

## CPP 30: New Perspectives of Scattering at Soft Matter

Time: Wednesday 15:00–18:45

Location: C 264

## Invited Talk

CPP 30.1 Wed 15:00 C 264

**Soft Matter Research at the ESS** — ●KEN ANDERSEN — European Spallation Source ESS AB, P.O.Box 176, 22100 Lund, Sweden

The European Spallation Source will be a world-leading centre for neutron scattering, based in Lund in Sweden. It will start operation in 2019 and will be fully operational with 22 neutron instruments in 2025. The ESS time structure will be particularly well-suited for cold neutron applications and is expected to outperform existing facilities by at least an order of magnitude. The current status of the project, as well as the plans for instruments and support labs, particularly those relevant for soft matter research, will be presented.

CPP 30.2 Wed 15:30 C 264

**Neutron spin echo instrumentation for the European Spallation Source** — ●STEFANO PASINI and MICHAEL MONKENBUSCH — Forschungszentrum Jülich, 52425 Jülich, Germany

Neutron spin echo (NSE) is the technique with the highest energy resolution for probing the dynamics of materials. At the European Spallation Source (ESS) three different instrument concepts are currently being developed together with Research Center Jülich and the Technical University of Munich. These are a high-resolution spin-echo spectrometer, a wide-angle spin-echo spectrometer and a combined MIEZE and neutron-resonance spin-echo spectrometer. We will present here the progress made in adapting the high-resolution spin-echo spectrometer to the ESS parameters. One part of the work is focused on the specification and conceptual layout of an optimized beam transport including polarization, frame-overlap choppers and avoidance of the direct view. These aspects are quite common between high-resolution and wide angle instrument. Besides the beam transport, the proper spin-echo part consists of magnetic fields for the manipulation of the spin state evolution. Some results on the specification and on the optimization of the magnetic layout of the NSE will be presented.

CPP 30.3 Wed 15:45 C 264

**Development of Direct Geometry Chopper spectrometers for the European Spallation Source** — ●NICOLO' VIOLINI<sup>1</sup>, JORG VOIGT<sup>1</sup>, THOMAS BRUCKEL<sup>1</sup>, MARGARITA RUSSINA<sup>2</sup>, KATHARINA ROLFS<sup>2</sup>, GIOVANNA SIMEONI<sup>3</sup>, WIEBKE LOHSTROH<sup>3</sup>, LUCA SILVI<sup>3</sup>, and PASCALE DEEN<sup>4</sup> — <sup>1</sup>Forschungszentrum Jülich GmbH, Jülich Centre for Neutron Sciences, Leo Brandt Strasse, 52425 Jülich, Germany — <sup>2</sup>Zentrum Berlin für Materialien, Hahn-Meitner-Platz 1, 14109 Berlin, Germany — <sup>3</sup>Technische Universität München, Forschungsneutronenquelle Heinz Maier-Leibnitz (FRM II) Lichtenbergstrasse 1, 85747 Garching, Germany — <sup>4</sup>European Spallation Source ESS AB, Box 176, 22100 Lund, Sweden

The long pulse of the ESS will provide a high neutron flux, comparable to the best existing steady state reactors. The main challenge in the instrument design at the future ESS is how to take full advantage of the high neutron peak flux and at the same time to take control over the pulse parameters to best suit the instruments and individual experiments. It has been shown that in particular direct geometry time of flight spectrometers using cold neutrons profit strongly from the long pulse at ESS. In addition the implementation of novel multiplexing techniques, such as RRM and WFM will allow the multispectral instruments to better exploit the source features. Within the German ESS Design Update Phase, we will present the recent progress in the Work Package I1 on chopper spectroscopy. We describe the main aspect of the instruments design, especially focusing on the purpose to achieve a high energy resolution (<0.5%) and its implications.

