAGEN

# NBIA7

Niels Bohr International Academy, Copenhagen, June 25 - 29 2018

*7th Annual Niels Bohr International Academy Workshop-School on ESS Science: Deciphering the hidden dynamics of Soft Matter*

**Organizers: Heloisa N. Bordallo, Juergen Eckert and Kenneth Dahl Knudsen.**

**Local Support: Margerie Pouteau, Johann Raillard, Mattias Sauzon and Gitte Michelsen.**

# Introduction and speakers

## Introduction

An optimal extraction of molecular level information contained in experimental data of soft matter systems depends heavily on the use of advanced data analysis and modeling for its interpretation. A close collaboration between experimentalists and theoreticians as well as the application of complementary experimental techniques is crucial in this process. This school will accordingly offer a series of lectures on ways in which Inelastic Neutron Scattering (INS), Nuclear Magnetic Resonance (NMR), Molecular Dynamics (MD) and other theoretical modeling methods can be combined to extract unique information on the dynamical behavior of a variety of soft matter systems.

## Speakers

**Christiane Alba-Simionesco - LLB, France**

**Ana R. Benetti - University of Copenhagen, Denmark**

**Gerd Buntkowsky - Technische Universität Darmstadt, Germany**

**Juan Colmenero - Materials Physics Center (CSIC-UPV/EHU), Spain**

**Juergen Eckert - Texas Tech University, USA**

**Félix Jimenez-Villacorta - ESS Bilbao, Spain**

**Sergey Kapishnikov - Niels Bohr Institute, Denmark**

**Gerald Kneller - Centre de Biophysique Moléculaire - CNRS, France**

**Maria Paula Marques - University of Coimbra, Portugal**

**Murillo L. Martins - Pontifical Catholic University of Goiás, Brazil**

**Tommy Nylander - Lund University, Sweden**

**Loukas Petridis - ORNL, USA**

**Edina Rosta, King's College, UK**

**Felix Roosen-Runge - Lund University, Sweden**

**Andreas Schreyer - European Spallation Source ERIC, Sweden**

**Mark Telling - University of Oxford and ISIS Neutron and Muon Facility, UK**

**Emanuella Zaccarelli - CNR Institute of Complex Systems, Italy**

## Access

The main door of Building C will be unlocked from 8:30 to 9:15 each day of the workshop. The reception in Building A, which is to the right, is unlocked.

## Lectures , Tutorials, Posters & Coffee breaks

All lectures will be held in Auditorium A of Building C at the Niels Bohr Institute (Blegdamsvej 17 - 2100 København Ø). Please try to be respectful and do not use your computers during the lectures.

The practical exercises on Monday, Tuesday and Wednesday will take place in rooms **BK-2 (MD-tutorials**) and **Auditorium A (QENS-tutorial)**.

All posters will be exposed in Auditorium C. Coffee breaks will be served by the posters.

## Lunch

Lunches are provided free of charge to the registered participants at the NBI canteen. You will find an envelop with lunch tickets on your folder. These tickets are to be handled at the canteen before each meal. If you want a soft drink, you can purchase it.

## Work space

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

## Wireless connectivity

The local networks are Eduroam and KUGuest network.

If you need to use the KUGuest network, you will be guided by the website in how to get access.

## Round Table with ESS Scientists

It will take place on Wednesday, 27 of June (14:00 – 16:00) in room **HB1.** This parallel session is aimed as a brainstorming meeting between the invited speakers and ESS scientists.

## Social Program

Tuesday, 26 of June: A dinner will be organized for the invited speakers (expenses not covered).

Thursday, 28 of June: Guided tour at the Danish Design Museum (https://designmuseum.dk/en/). We meet at the entrance at 13:45 (**sharp**). After the visit, we will all be taken by bus to Dragør (https://www.visitdenmark.com/denmark/day-trip-dragor-gdk917384). There will be time to visit this nice village before gathering for dinner at 18:00 at Restaurant Beghuset (https://www.beghuset.com).

**Attention!!!** Computers and personal belongs have unfortunately been stolen from the Institute. **Please never leave your bag and/or computer unattended.**

| Final Program | | |
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| *(1) All participants can take part on the lectures, only the students (20) will take part on the hands on exercises.*<br>*(2) Problem solving sessions are scheduled on Monday, Tuesday and Wednesday. These sessions will be supervised.* The results are presented on Thursday.<br>*(3) "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.* | | |
| *Time* | *Lecturer* | *Topic* |
| *Monday, 1st day* | | |
| 8:45 am – 9:15 am | Registration | |
| 9:15 am – 9:30 am | Poul Henrik Damgaard (Niels Bohr International Academy, Denmark) | *Welcome* |
| 9:30 am-10:15 am | Juan Colmenero (Materials Physics Center (CSIC-UPV/EHU, Spain) | Polymers, neutrons & computers: a guided tour through the relaxation map of polymers |
| 10:15 am-10:45 am | Coffee break | |
| 10:45 am-11:30 am | Gerd Buntkowsky (Technische Universität Darmstadt, Germany) | Studying Soft-Matter-Dynamics with Solid State NMR Spectroscopy |
| 11:30-12:00 | Maria Paula Marques (University of Coimbra, Portugal) | Shining the Beam on Cells – In Search of Improved Anticancer Drugs |
| 12:15 pm-1:30 pm | Lunch | |
| 1:30 pm-2:15 pm | Mark Telling (ISIS Facility, UK) | Macromolecular dynamics: what can high energy resolution neutron spectroscopy tell us? |
| 2:15 pm-3:00 pm | Loukas Petridis (ORNL, USA) | Molecular Simulation in Bioenergy |

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| 3:00 pm-3:30 pm | Coffee Break | |
| 3:30 pm-5:00 pm | Students divided in two groups | *QENS tutorial exercises: data analysis & MD* |
| *Tuesday, 2nd day* | | |
| 9:00 am-9:45 am | Clip presentation from the students | *Students give a 3 minutes presentation on their work* |
| 9:45 am-10:30 am | Gerald Kneller (Centre de Biophysique Moléculaire, France) | New perspectives for interpreting quasielastic neutron scattering spectra |
| 10:30 am-11:00 am | Coffee break | |
| 11:00 am-11:45 am | Edina Rosta (Department of Chemistry, King's College London, UK) | Molecular Simulations of Enzyme Catalysis |
| 11:45-12:30 | Juergen Eckert (Texas Tech, USA) | This (peak) must be a C-C-OH deformation, or is it"? Vibrational Spectroscopy has come of age thanks to computation |
| 12:30 pm-2:00 pm | Lunch | |
| 2:00 pm-5:00 pm | Students divided in two groups | Students chose project, hands on, data analysis, etc |
| 6:30 pm-8:30 pm | Dinner for the invited speakers | |
| *Wednesday, 3rd day* | | |
| 9:00 am-9:45 am | Tommy Nylander (Lund University, Sweden) | The structure of lipid assemblies in bulk and at interfaces revealed by neutrons and X-rays |
| 9:45 am-10:30 am | Murillo L. Martins (Pontifical Catholic University of Goiás, Brazil) | Using neutron scattering on medical research |

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| 10:30 am – 11:00 am | Coffee Break | |
| 11:00 am – 12:00 pm | Andreas Schreyer (ESS, Sweden) | ESS Science: Opportunities & Ideas |
| 12:00 pm -12:30 pm | Félix Jimenez-Villacorta (ESS-Bilbao, Spain) | MIRACLES – The time-of-flight backscattering spectrometer at the European Spallation Source |
| 12:30 pm-2:00 pm | Lunch | |
| 2:00 – 4:00 | Student Working Groups & Round table discussions | |
| 4:00 – 6:00 pm | Posters & Snacks | |
| *Thursday, 4th day* | | |
| 9:00 am-9:45 am | Emanuella Zaccarelli (Sapienza Università di Roma and CNR Institute of Complex Systems, Italy) | Slow dynamics in soft matter: insights from computer simulations |
| 9:45 am-10:15 am | Felix Roosen-Runge (Lund University, Sweden) | Analytical modeling of complex and hierarchical dynamics |
| 10:15 am-11:00am | Posters & Coffee break | |
| 11:00am – 12:00 pm | 2 Groups of Students (30 minutes each group) | Student presentations on their results |
| 12:15 pm-1:00 pm | Lunch | |
| 2:00 pm – | Guided to tour: https://designmuseum.dk/en/ Conference dinner at https://www.beghuset.com | |
| *Friday, last day* | | |
| 9:00 am-9:45 am | Sergey Kapishnikov (Copenhagen University, Denmark) | Multiple correlative X-ray microscopy study of the malaria parasites in human red |

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| | | blood cells |
| 9:45 am-10:30 am | Ana R. Benetti (University of Copenhagen, Denmark) | Neutrons combined to X-rays in Dentistry |
| 10:30 am – 11:00am | Posters & Coffee break | |
| 11:15 am – 12:00 pm | Christiane Alba-Simionesco (LLB, France) | Thermodynamics of glass forming liquids by neutron scattering |
| 12:00 pm-2:00 pm | Lunch and Good bye | |

