UM17 - Abstract Submission and Registration Staff & Invited Speakers

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CENTRAL LUND, STADSHALLEN & GRAND HOTEL

Book of Abstracts

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Understanding Water Purification - using a new sustainable technology

Author: Adrian Rennie[1]

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Pure water is essential for good health and the supply is still a major challenge. Technology that can be used without specialist support in remote and rural areas is still needed in many countries. An extract from the seeds of the *Moringa oleifera* tree that is principally a low molecular mass protein is known to be efficient as a coagulating agent for water purification. A purification process based on traditional methods used in tropical and sub-tropical Africa is attracting interest for wider use as a sustainable, environmentally friendly technology. The crystal structure of seed protein has been studied by synchrotron X-ray diffraction. Adsorbed layers of protein at different surfaces have been investigated by neutron reflection. The studies have identified that very compact flocs of impurity particles can be formed that are easy to separate. The amount of protein required to cover various different surfaces has been determined.

Sessions:

Environmental and Earth Sciences

1

The Versatility of Mesoscopic Solar Cells

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For solid-state dye-sensitized solar cells we have recently shown that copper phenanthroline complexes can act as an efficient hole transporting material, obtaining power conversion efficiencies of more than 11%. The intriguing electron transfer studies will be presented at the meeting. For perovskite solar cells (PSC) we have achieved efficiencies above 20% with a mixed composition of iodide/bromide and methyl ammonium/formamidinium. With the use of SnO2 compact underlayers as electron acceptor contacts, UPS data show an almost ideal band alignment between the conduction bands of SnO2 and the perovskite, and we have constructed planar perovskite solar cells with efficiencies above 20%. We have taken the cation mixing by including the Cs+ and Rb+. Larger grains are observed and reproducibility and device stability are improved. At the meeting we will present our champion data; up to 22% efficiency and a breakthrough in stability at 85 oC for 500 h under full solar illumination.

Sessions:

New Materials & Energy

2

Pseudo-Single-Bunch Mode for the MAX IV 1.5 GeV Storage Ring

Author: Teresia Olsson[1]

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Since the completion of the MAX IV detailed design report, a discussion on timing modes at the storage rings has been initiated by the user community. Several research areas have been identified where pulse length is not critical, but the experiments require kHz –MHz repetition rates which so far cannot be supplied by the facility. To serve these experiments, many synchrotron storage rings operate with inhomogeneous fill patterns. This is not planned for the MAX IV storage rings due to employment of passive harmonic cavities for beam lifetime and stability. Interest therefore exists for developing methods that could serve timing experiments while operating the storage ring in multibunch mode. One such method is Pseudo-Single-Bunch (PSB), where one bunch in the bunch train is kicked onto another orbit by a fast kicker. The light from this bunch is separated by an aperature in the beamline. We will present the development of such a mode for the MAX IV 1.5 GeV storage ring.

Sessions:

Quantum systems & processes

3

Time- and Space-Resolved Atomic Imaging of 3D Active Site by Micro-Photoelectron Holography at SPring-8: Towards collaboration with MAX IV

Author: Toyohiko Kinoshita[1]

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We have organized a research group to investigate "3D active site"by using photoelectron holography (see, http://www.en.3d-activesite.jp/). In this project, photoelectron holography measurements for a variety of materials, such as impurity sites of dopants, active sites of catalysis, and local structures of interfaces fulfil their important functions are performed at the soft-x-ray beamlines of SPring-8.

Some of the successful examples are introduced together with the apparatus used in the project (the Display-type Spherical Mirror Analyzer (DIANA), a hemispherical analyzer (DA30), the display-type ellipsoidal mesh analyzer (DELMA), compact display type analyzers such as PESCATORA and a retarding field analyzer and the lens part of DELMA (WAAEL)). The compact ones can be introduced into some beamlines at MAX IV. For the time-resolved measurements, we set experimental apparatuses, such as pump laser branch lines, soft-x-ray choppers and so on.