CPP 30.4 Wed 16:00 C 264

**Dynamics in an enzyme containing bicontinuous microemulsion: A quasielastic scattering study** — RALPH NEUBAUER<sup>1</sup>, STEFAN WELLERT<sup>2</sup>, ANDREAS RICHARDT<sup>3</sup>, MARC-MICHAEL BLUM<sup>4</sup>, and ●THOMAS HELLWEG<sup>1</sup> — <sup>1</sup>Phys. und Biophys. Chemie (PC III), Universität Bielefeld, Universitätsstr. 25, 33615 Bielefeld, Germany — <sup>2</sup>Stranski Lab. f. Physikalische und Theoretische Chemie, TU Berlin, Straße des 17. Juni 124, 10623 Berlin, Germany — <sup>3</sup>WIS Munster, ABC-Schutz, Humboldtstraße 100, 29633 Munster, Germany — <sup>4</sup>Blum-Scientific Services, Ledererstraße 23, 80331 Munich, Germany

The enzyme diisopropyl fluorophosphatase (DFPase) from the squid *Loligo vulgaris* is of relevance due to its ability to catalyze the hy-

drolisis of highly toxic organophosphates. In the present work, the enzyme structure in solution (native state) is studied by different scattering methods. The results are compared to hydrodynamic model calculations. Bicontinuous microemulsions (bME) made of sugar surfactants are discussed as reaction media for the DFPase. The bME remains stable in the presence of the enzyme, which is revealed by scattering experiments. It is shown that the DFPase still has a high activity in the bME [1]. The collective and the local motion of the surfactant interface in the bME is studied by means of neutron spin-echo. Moreover, it is tried to study the enzyme motion decoupled from the microemulsion by contrast variation.

[1]S. Wellert, B. Tiersch, J. Koetz, A. Richardt, A. Lapp, J. Gäb, O. Holderer, M.-M. Blum, C. Schulreich, R. Stehle und T. Hellweg; European Biophys. J., 40:761–774, 2011.

CPP 30.5 Wed 16:15 C 264

**Chain dynamics of n-alkanes studied by neutron scattering and MD simulations** — ●HUMPHREY MORHENN<sup>1</sup>, SEBASTIAN BUSCH<sup>1</sup>, and TOBIAS UNRUH<sup>2</sup> — <sup>1</sup>Physik Department E13 and Forschungs-Neutronenquelle Heinz-Maier-Leibnitz (FRM II), Technische Universität München, 85747 Garching, Germany — <sup>2</sup>Lehrstuhl für Kristallographie und Strukturphysik, Friedrich-Alexander-Universität Erlangen-Nürnberg, 91058 Erlangen, Germany

The analysis of local molecular dynamics on time scales shorter than the long-range diffusion relaxation time is challenging. Quasielastic neutron scattering probes the dynamics on a molecular length and a picosecond time scale. Corresponding data was used to validate MD simulations of liquid hexadecane with respect to the short time dynamics. From the analysis of the MD simulations a detailed picture of the local molecular motions in the liquid could be gained. It is e.g. possible to distinguish and specify local torsional dynamics and global rotational diffusion of the molecules. Using this information a physical model describing the short time motion of medium chain molecules is being developed.

CPP 30.6 Wed 16:30 C 264

**Influence of the Incident Wavelength on the Apparent Diffusion Coefficient of Au Nano Rods** — ●MARYAM HAGHIGHI<sup>1</sup>, MAKUS PLUM<sup>1</sup>, GEORGIOS GANTZOUNIS<sup>3</sup>, GEORGE FYTAS<sup>1,2</sup>, HANS-JÜRGEN BUTT<sup>1</sup>, and WERNER STEFFEN<sup>1</sup> — <sup>1</sup>Max Planck Institute for Polymer Research, Mainz, Germany — <sup>2</sup>Department of Material Science, University of Crete, Heraklion, Greece — <sup>3</sup>University of Athens, Section of Solid State Physics, Athens, Greece

Depolarized dynamic light scattering is a powerful method to measure the diffusion and the rotation of anisotropic particles in solution [1]. Compared to free diffusion in bulk solution, movement close to an interface is influenced by several factors, e.g. hydrodynamic or electrostatic double layer forces. To investigate the dynamics of nanoparticles close to an interface Resonance Enhanced Dynamic Light Scattering (REDLS) is employed [2]. We investigate the diffusion as well as the rotation of Au nano rods in bulk and compared to experiments performed with REDLS close to the solid-liquid interface. Our results show an alteration of the apparent diffusion coefficient of the Au nano rods depending on the incident wavelengths and on the aspect ratio of Au nano rods in bulk solution. We attribute these non-intuitive results to the interplay of surface plasmons generated at certain wavelength in the nano rods themselves and the incident field for the light scattering experiment. [1] Berne, B.J. and Pecora, R., Dynamic light scattering with applications to chemistry Biology and physics (Dover, 2000) [2] Plum M. A., Steffen W., Fytas G., Knoll W. and Menges B., Optics Express 17:10364, 2009