# Invited talks

**Polymers, neutrons & computers:**

**A guided tour through the relaxation map of polymers**

Juan Colmenero

*University of the Basque Country (UPV/EHU), Spain*

Polymers are condensed matter systems where the structural units are macromolecules – giant molecules built up by repetition of more or less simple chemical motifs called monomers. Due to their macromolecular character, the structural and dynamical properties of polymer systems strongly depend on a hierarchy of length and time scales. While at short and intermolecular length scales polymer melts display the 'universal' dynamical properties of glass-forming systems in general, at large length scales (of the order of the radius of gyration of the macromolecules) polymers exhibit unique dynamic properties related to the chain-like conformation of their structural units. The characteristic times of these dynamic processes spread out over a huge dynamic range (the so-called 'relaxation map') covering more than 12 orders in magnitude of time/frequency. Investigating these dynamic processes and identifying their interplay is not an easy task that usually demands for the combination of different techniques. Moreover, increasing the complexity of the system (e.g., by considering different macromolecular architectures, complex monomers, polymer blends, etc.) we may find profound modifications of the features observed in simple polymers or even novel properties can emerge. Over last years, the combination of neutron scattering techniques -together with selective deuteration - and molecular dynamic simulation methods has proved to be a highly successful strategy for characterizing and unraveling dynamic processes in polymer systems. In this talk we propose a guided tour through the relaxation map of polymer systems, showing examples of different complexity of this strategy.

**Studying Soft Matter-Dynamics with Solid State NMR Spectroscopy**

Gerd Buntkowsky

*TU Darmstadt, Germany*

Solid-state NMR spectroscopy (ssNMR), in particular when combined with molecular dynamics (MD) simulations provides a unique access to the details of dynamic processes in soft condensed matter. While deuteron-NMR spectroscopy reveals detailed information about reorientation dynamics of molecules or molecular groups, dipolar interactions give structural information about intermolecular arrangements and their changes. The lecture first presents a short tutorial on ssNMR tools for the investigation of dynamic processes and then discusses a number of examples taken from our resent work, employing multinuclear variable temperature solid-state NMR spectroscopy and dynamic nuclear polarization (DNP) enhanced $^{1}H$-$^{13}C$ solid-state NMR spectroscopy to illustrate the application of these tools.

**Shining the Beam on Cells – In Search of Improved Anticancer Drugs**

M.P.M. Marques[1,2], A.L.M. Batista de Carvalho[1], V. Garcia-Sakai[3] and L.A.E. Batista de Carvalho[1]

[1]*R&D Group "Molecular Physical-Chemistry", Univ. Coimbra, Portugal*

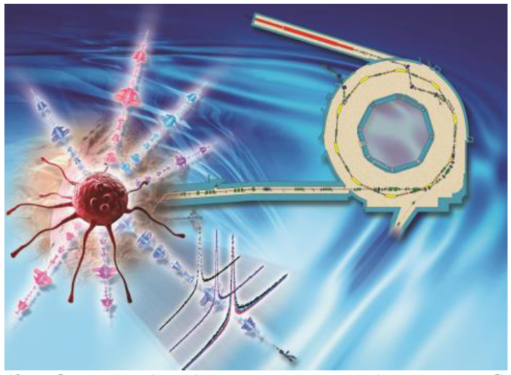
[2]*Dep. Life Sciences, Univ. Coimbra, Portugal*

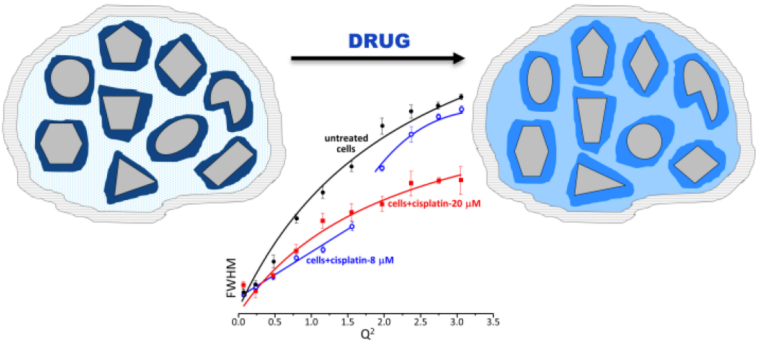
[3]*ISIS Facility, STFC Rutherford Appleton Laboratory, Chilton, Didcot, UK*

Development of new anticancer agents against metastatic breast carcinoma is of paramount importance, since this is the second most common type of cancer worldwide and the most frequent among women, with a very poor survival rate. Particular attention has been paid to new generation cisplatin-like polynuclear Pt(II) and Pd(II) chelates with alkylpolyamines, namely $Pt_2Spm$ and $Pd_2Spm$ (Spm=$H_2N(CH_2)_3NH(CH_2)4NH(CH_2)_3NH_2$). Some of these compounds show promising results towards triple-negative breast carcinoma, leading to more severe and less repairable DNA damage (formation of long-range interstrand drug-DNA adducts) than the clinically used platinum agents (*e.g.* cisplatin, *cis*-$(NH_3)2PtCl_2$).

Inelastic and quasi-elastic neutron scattering (INS and QENS) spectroscopy, coupled to complementary optical vibrational methods, have been used to develop novel Pt- and Pd-based anticancer agents. The first neutron scattering study of whole human cells (MDA-MB-231 triple-negative human breast cancer) is reported which addresses the subject of solvent-slaving to a drug by probing intracellular water, with a view to ascertain structural and dynamical variations upon drug exposure. This work is based on the assumption that the behaviour of cytoplasmic water determines the conformation and function of biomolecules, and hence cellular viability. This is an innovative way of tackling a drug´s pharmacodynamics, searching for alternative targets of drug action (apart from DNA), in order to improve chemotherapeutic efficiency.

Concentration-dependent dynamical changes evidencing a progressive reduction in mobility were unveiled for drug-exposed samples, concurrent with variations in the native organisation of water molecules within the intracellular medium [*PCCP* 19 (2017) 2702]. This constitutes the first experimental evidence of a drug´s impact on the cytomatrix by neutron techniques, and will hopefully lead to a better understanding of the *in vivo* mode of action of this type of metal-based antitumour compounds, at a molecular level. We hope that this will help the design of improved chemotherapeutic agents with optimised efficacy and minimal acquired resistance and deleterious side-effects.






(from [*PCCP* 19 (2017) 2702. DOI: 10.1039/C6CP05198G])

*Acknowledgements: Portuguese FCT – UID/MULTI/00070/2013 and PTDC/QEQ-MED/1890/2014 (within Project 3599 – to Promote Scientific Production and Technological Development as well as the formation of thematic networks (3599-PPCDT) –jointly financed by the European Community Fund FEDER). The STFC Rutherford Appleton Laboratory (UK) is acknowledged for access to neutron beam facilities.*

**Macromolecular dynamics:**

**what can high energy resolution neutron spectroscopy tell us?**

Mark Telling

*STFC Rutherford Appleton Laboratory, Chilton, Didcot, UK*

Neutron scattering has helped underpin our understanding of macromolecular phenomena by enabling researchers to answer two fundamental questions: 'where atoms are' and 'what atoms do'. Answers to such elemental queries are possible because neutron sources produce particles whose wavelengths not only span inter-atomic spacings, but also whose energies are comparable to the vibrational modes and diffusive motions of the molecular components. Moreover, the neutron is a highly penetrating, weakly perturbing, yet non-destructive, charming probe and the complementarity between neutron scattering and other experimental methods help expand the spatial and temporal view of many soft matter topics. However, for highly complex, multi-component systems it is the ability to selectively 'label', or mask, different molecular species using deuterium that sets neutron scattering apart; deuterium labeling allowing, where possible, researchers to ask specific questions.

Considering macromolecular motion, high energy resolution neutron spectroscopy affords access to a spatial and temporal scale that ideally matches the atomic and molecular vibrational displacements, jump distances and correlation lengths encountered in such systems. This particular spectroscopic regime, referred to as Quasi-Elastic Neutron Scattering (QENS) [1-4], is sensitive to the re-organization of atoms and molecules on a pico-second (ps) to nano-second (ns) time scale, and over length scales from 1 to ~500 Angstrom (Å); length scales covering both inter and intra molecular distances.

In this talk, the basic principles of the quasi-elastic neutron scattering method, pertinent to the study of dynamic processes in macromolecular materials, will be presented. An overview of the neutron instrumentation required for such studies will be given as will experimental results which highlight the spectroscopic information accessible using such an experimental technique.