Sessions:

Quantum systems & processes

4

Role of ultrafast dissociation in the fragmentation of chloromethanes

Author: Esko Kokkonen[1]

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Ultrafast dissociation (UFD) has been found to be an effective way of reorganizing molecular internal energy after an X-ray induced excitation. In the UFD scheme, the molecule decays while the Auger process is still ongoing. This is often experimentally seen as sharp atomic Auger states, which are different from broader molecular states.

In this work we have studied the UFD phenomenon in various chlorinated methane molecules. In each case, a Cl $2p$ electron was promoted to an antibonding σ^* type orbital. The subsequent fragmentation was studied using electron-ion coincidence spectroscopy. All cations were measured and coincidences between the fragments and the resonant Auger electrons were recorded. Clear indicators of UFD in the resonant Auger electron spectra were found. These states also correspond to an ejection of an atomic species from the parent molecule, which in this case was always atomic chlorine. UFD response was found to vary in different CHC molecules.

Sessions:

Quantum systems & processes

5

Calibration of the Fe/O-based spin detector FERRUM by a double-scattering experiment

Author: Matthias Escher[1]

Co-authors: Christian Datzer [2]; Christian Thiede [2]; Hubert Ebert [3]; Jan Minár [3]; Markus Donath [2]; Michael Merkel [1]; Nils B. Weber [1]; Stephan Borek [3]

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We report on the characterization of the FERRUM spin-polarization detector, a highly efficient, easy to handle detector based on exchange scattering from a Fe(100)-p(1x1)O surface [1]. The calibration used two scattering processes under the same geometry, eliminating the uncertainty of the primary-electron spin-polarization.
Low-energetic electrons are specularly reflected at an incidence angle of 15° and partially polarized at the first iron film. Subsequent energy and spin analysis is performed with the EasySPIN analyzer,

consisting of a cylindrical sector analyzer (CSA) and a FERRUM detector, where the second scattering process takes place.
Theoretical calculations are in good agreement with the experiments. We obtain a Sherman function of 27.5±1.0% in agreement with previous results [2].

References

[1] R. Bertacco, D. Onofrio and F. Ciccacci, Rev. Sci Instrum., 70, 3572 (1999)

[2] M. Escher, N.B. Weber and M. Merkel, e-J. Surf. Sci. Nanotech. 9, 340-343 (2011)

Sessions:

Quantum systems & processes

6

Time-resolved in-operando SAXS/WAXS studies of organic thin films and model devices at XMaS

Author: Oier Bikondoa[1]

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Organic and hybrid thin-films (OTFs) are implemented in a range of device types (solar cells, LEDs, TFTs, sensors, etc.) due to their appealing properties. Such devices do improve sustainability due to the use of more eco-friendly materials compared to the traditional electronics industry and also because of the use of more energy-efficient manufacturing technologies. The research and development in these fields are primarily pursuing the improvement of 1) device performance and 2) device lifetime. Both aspects are strongly influenced by the molecular and microstructural properties of the thin films and their evolution during operation. At XMaS (www.xmas.ac.uk), we have developed several environmental cells and metrologies to correlate the time evolution of OTF model devices as a function of applied electric fields and under controlled thermal and humidity protocols mimicking normal operational conditions. We present examples of studies performed on solar cells and TFTs.

Sessions:

New Materials & Energy

7

First experiments at the NanoMAX beamline

Author: Ulrich Vogt[1]

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NanoMAX is the first beamline to take full advantage of MAX IV's exceptional low emittance and resulting coherent properties. We will present results from the first experiments at NanoMAX that took place in December 2016. We used zone plates with outermost zone widths of 100 nm and 30 nm and performed experiments at 8 keV photon energy on x-ray fluorescence and ptychography, both in step-scan and fly-scan mode. Moreover, we investigated stability and coherence with a Ronchi test method. We could demonstrate spatial resolution below 50 nm after only few hours of beamtime on both test and nanowire samples.