## 15 min break

## Invited Talk

CPP 30.7 Wed 17:00 C 264

**Scanning small-angle X-ray scattering: Imaging nano-scale properties of extended samples** — ●OLIVER BUNK — Paul Scherrer Institut, Swiss Light Source, 5232 Villigen PSI, Switzerland

Small-Angle X-ray scattering (SAXS) is sensitive to the average nanoscale structure within the illuminated area. With the advent of 3rd generation synchrotron radiation undulator beamlines, X-ray optics of adequate quality and fast, low noise, high dynamic range 2D

X-ray detectors scanning SAXS turned from a proof-of-principle to a routinely applied imaging technique, applied in 2D and 3D. It allows imaging nano scale structures over extended, square centimeter sized areas.

After a brief introduction to the technique examples will be shown that include the detection of melt-flow induced alignment in injection moulding of polymers, carbon nanotube reinforced polycarbonate as a two-component system and examples from the biomedical field like bone and brain research that hint at future applications of this technique in the field of soft matter research.

CPP 30.8 Wed 17:30 C 264

**Resonant Soft X-Ray Reflectivity - A tool to study the near-surface structure of complex liquids** — •MARKUS MEZGER<sup>1</sup>, BENJAMIN OCKO<sup>2</sup>, HARALD REICHERT<sup>3</sup>, and MOSHE DEUTSCH<sup>4</sup> — <sup>1</sup>Max-Planck-Institut für Polymerforschung, Mainz — <sup>2</sup>Brookhaven National Laboratory, Upton NY, USA — <sup>3</sup>European Synchrotron Radiation Facility, Grenoble, France — <sup>4</sup>Bar-Ilan University, Ramat-Gan, Israel

X-ray reflectivity (XRR) became one of the leading techniques to study the near-surface structures of liquids. However, standard XRR is not atom-specific and can determine only surface-normal total electron density profiles. In complex liquids, this generally leads to ambiguities in the assignment of molecular moieties to reconstructed interfacial profiles. Resonant x-ray scattering techniques can overcome this limitation by enhancing and modulating the scattering contrast between different molecular moieties.

We present the first fluorine K-edge resonant soft-XRR study of the surface structure of a complex fluid, the ionic liquid  $[C_{18}mim]^+[FAP]^-$ . Analysis of the x-ray absorption spectroscopy and resonant XRR data reveal a depth-decaying near-surface layering. The contributions of specific molecular moieties was unambiguously determined with sub-molecular resolution. Temperature-dependent XRR, SAXS, and FTIR uncover an intriguing melting mechanism for the layered region, where alkyl chain melting drives a negative thermal expansion of the surface layer spacing that has hitherto never been observed for an isotropic liquid.

CPP 30.9 Wed 17:45 C 264

**Observing Molecular Reactions via Simultaneous Ultrafast X-ray Spectroscopies and Scattering** — •WOJCIECH GAWELDA, ANDREAS GALLER, ENRIQUE CUNA, and CHRISTIAN BRESSLER — European XFEL, Albert-Einstein-Ring 19, 22761 Hamburg

Structural dynamics research on chemical and biological systems seeks to extend the use of optical probes to the atomic-scale sensitive tools with either x-ray absorption spectroscopy (XAS) or x-ray (and electron) scattering (XRS). These tools were developed at synchrotron radiation sources, and thus ultimately limited to 50-100 ps time resolution due to the x-ray pulse widths.

We have recently succeeded to extend the capabilities of such laser-x-ray studies towards MHz pump-probe repetition rates at different synchrotron radiation sources, with quasi-static S/N. We studied different Fe-based spin transition compounds, via XAS, but now also with x-ray emission spectroscopy (XES) and XRS in one single setup. XES is sensitive to the actual spin state of the system, and XRS allows investigating the global structural environment of the thermally equilibrated sample. In addition, the electron transfer between a Ru-donor and a Co-acceptor atom was observed via TR-XES in a bimetallic bipyridine-based Ru-Co complex.

More intense x-ray pulses from x-ray free electron lasers (XFELs) are required in order to permit simultaneous femtosecond scattering and spectroscopic studies. This was done for the first time in liquid solutions of Fe-based spin transition compounds at the XPP end station of the LCLS, next to a Ru-Co based compound, and results discussed.