[1] M. Bée, "Quasi-elastic Neutron Scattering Principles and Application", Adam Hilger (1988)

[2] J. Fitter et al (Eds.), "Neutron Scattering in Biology", Spinger (2006)

[3] J.S. Higgins et al, Polymers and Neutron Scattering, Clarendon Press, (1996)

[4] M.T.F. Telling, "QENS: A Tool for the Study of Biological Molecules and Processes" in "Dynamics of Biological Macromolecules by Neutron Scattering" eds S. Magazù et al, 4 (2012) 18

**Molecular Simulation in Bioenergy**

Loukas Petridis

*ORNL, USA*

The conversion of plant cell-wall lignocellulosic biomass to chemicals for renewable bioenergy and other high-value uses requires overcoming the evolved recalcitrance of biomass to deconstruction. To increase yields biomass is commonly pretreated using physical and/or chemical methods. Recent experimental and computational work has led to significant progress in understanding the molecular-level driving forces governing the structure of native biomass and its deconstruction during pretreatment. The thermodynamics and kinetics determining the three- dimensional configurations and associations of the principal biopolymers involved - cellulose, lignin and hemicellulose - has been characterized. The energetic requirements for the effective fractionation of biomass into lignin and cellulose components for co-valorization have been determined. Of fundamental interest is the detailed understanding of the origin of the kinetic barriers leading to irreversibility of pretreatment processes. A pervading theme is solvation thermodynamics, which plays a critical role in determining biomass structure and susceptibility to breakdown, and provides a path to obtaining a predictive understanding of requirements for effective biomass pretreatment.

**New perspectives for interpreting quasielastic neutron scattering spectra**

Gerald Kneller[1,2,3]

[1]*Centre de Biophysique Moléculaire, CNRS, Orléans, France*

[2]*Synchroton SOLEIL, Saint Aubin, Gif-sur-Yvette CEDEX*

[3]*Université d'Orléans, Université d'Orléans, Orléans, France*

In this talk it is shown that quasielastic neutron scattering (QENS) experiments at moderate momentum transfers can be described by a "model-free" approach [1], which is based on the Gaussian approximation of the intermediate scattering function [2] and the asymptotic form of the quantum mean square displacement of the hydrogen atoms in the system. Both diffusive and quantum properties of dynamics of the hydrogen atoms are here accounted for with a few parameters. The second part of the talk is devoted to a new representation of neutron scattering functions in terms of neutron-induced transition probabilities between different levels of the protein energy spectrum [3]. The formalism is the momentum-space analogue of the Frank-Condon theory for vibronic transitions in molecules due to the absorption or emission of photons and emphasizes an energy landscape-oriented interpretation of neutron scattering experiments. It shows in particular that the dynamic structure factor of complex systems with a quasi-continuous distribution of energy levels can be given a truly probabilistic interpretation, which emphasizes a continuous transition from elastic to inelastic scattering.

[1] G. R. Kneller, *J Chem Phys* **145**, 044103 (2016).

[2] A. Rahman, K. S. Singwi, and A. Sjölander, *Phys. Rev.* **126**, 986 (1962).

[3] G. R. Kneller, manuscript under revision

**Molecular Simulations of Enzyme Catalysis**

Edina Rosta

*King's College London, UK*

The formation and cleavage of phosphate bonds is essential in most biological processes including nucleic acid processing. Many enzymes that catalyze phosphate hydrolysis require bound divalent metal ions. Most commonly, $Mg^{2+}$ ions are required for catalysis, while similar $Ca^{2+}$ ion abolishes the catalytic activity. To elucidate the poorly understood mechanism of these ubiquitous metal ion catalyzed reactions, we carry out hybrid quantum-classical QM/MM free energy simulations. In our calculations, we focus on specific systems, including Ribonuclease H (RNase H) [1] and dUTPase [2]. To gain a more general picture of the key requirements for $Mg^{2+}$ coordination, we also performed a PDB-wide analysis enumerating possible NTP hydrolysis enzyme crystal structures. Our results highlight key structural requirements for the $Mg^{2+}$ ion to serve as a "Mg-pinch" motif in phosphate catalysis over a wide range of enzymes.

[1] E. Rosta, W. Yang and G. Hummer, J. Am. Chem. Soc., Vol. 136, 3137, 2014

[2] (a) Lopata, A.; Jambrina, P. G.; Sharma, P. K.; Brooks, B. R.; Toth, J.; Vertessy, B. G.; Rosta, E., ACS Catalysis 2015, 5 (6), 3225-3237; (b) Nagy, G. N.; Suardíaz, R.; Lopata, A.; Ozohanics, O.; Vékey, K.; Brooks, B. R.; Leveles, I.; Tóth, J.; Vértessy, B. G.; Rosta, E., J. Am. Chem. Soc. 2016, 138 (45), 15035-15045.

**"This (peak) must be a C-C-OH deformation, or is it"?**

**Vibrational Spectroscopy has come of age thanks to computation**

Juergen Eckert

*Department of Chemistry and Biochemistry, Texas Tech University, USA*

Vibrational spectroscopy is, in principle, a very powerful experimental technique that can connect molecular vibrations, especially their amplitudes, with the potential energy surface (PES) given by the intra- and intermolecular interactions that define the PES. The traditional approach of "assignments" of peaks in a vibrational spectrum does this in a highly oversimplified manner. The missing link is a detailed description of these interactions, along with the methodology to compute vibrational spectra for comparison with observation. Neutrons and computers may be said to be a nearly ideal match since the simplicity of the interaction of neutrons with atomic nuclei in matter greatly facilitates computational modeling of neutron scattering experiments. These interactions are commonly described by force fields in large molecules for reasons of simplicity, or by 'ab-initio' DFT methods for smaller systems, and the dynamics typically by harmonic vibrational analysis, or MD simulations. Remarkable agreement between observed inelastic neutron scattering vibrational spectra and their calculation can be achieved, but the *caveat* remains, namely, "if you do not have the right model (or methodology) you cannot expect to get the right answer".

**The structure of lipid assemblies in bulk and at interfaces revealed by neutrons and X-rays**

Tommy Nylander

*Lund University, Sweden*

Biological membranes do not only occur as planar bilayer structures, but bilayers have also been shown to, depending on the lipid composition, curve into intriguing 3D structures. In fact the important role of curvature of lipid membranes has been increasingly recognized. Understanding biological implications of such curved lipid interfaces as well as exploiting their full potential in applications, for e.g. drug delivery and other biomedical applications, poses a challenge that requires the development of novel, well-defined and versatile model system.

In this talk, we will discuss how this can be achieved by using bulk dispersions as well as deposition of lipids from solution followed by hydration. The properties of the obtained nanostructured dispersions and the formed layer will be considered in terms of structure and dynamics as revealed by neutron and x-ray scattering techniques. We will show that non-lamellar liquid crystalline particles and surfaces layers of different phases can formed and will discuss on the implications for enclosing other functional molecules.

**Using neutron scattering on medical research**

Murillo Longo Martins

*Pontifical Catholic University of Goiás, Brazil*

This talk will focus on two applications of neutron scattering techniques on medical research. First, the characterization of a bio-nanocomposite to be used as a drug carrier for breast cancer will be discussed. Here, neutron scattering was combined to several state-of-the-art techniques to depict the properties of the composite itself as well as the behavior of an encapsulated anti-cancer drug [1]. The observed results are then discussed in combination with some of the biological properties of the material, for example, toxicity against healthy and cancer cells. Sequentially, I will discuss the application of neutron scattering on the characterization of water populations within breast cancer cells. Most importantly, I intend to show how the action of an anti-cancer drug may change the properties of cellular water and how this methodology can be combined to clinical procedures to predict the prognosis of a disease.

[1] M.L. Martins, R. Ignazzi, J. Eckert, B. Watts, R. Kaneno, W. F. Zambuzzi, L. Daemen, M. J. Saeki and H.N. Bordallo (2016) Restricted mobility of specific functional groups reduces anti- cancer drug activity in healthy cells. Sci. Rep. **6**, 22478.

**ESS Science: Opportunities & Ideas**

Andreas Schreyer

*European Spallation Source (ESS), Sweden*

The European Spallation Source (ESS), which is currently under construction in Lund, Sweden, is designed to push the limits of research with neutrons to new horizons. ESS will open up new scientific opportunities, which are complementary to those at X-ray sources. These will include unprecedented in-situ and in-operando experiments, which are only possible with neutrons due to their special properties.

After a short summary of the design and the specifications of the European Spallation Source an overview of the current status and schedule of the ESS construction project will be given with a strong focus on the instruments and the surrounding scientific infrastructure. The overall goal of ESS is to begin user operation in 2023/24 and ramp up to 15 instruments by 2026. Selected examples of new scientific opportunities in the field of materials and life science will be discussed.

**MIRACLES**

**The time-of-flight backscattering spectrometer at the European Spallation Source**

Félix Jimenez-Villacorta

*ESS-Bibao, Spain*

MIRACLES will be the time-of-flight backscattering spectrometer at the ESS. Neutron backscattering spectroscopy is a unique experimental technique to unambiguously access dynamics at the ns-ps time scale. Ideal to carry out studies on an extended list of topics, from soft matter (life sciences, polymers) to energy science (catalysis, fuel cells).