Sessions:

New Materials & Energy

8

In operando X-ray characterization of single nanowire devices

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Hard X-rays offer the ability to measure nanoelectronic devices in more or less realistic operational conditions. Nanofocused hard X-rays were used to quantitatively measure both strain and bending in a single nanowire device under electric bias. Furthermore, the X-ray beam induced conductance (XBIC) was measured in several single nanowire devices. Scanning X-ray Bragg diffraction was performed with 100 nm real-space resolution along the nanowire axis, also within the metal contacts. The 3D shape of the nanowire was reconstructed from the XRD data. In the as-processed device, the strain was small but the nanowire was bent in an arch between the contacts. The device was then exposed to increasing bias voltages until breakdown, while simultaneously measuring the electrical current. The structural changes were correlated with a reduction in electrical conductance.

Sessions:

New Materials & Energy

9

Recent topics of X-ray fluorescence holography

Author: Koichi Hayashi[1]

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X-ray fluorescence holography (XFH), which was first demonstrated in Europe, can determine atomic arrangements around a specific element without any prior knowledge of structures. To date, using XFH we have obtained new information on the structures of some advanced materials. Since 2014, we have conducted the "3D active site"project (http://www.en.3d-activesite.jp/), whose aims are analyses and designs of active sites in materials. XFH is one of the main methods in the project. Although XFH is interesting and important method to understand mechanisms of functional materials, it is still not widespread in the world. Therefore, we should make many opportunities to advertise our activities. Moreover, we are now seeking good beamlines to carry out XFH experiments in Europe. MAX IV is a strong candidate for us. In our poster presentation, we show our XFH setup in SPring-8 and its several recent topics.

Sessions:

New Materials & Energy

10

Atomic and Electronic Structure study of Silicene and hydrogenated Silicene on Ag(111)

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We report a detailed study of the atomic and electronic structure of the "2√3"silicene on Ag(111) using LEED, STM and ARPES. Our ARPES data show three dispersive bands around normal emission which is qualitatively consistent to the DFT calculations of the electronic structure of a relaxed 2√3 model that will be presented. Theoretical calculations suggest that hydrogenated silicene has the same hydrogen chemisorption geometry and band gap opening as graphane. After hydrogenation of the "2√3"silicene on Ag(111), the change in the LEED pattern indicates that the buckling of the silicene sheet on Ag(111) is reduced. STM images reveal a hexagonal structure with the periodicity of the silicene (1×1) lattice which is consistent with the chair-like model. The ARPES data show two dispersive bands around normal emission which are in good agreement with the theoretical band structure of our DFT calculations based on a chair-like model of free-standing half-silicane.

Sessions:

New Materials & Energy

11

Temperature-dependent surface propensities of solutes in a water liquid jet

Author: Clara-Magdalena Saak[1]

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The aqueous interface is a unique environment, distinct from the liquid continuum due to geometric constraints and energetic considerations not found in the bulk. Surface effects are mainly driven by the competing solute-water and water-water interactions, as well as larger scale entropic contributions, however disentangling these individual contributions remains a significant challenge.
Here we present surface-sensitive temperature-dependent soft X-ray photoelectron spectroscopic measurements of a water liquid jet containing inorganic salts. Tracking the behaviour as a function of temperature allows us to estimate the relative strengths of the driving forces that govern surface propensity. From this work we aim to quantify the molecular processes that underpin interfacial solvation behaviour, thereby contributing to a more fundamental understanding of the energetics of the aqueous interface.

Sessions:

Quantum systems & processes

12

The impact of organic acids on the surface enrichment of sodium and calcium ions in sea spray aerosols

Authors: Clara-Magdalena Saak[1]; Ilona Riipinen[2]; Isaak Unger[3]; Matthew Salter[2]; Minna Patanen[4]; Olle Björneholm Björneholm[5]; Paul Zieger[2]

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Aerosols in the atmosphere impact the radiative balance of the earth and according to the IPCC their influence is one of the major uncertainties in climate models. One of the most common natural aerosol species is sea spray aerosols. Their composition affects the chemistry at the gas-particle interface and their ability to act as cloud condensation seeds. Until recently, it has been consensus that the composition of sea spray aerosols mimics the composition of seawater. We used X-ray photoelectron spectroscopy to probe the topmost atomic layers of sea spray aerosols to investigate the enrichment of Ca2+ therein. Experiments have been carried out on aerosols from a sea salt solution and from solutions of sea salt and different amounts of acetic acid, which we utilized to mimic the presence of surface-active organic molecules in seawater and their impact on the amount of Ca2+ at the gas-particle interface.