CPP 30.10 Wed 18:00 C 264

**X-Ray Nano-Diffraction on Intracellular Keratin Bundles** — •BRITTA WEINHAUSEN<sup>1,2</sup>, JANNICK LANGEFAHL-KLABES<sup>1,2</sup>, CHRIS-

TIAN OLENDROWITZ<sup>1</sup>, TIM SALDITT<sup>1,2</sup>, and SARAH KÖSTER<sup>1,2</sup> — <sup>1</sup>Institute for X-Ray Physics, University of Göttingen, Germany — <sup>2</sup>Courant Research Centre Nano-Spectroscopy and X-Ray Imaging, University of Göttingen, Germany

The cytoskeleton of eukaryotic cells is a complex network of filamentous biopolymers, which gives cells their versatile shapes and specific mechanical properties. It mainly consists of three different types of filaments: actin filaments, microtubules and intermediate filaments. Keratin intermediate filaments mainly occur in epithelial cells, where they form about 100 nm thick bundles that are organized in a crosslinked network and provide these cells with a high tensile strength as well as the capability to withstand external stresses.

Our goal is to probe the native structure of keratin bundles in live eukaryotic SK8/K18 cells in a physiological environment. For this purpose we use X-ray diffraction with a nanofocused X-ray source, which enables us to achieve high-resolution structural information in combination with a non-destructive sample preparation. Nevertheless, to simplify the experimental set-up, first synchrotron experiments were performed on fixed and freeze-dried cells. High-resolution dark-field contrast image, where the cellular substructure is visible, were obtained and the analysis of single diffraction patterns obtained on keratin bundles showed oriented scattering corresponding to a high degree of orientation in the sample.

CPP 30.11 Wed 18:15 C 264

**Investigation of structural changes of polymer surfaces during friction by GISAXS** — •KONRAD SCHNEIDER<sup>1</sup>, DAVID NITSCHKE<sup>1</sup>, and STEPHAN ROTH<sup>2</sup> — <sup>1</sup>Leibniz-Institut für Polymerforschung Dresden, Germany — <sup>2</sup>HASYLAB at DESY Hamburg, Germany

The materials behaviour during friction is not yet well understood. On macro-scale mainly the contact between certain points or asperities happens and wear is observed. Measuring on nano-scale by a SFM mainly topography and local stiffness are mapped. By a new friction device we investigate friction between a well-defined glass sphere and a polymer surface. This surface is created by grafting of polymer layers with thickness of some nm on a wafer. Friction is performed in dependence of normal load. The changes in surface morphology were characterized by GISAXS (grazing incidence small angle X-ray scattering). This enables to monitor flattening and destruction of the polymer layer on the surface as well as the creation of certain ripple structures.

CPP 30.12 Wed 18:30 C 264

**Millisecond time resolution GISAXS investigation of metal nanoparticle growth on soft and hard surfaces** — EZZELDIN METWALLI<sup>1</sup>, VOLKER KÖRSTGENS<sup>1</sup>, ADELIN BUFFET<sup>2</sup>, JAN PERLICH<sup>2</sup>, STEPHAN V. ROTH<sup>2</sup>, and •PETER MÜLLER-BUSCHBAUM<sup>1</sup> — <sup>1</sup>TU München, Physik-Department, LS Funktionelle Materialien, James-Frank-Str. 1, 85748 Garching, Germany — <sup>2</sup>HASYLAB at DESY, Notkestr. 85, 22603 Hamburg, Germany

Metal deposition on solid supports and polymer surfaces is of importance in many areas such as metal electrodes and engineered nanomaterials [1]. Here, gold in its atomic state is deposited on both soft homopolymer films and hard silicon surface by utilizing a DC magnetron sputtering deposition system. With the unprecedented time resolution of ten milliseconds, the nucleation/growth dynamics of gold nanoparticles on both surfaces is monitored using in situ real-time grazing incidence small angle x-ray scattering (GISAXS). An initial rapid change of the particle size and shape is detected and a large particle size distribution becomes narrower with increasing the particle size. At silicon surface, metal deposits exhibit heterogeneous distributions and asymmetric nanoparticle growth compared to those on soft polymer film. At high metal load, a smooth and uniform metal layer on the polymer surface is attributed to an initial high particle mobility and bridging interactions between particles. A transient network between the bridges and strong metal-metal interactions may explain the progressive slow dynamics at concentrated metal particle dispersions. [1] Kaune et al. ACS Appl.Mater.Interfaces 3, 1055 (2011)