MIRACLES will have a broad energy bandwidth, $\hbar\omega$, of about ±500 μeV centered at the elastic line. Variations in energy of the incoming neutrons interacting with the samples will be analyzed using Si(111) crystals in near-backscattering geometry reflecting neutrons with energy $E_f$ =2.08 meV to the detectors area near the sample. Contributions from the primary (beamline) and secondary (backscattering system) spectrometers to the energy resolution are optimized to reach an elastic resolution, $\delta(\hbar\omega)$, around 2 μeV in the high-resolution mode. This energy resolution can be tuned and relaxed to achieve record values of flux, taking advantage of the excellent brilliance provided by the ESS source. The large observation time, large energy bandwidth, energy range and tuneable resolution offered by MIRACLES, will provide complete information using a single spectrometer.

**Slow dynamics in soft matter: insights from computer simulations**

Emanuella Zaccarelli

*CNR Institute for Complex Systems, Italy*

Dynamic arrest in soft matter systems manifests in a variety of arrested states, including gels, attractive and repulsive glasses. Usually, the approach to an arrested state happens through a two-step relaxation of the dynamic auto-correlation functions, where the microscopic, fast relaxation is separated from the structural, slow relaxation by an intermediate plateau often interpreted in terms of the so-called cage effect.

After discussing simulation results for typical colloidal glassy models, such as hard spheres, I will also discuss situations in which the standard two-step picture does not hold in soft matter systems. In this case, anomalous dynamics occurs, which is manifested by a logarithmic relaxation of the density auto-correlation functions and a sub-diffusive behavior of the mean-squared displacement. If time permits, I will also discuss other kinds of anomalous dynamics where the long-time relaxation becomes faster than exponential.

**Analytical modeling of complex and hierarchical dynamics**

Felix Roosen-Runge

*Lund University, Sweden*

Dynamics in soft matter systems occurs on a broad range of length and time scales, and encompasses a variety of dynamical processes. Given this complexity, linking experimental observables to underlying mechanisms in a reliable way is a central challenge for data analysis and interpretation.

In this talk, two central philosophies of data analysis are discussed – model fitting and model-free approaches. Although the presented methodology is motivated on neutron spectroscopy, many ingredients can also be transferred to other techniques.

First, model fitting builds upon physical reasoning and previous knowledge about the experimental system. An ideal model allows characterizing experimental data with few model parameters with a specific physical meaning. As a specific case, dynamics of proteins in solution are discussed. For protein solutions, the hierarchical structure – atoms, side-chains, backbone, macromolecule, aggregates – is reflected in a complex dynamical behavior ranging from global diffusion over interdomain and backbone motions to localized internal relaxations. Starting from the experimental observables, the essential model ingredients are identified [1,2,3] and common choices are reviewed. In this context, a novel method for the derivation of analytical correlation functions for complex and switching dynamics is presented [4], along with its potential for dynamics in complex soft matter systems.

Second, model-free approaches allow obtaining general information on the system dynamics without assuming a specific underlying process. As an example, the model-free access to the real atomic mean-squared displacement $\langle \Delta r^2 \rangle$ based on incoherent neutron spectroscopy is presented. In addition, the extension towards a model-free indicator for confined and anomalous diffusion is discussed [5].

[1] F Roosen-Runge, M Hennig, et al. Proc. Nat. Acad. Sci. USA 108 (2011) 11815-11820

[2] M Grimaldo, F Roosen-Runge, et al. Phys. Chem. Chem. Phys. 17 (2015) 4645-4655

[3] M Grimaldo, F Roosen-Runge, et al. EPJ Web of Conf. 83 (2015) 02005

[4] F Roosen-Runge, DJ Bicout, JL Barrat, J. Chem. Phys. 144 (2016) 204109

[5] F Roosen-Runge, T Seydel, EPJ Web of Conf. 83 (2015) 02015

**Multiple correlative X-ray microscopy study of the malaria parasites in human red blood cells**

Sergey Kapishnikov[1], *Leslie Leiserowitz[2] and Jens Als-Nielsen[1]*
[1]*Niels Bohr Institute, University of Copenhagen, Denmark*
[2]*Weizmann Institue of Science, Israel*

Alarming signs of the malaria parasite resistance to current drug treatments highlight the need for identification of efficient targets to improve present antimalarial therapies. Residing in a human red blood cell the malaria parasite consumes hemoglobin and digests it in an organelle called the digestive vacuole. Hemoglobin digestion liberates large quantities of heme. This iron-containing molecule is toxic to the parasite. The parasite detoxifies heme by turning it into inert hemozoin crystals. This waste-disposal mechanism is a promising drug target. How heme is crystallized remains uncertain, but current models predict very different rates of crystallization. To this end we have developed a unique correlative X-ray absorption cryo-tomography and X-ray fluorescence cryo-microscopy method that enables us to determine the distribution and concentration of chemical elements relative to the three-dimensional cellular structure of instantly frozen snapshots of the malaria parasites in red blood cells [1].

Our measurements of heme crystallization rate and our discovery of considerable amounts of hemoglobin in the digestive vacuole suggest an assembly line process of heme detoxification: heme monomers liberated from hemoglobin are dimerized via the heme detoxification protein (HDP) and the dimers crystallize into hemozoin [2]. According to this model, the rates of heme monomer release, heme dimerization and hemozoin formation must closely match. Thus, two targets for drug development become apparent: Inhibition of the creation of HDP, a subject of ongoing studies, and inhibition of hemozoin crystallization. Both targets will lead to accumulation of toxic heme monomers and self-poisoning of the parasite. Indeed, quinoline-family drugs are believed to act by targeting hemozoin crystallization. Specifically, molecular simulation studies predict that the drugs adsorb onto the surface of hemozoin crystals thereby inhibiting their growth [3,4]. To investigate this model, we used our X-ray cryo-microscopy method to quantitatively map the distribution of bromoquine, an analog of the classical chloroquine drug, within the malaria parasites. To avoid altering distribution of chemical elements due to sample preparation, the parasites were rapidly vitrified by cryo-freezing avoiding chemical fixation, staining, embedding or sectioning. Our results strongly support the predicted affinity of bromoquine to hemozoin crystals. Interestingly, we also detect accumulation of bromoquine at the nucleus of the parasite indicating an additional antimalarial activity. In conclusion, our correlative X-ray cryo-microscopy method establishes a new approach for the measurement of element-specific concentrations within intact cellular ultrastructure at high spatial resolutions of ~50 nm or better. This, in-turn, enables us to further investigate heme metabolism, antimalarial drug action and resistance in the malaria parasites.

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**Neutrons combined to X-rays in Dentistry**

Ana R. Benetti

*Department of Odontology, Faculty of Health and Medical Sciences, University of Copenhagen, Denmark*

Neutrons and X-rays combined are able to disclose important information during the investigation of dental materials and dentine. The water-based cements used in Dentistry offer a number of biologic advantages but have somewhat limited strength. By using X-rays, detailed structural information was gathered. Combined with neutrons, insight on proton mobility within the water-based cements was achieved [1]. By using different spectrometers covering distinct timescales, different proton populations were identified and the influence of free water on the strength of these materials was also assessed [2,3]. Neutrons were also used to investigate proton mobility within dentine, a dental hard tissue rich in organic content and water [4].

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**Thermodynamics of glass forming liquids by neutron scattering**

Christiane Alba-Simionesco

*Laboratoire Léon Brillouin (LLB), France*

The viscosity of liquids that can be supercooled below the first-order freezing transition increases greatly as temperature is lowered, and at some temperature $T_g$, the viscosity becomes too great to measure, *i.e.*, the liquid-like flow becomes too slow to measure, and below $T_g$ the substance is denoted a glass or amorphous solid. The complexity of the problem, which involves concomitantly Thermodynamics, Dynamics and Structure, is of current and likely future interest in the diverse areas of Soft Matter; it requires studies with multiple techniques over broad length and time scales. Elastic, Quasielastic and Inelastic Neutron Scattering experiments are providing THE observables that contribute to understand the phenomenon and its complexity; when combined with other methods such as Calorimetry, Dielectric and Mechanical spectroscopies, NMR, X-rays Scattering and Numerical Simulations, it makes a unique input for any theoretical approaches.

# Students contributions

**In silico modelling of microgel particles**

Fabrizio Camerin, Nicoletta Gnan, Lorenzo Rovigatti and Emanuela Zaccarelli

*Università di Roma La Sapienza, Italy*

In contrast to solid colloidal particles, microgels promptly respond to external stimuli such as the temperature and the pH of the solution. This peculiarity has been widely applied in bulk experiments, where the subsequent size changes can be used to tune the particle volume fraction with no change in its number density. Despite the plain experimental interest, theory stands behind, as models lack a comprehensive description in terms of the internal polymeric nature of the microgels, which is fundamental to describe correctly their elasticity and deformability, especially in high density states [1].