Sessions:

Environmental and Earth Sciences

13

Prospects of time resolved photoluminescence spectroscopy at the FinEstBEAMS beamline

Author: Sebastian Vielhauer[1]

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The upcoming FinEstBEAMS beamline at the MaxIV 1.5 GeV ring, which is planned to go into operation later this year, will provide a wide range of photon energies from the VUV to soft X-Ray range (~4.3 eV to 1000 eV). One of the permanent stations for this beamline will be dedicated to photoluminescence spectroscopy (PLS) of solids. New technologies, e.g. in HEP detector design and medical applications, drive the demand for novel luminescent materials such as ultrafast scintillators or nano-sized particles. PLS at FinEstBEAMS allows to examine the luminescence properties under excitation of valence and inner shell electrons. Time-resolved spectroscopy plays a crucial role for studying the dynamics of the energy transfer processes and for identifying characteristic emissions by their lifetimes. It is also used for separating spectrally overlapping luminescence channels with time gating. Examples for applications of time resolved PLS in the sub-ns to µs range are presented in this talk.

Sessions:

Quantum systems & processes

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LP3 and DEMAX

Author: Wolfgang Knecht[1]

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Wolfgang Knecht (1) and Zoe Fisher (1,2)

1) LP3, 2)ESS

Proteins are of enormous importance to life and a prominent topic in life sciences. Access to both X-ray (MAX IV) and neutron sources (ESS) will increase the capacity for innovation in the life sciences. To enable use of these unique facilities, Lund University hosts the protein production facility, LP3 (www.lu.se/lp3). LP3 assists users with: 1) Recombinant protein production, 2) High-throughput crystallization, and 3) Stable isotope labelling and bio-deuteration of biological macromolecules. In 2016, the DEuteration and MAcromolecular Xtallization (DEMAX) platform of the European Spallation Source ERIC (ESS) co-localized with LP3. LP3 and DEMAX are coordinating in their efforts to develop cost-effective production of deuterated proteins for macromolecular crystallography, enable crystallization of interesting proteins for neutron work, and for the production of labeled proteins/lipids for neutron reflectometry.

Sessions:

Life Sciences

15

Electronic structure study of ionic liquids

Author: Ivar Kuusik[1]

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Although ionic liquids have very low vapor pressures and are UHV compatible liquids (!), it is still possible to vaporize them and do gas phase studies. It has been shown that in most cases intact ion-pairs are evaporating from the ionic liquid - ionic liquid molecules. Very few gas phase studies of ionic liquids have been done to date, while the liquid phase has been studied extensively. The valence band UPS spectrum of the EMIM-BF4 ionic liquid reveals interesting electronic structure. We compare gas and liquid phase electronic structures with different quantum chemistry calculations and show that electronic relaxation during photoemission is happening in the inner valence band, while little or no relaxation occurs in the anion.

Sessions:

Quantum systems & processes

16

Studying materials by combining analysis techniques and sample environments at Diffabs beamline (Synchrotron SOLEIL)

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The wide range of instrumental techniques at DiffAbs beamline concerns numerous sectors of fundamental and applied research among which the science of materials holds a predominant position. In particular, in situ studies of the transformations in materials at (ultra-)high temperature is the domain of excellence of the beamline. The interest of coupled absorption and diffraction measurements is to ensure that both experiments are carried out on the same zone of the sample, in absolutely identical physico-chemical conditions (T, p, reactive atmosphere), i.e. establishing correlations between the information provided by both types of measurements. Local probe approach (few microns X-ray beams) can be also used.
After a brief description of the characteristics of the beamline and the users communities, several examples will be given. In the context of rapid data acquisition schemes (N-dimensions large datasets), issues like data handling, mining, storage and treatment will be addressed.