We are now able to provide novel theoretical insights in this respect, thanks to a cutting-edge model that reproduces in silico realistic PNIPAM microgels. Indeed, we reconstruct the polymer network via an ensemble of bi- and tetra-valent patchy particles, whose topology is subsequently fixed via a bead-spring model [2]. The computational protocol is validated, in the first place, by comparing the calculated form factors to the ones obtained via x-ray and neutron scattering experiments. Secondly, we verify that designed and experimental microgels with equal crosslinks ratio undertook the same swelling behavior. Further improvements have allowed to introduce in the model a coarse-grained explicit solvent [3]. Indeed, we demonstrate that a likely description shall include hydrodynamics interactions, for which the solvent behaves as a continuous fluid that permeates the polymer network. The newly designed protocol paves the way to the calculation of effective interactions acting among multiple microgels in bulk, and where the presence of the solvent has revealed to be crucial, such as at interfaces [4].

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**Local Dynamics in Ionic Liquids**

Filippa Lundin[1], Kristine Niss[2], Alexandar Matic[1]and Henriette Wase Hansen[2]

[1]*Chalmers University of Technology, Sweden*

[2]*DNRF center "Glass and Time", IMFUFA, NSM, RUC, Denmark*

Ionic liquids are salts with a melting temperature below 100 °C. They typically consist of a large organic cation with an asymmetry introduced by adding alkyl side chains of varying lengths, and an inorganic anion. The asymmetric shape of the ions prevents efficient packing, thus reducing the melting point. The flexibility in the design of the anions and cations makes it possible to tune the properties of the ionic liquid to suit a particular application. In particular, there has been a large interest towards their implementations in Li-ion batteries and fuel cells due to properties such as low vapor pressure, large electrochemical window and high thermal stability.

However, ionic liquids are also interesting from a more fundamental point of view. Unlike most other liquids they show structural heterogeneities on mesoscopic length scales. The heterogeneities are suggested to originate from the segregation of the alkyl side chains in a charge matrix. The length scale and interactions of these heterogeneities can be tuned by the architecture and constituent ions of the ionic liquid, providing a systematic way to investigate their influence on the dynamics of the liquid.

In this project we are investigating the dynamics of ionic liquids directly on the mesoscopic length scales of the heterogeneities present in these systems. The aim is to understand the correlation between the local dynamics, the structural heterogeneities, and the ionic conductivity. For this, neutrons are the ideal probe as they give us access to the dynamics on relevant length scales. With the back-scattering spectrometer IN16B at ILL we can access the relevant time and length scales. A key feature of our experiment is that we will use a newly developed sample cell where we can perform neutron scattering and dielectric spectroscopy at the same time [1]. In addition, this cell allows also changing the pressure, going to high pressures of up to 5000 bar. Thus, we can monitor the conductivity directly at a given pressure and temperature as we are doing the neutron scattering experiment. By being able to explore effects of both pressure and temperature we aim to investigate the dynamics at different state points (P,T) where the conductivity is the same. A key question is if the local dynamics is the same in these points, which will give us insight in the mechanism of ion transport.

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**A computational approach to estimate absolute free energy of drug-target binding**

Dorothea Gobbo[1], Pietro Ballone[2], Sergio Decherchi[2] and Andrea Cavalli[1]

[1]*Italian Institute of Technology, University of Bologna, Italy*

[1]*Italian Institute of Technology, Italy*

Equilibrium properties and transformations in chemical physics systems are often determined by free energy considerations. This is the case, for instance, of binding and unbinding events of drugs to their physiological targets, whose rate is crucial for the pharmacological activity of drugs. A popular method to determine free energies of molecules in solution relies on the exact computation for a simple representative system, complemented by the estimate of the excess free energy by perturbation approaches. In practice, the reference free energy is computed by resorting to an Einstein model in which atoms are confined by harmonic restrained to their equilibrium position. Here, to provide a better reference system, we introduce an atomistic network model, consisting of point particles (atoms) and harmonic springs, hence defining a more reliable starting representation of the system dynamics. The enhanced realism of the reference model allows therefore limiting the perturbation part, which therefore requires much shorter simulations relative to the Einstein model. In our study, we develop and validate the method on neutral and charged organic molecules in water, and we outline the computational path towards scaling the method to the large systems of biophysical and pharmacological systems. The role of neutron scattering data in the parametrization of the network model is also discussed.

**Complementary Neutron scattering methods to study drug phospholipid interactions**

Henrich Frielinghaus[1,2], Gaetano Magiapia[1,2] and Manchar Gvaramia[1,2]

[1]*JCNS, Germany*

[2]*HZG, Germany*

[3]*Iv.Javakhishvili Tbilisi State University, Georgia*

Phospholipid-based bilayers are widely used as model systems for studying the more complicated biological cell membranes, providing information about their structure and interactions. In particular, we are interested in understanding the effect of drugs on phospholipid-based membranes, i.e. the action mechanism, and the eventual toxicity when administered at high concentrations. This knowledge can in principle support a chemical design of more efficient variants having lower side effects.

In the present study, we have investigated the effect of some active principles, namely benzocaine and propranolol on bilayers composed of L-α-phosphatidylcholine (SoyPC) by means of Neutron Reflectivity (NR) Grazing Incidence Small Angle Neutron Scattering (GISANS) and Small Angle Neutron Scattering (SANS). Benzocaine is a commercial drug that serves as topical pain reliever, used for instance in cough drops. It is also found as main component in many anesthetic ointments such as products for oral ulcers. Propranolol is a beta-blocker, affecting the heart and blood circulation: it is used for treating tremors, angina, hypertension and other heart or circulatory conditions. We generally found a variation of the structural parameters of the membranes with incorporated drug molecules, with a destabilization found at high drug concentrations, through the formation of ruptures inside the double layers,randomly distributed over the space. Propranolol has a bigger perturbative effect on the membranes, due to the structure of his hydrophobic part.

## Eating the bone! An enzymatic protocol aiming at bone's organic matrix removal

Adriana Pires Mamede[1,2,3], Ana Rita Vassalo[2,3], David Gonçalves[2,3,4], Stewart Parker[5], Luís Alberto Batista de Carvalho[1] and Maria Paula Marques[1,6]
[1]*R&D Group "Molecular Physical-Chemistry", Univ. Coimbra, Portugal*
[2]*Forensic Anthropology, Centre of Functional Ecology, University of Coimbra, Portugal*
[3]*Research Centre for Anthropology and Health (CIAS), University of Coimbra, Portugal*
[4] *Archaeosciences Lab., Directorate General Cultural Heritage (LARC/CIBIO/InBIO), Portugal*
[4]*ISIS Facility, STFC Rutherford Appleton Laboratory, Chilton, Didcot, UK*
[6]*Dep. Life Sciences, Univ. Coimbra, Portugal*

Human bone tissue is composed of an inorganic matrix, bioapatite; a hydroxyapatite ($Ca_{10}(PO_4)_6OH_x$, HAp)) analogue substituted by carbonate at both phosphate and hydroxyl sites; and an organic matrix comprising lipids and proteins (mainly type I collagen) [1,2]. In several fields of study such as anthropology, forensics, archaeology (*e.g.* radiocarbon dating), biochemistry (*e.g.* enzyme immobilisation substrates), pharmacology (*e.g.* drug delivery matrices) and medicine. Regarding the latter, both orthopaedic xenografts (from a different animal species) and allografts (from the same species with a different genotype) [3,4] are used as implants or as inducers of bone regeneration, and their preparation includes bone defatting and deproteination in order to obtain biocompatible systems with a suitable bioactivity and osteoconductivity [5,6] while preserving bone's inherent structural and physical properties.
However, care must be taken regarding the negative effect of the chemical treatments [2,4,7–9] on bone's inorganic matrix, namely in bioapatite's structure and crystallinity degree [10–12]. Moreover, none of the reported protocols achieved a total removal of the organic components of bone. Hence, the present study aimed at the development of a new experimental protocol allowing a maximum deletion of bone's organic components (both protein and lipids) with a minimum impact on bioapatite´s structural properties. A multi-enzymatic procedure – Aspergillus niger lipase [3] followed by Clostridium histolyticum clostridiopeptidase A [13,14] – was carried out on human femur and humerus samples from unidentified skeletons whose provenance is the same as the one from the 21st century Collection of Identified Human Skeletons [15]. The results were compared with those yielded by the widely used petroleum ether/hydrazine protocol, through Inelastic Neutron Scattering (INS, at the ISIS Neutron Pulsed Source, UK – MAPS and TOSCA spectrometers) and Fourier-transform Infrared Spectroscopy in Attenuated Reflectance mode (FTIR-ATR, at the Molecular Physical-Chemistry R&D Group, Coimbra University, Portugal).

FTIR-ATR analysis evidenced the removal of most organic matter by both protocols, although traces of protein (amide I signal at 1650 $cm^{-1}$) were still detected in the enzymatic-treated bones. In turn INS, which was shown to be an extremely suitable method for studying bone tissue [16], allowed to conclude that petroleum ether efficiently eliminated the lipids from bone (hardly any $\delta(CH_2)$ bands were observed) while hydrazine was not as successful for protein extraction (both amide I and amide A bands were detected, at 1650 and ca. 3300 $cm^{-1}$, respectively). On the other hand, all protein was removed upon enzymatic digestion but there were still lipid components present ($\delta(CH_2)$ features). The complementarity of these spectroscopic results is a consequence of the high sensitivity of INS to H-associated vibrational modes.

Regarding the impact of both experimental protocols on the crystallinity of bioapatite, INS data showed that the characteristic ($Ca\text{-}PO_4$) signals were more affected by the hydrazine treatment than by enzymatic extraction. Also, the crystallinity index calculated through FTIR (CI=(565+603 $cm^{-1}$)/595 $cm^{-1}$) confirmed a higher impact of the petroleum ether/hydrazine procedure: 2.89, 3.04 and 3.49, respectively for intact bone, enzyme- and hydrazine-exposed samples.

Overall, the newly proposed enzymatic process for bone tissue defatting and deproteination was found to be quite promising. Still, further optimisation of the method is needed: while the main protein component (type I collagen) was efficiently degraded by Clostridium histolyticum collagenase, Aspergillus niger lipase (which recognizes only mono-, di- and triacylglycerols) could not digest the vast variety of lipids present in bone tissue leaving a considerable amount of these components in the treated samples. This prompts for a future use of a mixture of different lipases.

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**Neutron Scattering Experiments Under Illumination**

Maksym Golub[1], Marcus Moldenhauer[2], Franz-Josef Schmitt[2], Wiebke Lohstroh[3], Artem Feoktystov[3], Thomas Friedrich[2] and Jörg Pieper[1]

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

[2]*Technical University Berlin, Germany*

[3]*FRM2, Germany*

The structure-dynamics-function relationship in proteins remains a field of great scientific interest. Photoactive proteins form a specific class, whose function can be activated by illumination. For instance, photosynthesis in cyanobacteria is initiated by light-absorption in protein complexes referred to as phycobilisomes (PBs). In the case of excess light energies, photodamage of the photosynthetic apparatus is prevented by a protection mechanism called non-photochemical quenching (NPQ). In cyanobacteria, NPQ requires a light-sensitive effector denoted as Orange Carotenoid Protein (OCP). OCP is photsensitive and undergoes a pronounced structural change to its active state under illumination with blue light. The underlying structural changes are currently a field of intensive research (see e.g [1-3]). We have used SANS and QENS experiments in the dark and under defined illumination in order to investigate structural and dynamical changes of OCP during its activation.

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**Characterization of Framework and Extra-Framework Aluminium Species in Zeolite Y by Solid-State NMR**

Monica Pinto[1], Gerd Buntkowsky[1], Hergen Breitzke[1], Juan Carlos Poveda[2], Daniel Molina[2] and Alexander Guzmán[3]

[1]*Technische Universität Darmstadt, Germany*

[2]*Universidad Industrial de Santander, Colombia*

[3]*Instituto Colombiano del Petroleo (ICP) , Colombia*

Brönsted and Lewis acid sites in zeolites play an important role as active sites in heterogeneous catalysis. Brönsted acid sites of zeolite catalysts are bridging hydroxyl protons in the vicinity of tetrahedral framework aluminum atoms. Frequently, Lewis acid sites are caused by extra-framework aluminum species formed upon calcination or steaming of the zeolite catalyst. Preparation of active and stable zeolite catalyst normally requires post-synthesis modifications, such as thermal and hydrothermal treatment, acid leaching and selective extraction of extra-framework species.

A multinuclear solid-state NMR investigation was carried out to characterize the possible structural changes in zeolites Y modified by hydrothermal treatment to obtain USY zeolite [1]. USY zeolite was chemically modified with aqueous solutions of EDTA and HCl to remove extra-framework aluminum species (EFAl), which could be obstructing the pore system.

Brönsted acid sites, silanol groups and non-framework Al were identified on $^{1}$H MAS NMR spectra. Two different Brönsted acid sites at the supercage were detected in all the samples, with signals at 3.7 and 4 ppm. The latter was assigned to a Brönsted acid site nearby oxygen from EFAl species [2]. In addition to that, $^{1}$H MAS NMR and $^{29}$Si MAS NMR spectra have revealed that both aqueous solutions are very effective in removing non-framework Al. $^{27}$Al MAS NMR experiments show the presence of aluminium in IV, V and VI coordinations in the samples under hydrothermal, salt solution and acid solution treatments, whereas $^{27}$Al MQMAS NMR spectra reveal two different tetrahedral Al environments (IVa, IV b), three octahedral signal (Al VIa, Al VIb, AlVIc) and one five-coordinated signal Al(V). The latter showed decreasing intensity in USY Zeolite samples after EDTA and HCl solutions treatments.

Finally, FSLG-HETCOR was used to obtain direct information about the proton connectivity of extra-framework Al species and silanol groups.

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**In silico analysis of subtype specific potassium channel blockage by the conotoxins μ-PIIIA, μ-SIIIA and μ-GIIIA**

Desirée Kaufmann and Daniel Tietze*

*Darmstadt University of Technology, Germany*

μ-conotoxins, obtainable from marine cone snails, are known as a very powerful substance blocking many different types of ion channels by occluding their pore[1] and thus interrupting signal transmission between neurons. – A reason for why they bear a great potential as analgesics.[2] As an example, ziconotide, also known as ω-conotoxin MVIIA, is approved as drug for the treatment of severe chronic pain.[3] However, ziconotide also exhibits neurological side effects,[4] resulting from its high sensitivity and coincident lack of subtype specificity towards voltage-gated ion channels.

Similarly and remarkably, μ-PIIIA, which is known to specifically block Nav1.4 channels[5] was recently found to possess significant affinity also towards some voltage gated potassium channels.[6] More specifically, μ-PIIIA is active on the Kv1.6 potassium channel while being completely insensitive to Kv1.5,[6a] which shows its overarching subtype specificity.

To date there is still a lack of knowledge considering the distinct contributions of specific key residue interactions and toxin conformations making up this remarkable feature of recognition. It is therefore important to track down the interplay of these complex dynamics in order to gain an understanding of their underlying mechanism.

This study takes up known experimental data published by Leipold et al.,[6a] applying comparative molecular dynamic simulations in a membrane environment of up to 500ns on combined systems of docked μ-conotoxins μ-PIIIA, μ-SIIIA and μ-GIIIA on the different potassium channel subtypes Kv1.5 and Kv1.6 and chimeras in water.

In accordance with to date published literature,[7] results of our simulations show characteristic and recurrent modes of toxin binding and un-binding when combined with the different channel types.

The gained knowledge on subtype specificity determinants enables us to take a further step towards subsequent (in-silico) optimizations or adjustments of detected lead structures towards different subtypes of ion channels. In this context, μ-PIIIA being active on Kv1.6 could serve as exemplary and very potential precursor combination for the determination of a preliminary μ- conotoxin-pharmacophore.

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**Synthesis and characterization of Poly Amic Acid and Polycyclic Imide for Ammonia Capture**

Rodrigo Lima[1,2], Ji-Woong Lee[3], Mark Telling[4], Heloisa N. Bordallo[1]

[1]*The Niels Bohr Institute, University of Copenhagen, Denmark*

[2]*Universidade Federal de Campina Grande, Portugal*

[3]*Department of Chemistry – University of Copenhagen, Denamark*

[4]*ISIS Facility, STFC Rutherford Appleton Laboratory, Chilton, Didcot, UK*

The organization of H-bonding networks in 3D structures is of great interest in various fields of science, encouraging artificial construction of materials with personalized functionality and performance. In this direction, and as a result of the high degree of functional and structural control, materials with permanent porosity as metal organic frameworks (MOF), covalent organic frameworks (COF) or porous polymers have been widely applied in specific applications such as separation, storage and gas capture. Porous polymers stand out because of their covalent nature and high level of synthesis control. Thus, polyamic acid (PAA) and polycyclic imide (PI) can be seen as new potential candidates to be used as solid-state absorbents.

This work aims to better understand the mechanism of ammonia capture in PAA and PI, i.e. how the H-bonding interactions change during gas adsorption using neutron spectroscopy. Previous to the neutron experiments, PAA and PI samples, synthesized according to the work of Lee et al. [1], were characterized by thermogravimetric analysis coupled to Fourier Transform Infrared (TGA-FTIR), differential scanning calorimetry (DSC), elemental analyses and X-rays powder diffaction (PXRD). The results from TGA-FTIR for PAA samples shows that the first mass loss is dependent on the washing process: if washed with N,N-dimethylformamide (DMF), the solvent accounts for 20% of the mass of the PAA sample, while without DMF the mass loss is ~1%. For PI sample, the first mass loss is also attributed to the solvent, in this case, 1,4-Dioxane. The DSC results show a clear endothermal transition between 100–250°C attributed to the imidization process in PAA. Based on the PXRD data we show that both samples are amorphous. The very first gas adsorption *in-situ* quasi-elastic neutron scattering (QENS) data are also presented.

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**Solid State NMR & MD Simulation Studies of Water-Octanol Mixture Confined in Mesoporous Silica**

Bharti Kumari, Martin Brodrecht, Mayke Werner, Sandra Forg, Elvira P. Sanjon, Barbara Drossel, Torsten Gutmann and Gerd Buntkowsky (TU Darmstadt)

*Technische Universität Darmstadt, Germany*

Solid-state NMR is a versatile technique for the determination of local structures and dynamics of small guest molecules in confined systems. CP-MAS HETCOR experiments with FSLG (Frequency Switched Lee-Goldburg) homonuclear decoupling allow estimating the strength of dipolar interactions and thus distances between protons and hetero nuclei such as $^{29}Si$ or $^{13}C$ in a sample via variation of the contact time. The combination of solid-state NMR spectroscopy and MD simulations is employed to study the behavior of water-octanol and its isomers in different mol ratio confined in the mesoporous silica SBA-15. Two dimensional $^{1}H$-$^{29}Si$ FSLG-HETCOR NMR spectra help to inspect the intermolecular interaction of these mixtures with the pore walls. This NMR study reveals that the hydroxyl groups of octanol and water stay near the pore surface through hydrogen bonds with silica sites, while the hydrocarbon chains are located in the range between surface and center. These results are supported by MD simulations, which shows the high -OH molecular density (from water and Octanol) near the pore surface. The orientation of water-octanol molecules tends to be nearly independent from the ratio between water-octanol molecules used in the experiments (0-30 mol%) of water. The investigation of water-alcohol interactions with surfaces at a molecular level is the basis to understand the effect of confinement in porous media. This will be the basis to optimize separation techniques such as lubrication, elimination of contamination and oil recovery.

**Tailoring molecular potentials for dynamics using quasi-elastic neutron scattering**

Thomas Farmer[1], Anders Markvardsen[1], Heloisa Bordallo[2], Thomas Holm Rod[3]

and Jan Swenson[4]

[1]*ISIS Facility, STFC Rutherford Appleton Laboratory, Chilton, Didcot, UK*

[2]*The Niels Bohr Institute, University of Copenhagen, Denmark*

[3]*European Spallation Source (ESS), Sweden*

[4]*Chalmers University of Technology, Sweden*

As experimental techniques are used to probe increasingly complex systems, subtle emergent behaviour can lead to significant difficulties when interpreting the data. This is particularly evident in quasi-elastic neutron scattering (QENS), where simple analytical models may be unrepresentative of the underlying dynamics. By augmenting QENS with molecular dynamics (MD) or other simulation techniques, it is possible to observe this complex behaviour. However achieving agreement between scattering and simulation is frequently challenging; a significant source of the disparity is because intermolecular potentials are commonly established using structural rather than dynamic data, and often only at ambient conditions. In order to address this problem, we are in the process of developing a dynamic analogue to empirical potential structure refinement. This approach uses Monte Carlo methods to minimize the difference between MD and neutron observables (both dynamic and structural) by optimizing the intermolecular potential parameters. Here we describe the underlying algorithm and present our initial results on water.

**Room temperature ionic liquids in protein amyloidogenesis: a comprehensive neutron scattering, atomic force microscopy and molecular dynamics simulation studies**

Visakh VS Pillai and Antonio Benedetto

*University College Dublin, Ireland*

Room temperature ionic liquids (RTIL) are vast class of non-aqueous electrolytes whose interactions with bio molecules is receiving great attention for potential applications in bio-nano-technology. Recently it has been shown that RTILs can affect protein amyloidogenesis. Whereas some RTILs favor the aggregation of proteins into amyloids, others inhibit their formation. Moreover, RTILs can dissolve mature fibrils and restore the protein biochemical function. The main aim and scope of our research is toward unraveling the microscopic picture underlying the observed mesoscopic effects. In our investigations we combine neutron scattering techniques and computer simulation approaches along with atomic force microscopy.

## Unraveling the mystery: FTIR-ATR and inelastic neutron scattering (INS) spectroscopies applied to the analysis of burned human skeletal remains

Ana R. Vassalo[1,2], Adriana P. Mamede[3], Eugenia Cunha[2], Stewart F. Parker[4], Maria P.M. Marques[3,5], David Gonçalves[1]and Luís A.E. Batista de Carvalho[3]

*[1]Research Centre for Anthropology and Health (CIAS), University of Coimbra, Portugal*
*[2]Forensic Anthropology, Centre of Functional Ecology, University of Coimbra, Portugal*
*[3]R&D Group "Molecular Physical-Chemistry", Univ. Coimbra, Portugal*
*[4]ISIS Facility, STFC Rutherford Appleton Laboratory, Chilton, Didcot, UK*
*[5]Dep. Life Sciences, Univ. Coimbra, Portugal*

Burned human skeletal remains can be found in forensic (terrorist attacks, fires, attempts to conceal the corpse in case of homicides) or archaeological contexts (funerary practices of the past populations). The problem here is that heat causes numerous changes in bones pand teeth that complicate bioanthropological analyses. Vibrational spectroscopy techniques have been shown to be very useful for understanding and quantifying heat-induced changes in bones composition and structure. In the present work, FTIR-ATR and inelastic neutron scattering (INS) spectroscopies were applied in order to identify markers that hopefully will allow relating heat-induced bone diagenesis to the pre-burned conditions of the remains.

Femoral and humeral of the skeleton CC_NI_42, with the same provenance of those from the 21st Century Identified Skeletal Collection of the Laboratory of Forensic Anthropology, were used. Diaphyses were sectioned and 7 sections of each bone were burned under controlled conditions in an electric oven (model Barracha K-3 three-phased 14A): 400, 500, 600, 700, 800, 900 and 1000 °C, for 120 minutes, at a heating rate of 6 – 10 °C/min. The combined application of the optical and neutron spectroscopic techniques allowed access to the whole vibrational profile of the both unburned and burned human bone samples. In particular, using an incident energy of 5240 $cm^{-1}$, with the MAPS spectrometer it is possible to simultaneously assess both OH libration and stretching signals of hydroxyapatite, thus unequivocally proving the assignment of these bands and ruling out the possible origin of the libration signal to water sequestered in the bone. Moreover, while the $OH_{Iib}$ band was present in all samples, the ν(OH) band was only visible for samples burned at 600 °C or above. At temperatures higher than 600 °C, the 1st overtone of the $OH_{Iib}$ and a band arising from the combination of the OH libration and stretching modes (comb) became observable. In turn, the 2nd and 3rd overtones of the librational mode were visible in the spectra from samples burned at 800 and 1000 °C, respectively. On the other hand, as the temperature increase, a progressive loss of carbonate content and crystallinity changes were observed and, additionally a shift of the OH libration and stretching bands was detected.

The good quality INS data obtained allowed us to validate the information retrieved from the FTIR spectra. The knowledge presently gathered, coupled to the macroscopic information obtained from bone analysis (before and after burning), is expected to lead to a quantitative correlation between the bone's crystalline structure and heat-induced changes. As previous mentioned, this approach will be useful in archaeological and forensic sciences.

**Development and Application of MnFe2O4 @ ɣ-$Fe_2O_3$ @ CTAB Magnetic Nanoadsorbents for Removal of Direct Yellow 12 from Aqueous Solutions**

Paulo Henrique Michels Brito[1,2], Renata Aquino[1], Jerome Depeyrot[1], Alex F. C. Campos[1] and Franciscarlos G. da Silva[1]

[1]*University of Brasília, Brazil*

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

The textile and dye manufacturing industries produce large quantities of dangerous dyes, pigments and metals with a high potential to pollute wastewaters. In this context, some methods for color removal from water and waste waters are available such as membrane separation, biologic degradation, chemical oxidation, coagulation and flocculation [1]. More recently, some methods based on magnetically assisted chemical separation have been proposed to be more efficient and produce less waste [2]. In this work, we investigate the removal of direct yellow 12 (DY12) from aqueous solutions using magnetic nanosorberts based on ferrite nanoparticles (NP) modified with cetyltrimethylammonium bromide (CTAB).

*Materials and Methods:* The nanosorbents were synthesized using the hydrothermal coprecipitation method in alkaline medium followed by a surface treatment with $Fe(NO_3)_3$ leading to $MgFe_2O_4$@γ–$Fe_2O_3$ core-shell NP. The surface modification was carried out by mixing the NP and CTAB in aqueous solution at pH = 10 and then sonication. The influence of time, solution pH and initial dye concentration were evaluated from batch studies using 0.50 g/L of the nanosorbent. After chemical adsorption, the NP were separated using a hand-held magnet and the final concentration of DY12 in decanted solution was determined by UV-VIS spectroscopy at 396 nm.

*Results and Conclusions:* The results of the batch studies were analyzed in the framework of Langmuir and Freundlich models and showed that the nanoparticle size has an important effect on the DY12 adsorption. The nanosorbents were more effective in slightly low pH conditions (pH = 5.0), using a shaking rate of 400 RPM. The contact time required to reach the equilibrium was relatively short (30 min). Finally, it was evidenced that the maximum adsorption capacity was nearly 108% higher for the nanosorbent of the smaller mean size (58.49 mg/g against 28.10 mg/g) due to its higher surface area. Finally, the nanoadsorbents were recovered from wash cycles and reused in removal tests with efficiency between 50% and 55%.

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**Origin of enzyme's catalytic capabilities:**
**A computational case study on monoamine oxidase A**

Eric Franciskovic[1], Alja Prah[2], Jernej Stare[2], Janez Mavri[2]
[1]*Department of Pharmacy, University of Copenhagen, Denamrk*
[2]*National Institute of Chemistry, Ljubljana, Slovenia*

The final answer on where does the enzyme's catalytic capability come from has proven to be highly elusive. Despite the best efforts of scientists from different areas of expertise we don't know much more than that enzymes lower the energy barrier of chemical reactions and thus speed them up. It has not yet been confirmed whether dynamical effects or preorganized electrostatics are the main driving force behind catalytical abilities of enzymes [1, 2]. In this study we used computational methods to learn more about the catalytic origins in monoamine oxidase A (MAO A).

Located on the outer membrane of the mitochondrion, MAO A catalyses the oxidative deamination of biogenic amines. Since it is important in the metabolism of several neurotransmitters it is not surprising that it plays a key role in the development of some psychiatric disorders (for example Parkinson's disease, dementia, anxiety and other mood disorders) [3]. An endogenous amphetamine, phenylethylamine (PEA), is a neuromodulator capable of affecting neurons beyond the synaptic contact, whose levels increase after intense physical activities and is responsible for mood-enhancing effects.

With a simple multiscale model we built for this purpose we were able to elucidate the effect of electrostatics in the rate-limiting step of the reaction between PEA and MAO A. Snapshot structures representative of the transition state and the state of the reactants were obtained from our previous molecular dynamics simulations of this reaction [4]. The reacting moieties (PEA and MAO A cofactor lumiflavin ※) comprised the quantum part, while the protein environment was represented by point charges. Quantum calculations were performed at the M06-2X/6-31G+(d, p) level of theory. This allowed us to quantify the effects of manipulating those point charges by scaling them by various factors (k between -1 and 2, with k = 1 representing the full unchanged enzymatic environment and k = 0 representing the gas phase) and also by performing several other manipulations (randomizing the point charges, placing large point charges close to the reacting moiety, switching the protein environment of the two representative states). Several parameters were studied including the energy barrier, charge transfer within the reacting moiety and the HOMO-LUMO gap, and it was established that the electrostatic environment enhances the reaction by all the considered criteria. This is consistent with the view that preorganized electrostatics are responsible for enzyme catalysis abilities.

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## Solid-state NMR and Dynamic Nuclear Polarization (DNP) studies of inorganic-organic functional materials

Timmy Schäfer[1], Steffen Vowinkel[2], Markus Gallei[2], Torsten Gutmann[1*]

[1] *Eduard-Zintl-Institute for Inorganic Chemistry and Physical Chemistry, Technical University Darmstadt, Alarich- Weiss-Str. 4, D-64287 Darmstadt, Germany*
[2] *Ernst-Berl Institute for Chemical Engineering and Macromolecular Science, Technische Universität Darmstadt, Alarich-Weiss-Str. 4, D-64287 Darmstadt, Germany.*

Cellulose is the major constituent of plant cells and is the world's most abundant biopolymer. In recent years, cellulose has been established as a carrier material for special functional materials e.g. as a membrane for fuel cells, [1] as a carrier for optically active materials [2] or for catalysts [3]. In addition, there is currently a trend to design special papers for controlled fluid flow, in biosensing or diagnostic [4].

To understand and design custom-made cellulose or polymer hybrid materials for these applications, their chemical structure has to be explored in detail on the molecular level [5]. This is a challenging task due to the complexity of such materials.

The often highly disordered structures of these materials require analytical methods that address local environments.

Solid-state NMR (ssNMR) spectroscopy is an important method that allows measuring local interactions. To achieve the necessary sensitivity to access systems with small specific surface areas or less surface functionalization it is necessary to combine ssNMR with dynamic nuclear polarization (DNP) [6]. Hereby the sensitivity can be enhanced by several orders of magnitude and enables the measurement of nuclei such as $^{13}C$, 15N even in natural abundance.

In this presentation, the selective signal enhancement for cellulose based systems and the potential of solid-state DNP for structure determination of polymer hybrid materials is demonstrated [4, 7].

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# Participants list

| Name | Institution | Email |
|---|---|---|
| Christiane Alba-Simionesco | LLB-CEA-CNRS | christiane.alba-simionesco@cea.fr |
| Ken Andersen | ESS | ken.andersen@esss.se |
| Ana Benetti | University of Copenhagen | arbe@sund.ku.dk |
| Heloisa N. Bordallo | University of Copenhagen (NBI) | bordallo@nbi.ku.dk |
| Gerd Buntkowsky | TU Darmstadt | gerd.buntkowsky@chemie.tu-darmstac |
| Fabrizio Camerin | Università di Roma La Sapienza | fabrizio.camerin@uniroma1.it |
| Juan Colmenero | University of the Basque Country (UPV/EHU) | juan.colmenero@ehu.eus |
| Juergen Eckert | Texas Tech University | juergen@usf.edu |
| Thomas Farmer | ISIS | tom.farmer@stfc.ac.uk |
| Eric Franciskovic | University of Copenhagen | ericfrancisko95@gmail.com |
| Denitsa Georgieva | Sofia University “St. Kliment Ohridski” | dgeorgievak@gmail.com |
| Dorothea Gobbo | Italian Institute of Technology (IIT) | dorothea.gobbo@iit.it |
| Maksym Golub | Institute of Physics, Tartu University | maksym.golub@hotmail.com |
| Manchar gvaramia | Iv.Javakhishvili Tbilisi State University | m.gvaramia@fz-juelich.de |
| Felix Jimenez-Villacorta | ESS-Bilbao | fjimenez@essbilbao.org |
| Sergey Kapishnikov | University of Copenhagen (NBI) | sergey.kapishnikov@nbi.ku.dk |
| Desiree Kaufmann | TU-Darmstadt | kaufmann@chemie.tu-darmstadt.de |
| Gerald Kneller | University of Orleans and CBM CNRS Orleans | gerald.kneller@cnrs.fr |
| Bharti Kumari | Technical university of Darmstadt | kumari@chemie.tu-darmstadt.de |
| Bela Lilova | Sofia University “St. Kliment Ohridski” | bmlilova@gmail.com |
| Rodrigo Lima | University of Copenhagen (NBI) | rodrigo@nbi.ku.dk |
| Filippa Lundin | Chalmers University of Technology | flundin@chalmers.se |
| Adriana Mamede | University of Coimbra (QFM-UC) | adrianampmamede@gmail.com |
| Maria Paula Marques | University of Coimbra (QFM-UC) | pmc@ci.uc.pt |
| Murillo Martins | Pontifical Catholic University of Goias | murillolongo@gmail.com |
| Paulo Henrique Michels Brito | NTNU | paulo.h.m.brito@ntnu.no |
| Gitte Michelsen | University of Copenhagen (NBI) | gittem@nbi.ku.dk |
| Tommy Nylander | Lund University | tommy.nylander@fkem1.lu.se |
| Loukas Petridis | Oak Ridge National Laboratory | petridisl@ornl.gov |
| Monica Patricia Pinto Salazar | Technische Universität Darmstadt | pinto@chemie.tu-darmstadt.de |
| Margerie Pouteau | Université Grenoble Alpes | margerie.pouteau@gmail.com |

| | | |
|---|---|---|
| Johann Raillard | Université Grenoble Alpes | johann.raillard.jr@gmail.com |
| Felix Roosen-Runge | Lund University | felixroosenrunge@gmail.com |
| Edina Rosta | King's College London | edina.rosta@kcl.ac.uk |
| Mattias Sauzon | Université Grenoble Alpes | mattias.sauzon@gmail.com |
| Timmy Schäfer | TU-Darmstadt | timmy.schaefer@chemie.tu-darmstadt |
| Andreas Schreyer | ESS | andreas.schreyer@esss.se |
| Mark Telling | STFC | mark.telling@stfc.ac.uk |
| Ana R. Vassalo | University of Coimbra (QFM-UC) | ana_rita_vassalo@hotmail.com |
| Visakh V.S. Pillai | University College Dublin, Ireland | visakh.vspillai@ucdconnect.ie |
| Emanuela Zaccarelli | CNR Institute for Complex Systems | emanuela.zaccarelli@cnr.it |