Sessions:

New Materials & Energy

17

Tender X-ray Spectroscopies on isolated Atoms and Molecules

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Tender x-ray spectroscopy.
Recoil
Post Collision Interaction
Localization/ Delocalization

Sessions:

Quantum systems & processes

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3D measurement of strain around a tin whisker

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Tin whiskers are a growing problem in the electronics industry as they can lead to short circuits and catastrophic failures of components. Whiskers are hair-like grains of tin that grow spontaneously out of tin plated surfaces. The underlying mechanisms of whisker growth are still not fully understood. The main hypothesis is that whiskers grow to release stress built up in the tin layer.

We have measured the strain field around a tin whisker using the Laue microdiffraction setup at BM32 of the ESRF. Conventional Laue diffraction gives results averaged over the volume probed by the x-ray beam. To achieve spatial resolution along the beam we have used the DAXM-technique being developed at the ESRF, which makes it possible to reconstruct the crystal orientations and the (deviatoric) strain field in three dimensions. For this study, this approach allows analysis of the in-depth strain gradients believed to be an important factor behind whisker growth.

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UPS AND DFT Investigation of the electronic structure of gas-phase Trimesic acid

Author: Liis Reisberg[1]

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One of the promising self-organizing molecules of supermolecular structures is benzene-1,3,5-tricarboxylic acid (trimesic acid, TMA, C6H3(COOH)3), which is composed of three peripheral carboxyl groups attached to central benzene ring.

In this study, we have utilized Ultraviolet Photoelectron Spectroscopy (UPS), carried out at beamline I411 of the MAX II storage ring, and Density Functional Theory (DFT) to investigate and resolve valence band electronic structure of TMA.

In the current study outer valence band electronic structure of TMA was interpreted. Furthermore, experimental and calculated TMA spectrum were compared to ones of benzene and benzoic acid. Ab initio DFT calculations are in good accordance with experimental binding energies. It is shown that similarities between molecular orbitals energies and shapes of benzene and TMA exists. It is demonstrated that the addition of carboxyl groups to the benzene ring clearly correlates with increasing binding energy.

Sessions:

Quantum systems & processes

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STATUS OF THE FINESTBEAMS BEAMLINE AT MAX-IV LABORATORY

Author: Rainer Pärna[1]

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The FinEstBeaMS is a materials science beamline mounted at the 1.5 GeV storage ring of the MAX IV facility. The beamline has two branch lines and three permanent end stations. The gas-phase end station has been mounted at the beamline, the photoluminescence end station is in installation and the solid state end station will be commissioned by the end of 2017.

Dedicated end stations cover wide range of sciences from processes occurring in the upper part of atmosphere, fragmentation pathways of bio- and organic molecules to formation of nanoparticle. It will be possible to characterize luminescent materials, investigate nanomolecular layers on alloy surfaces and electrochemical double layer capacitors in situ.

The FinEstBeaMS will receive first light in autumn 2017.

Main funding for the beamline has been received from the Academy of Finland through the FIRI funding projects and from the EU.

Sessions:

Quantum systems & processes

21

Visualization of Gas Distribution in a Model AP-XPS Reactor by PLIF: CO Oxidation over a Pd(100) Catalyst

Author: Jianfeng Zhou[1]

Co-authors: Edvin Lundgren [1]; Johan Gustafson [1]; Johan Zetterberg [1]; Sara Blomberg [1]

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In situ knowledge of the gas phase around a catalyst is essential to make an accurate correlation between the catalytic activity and surface structure in operando studies. In this work, planar laser-induced fluorescence (PLIF) is used to visualize the CO2 distribution in a model AP-XPS reactor, during CO oxidation over a Pd(100) catalyst. The results show that the gas composition in the vicinity of the sample measured by PLIF is significantly different from that measured by a conventional mass spectrometer connected to a nozzle positioned just above the sample. In addition, the gas distribution above the catalytic sample has a strong dependence on the gas flow and total chamber pressure. The technique presented has the potential to increase our knowledge of the gas phase in AP-XPS, as well as to optimize the design and operating conditions of in situ AP-XPS reactors for catalysis studies.

Sessions:

New Materials & Energy

22

Combining synchrotron light with laser technology in catalysis research

Author: Sara Blomberg[1]

Co-authors: Jianfeng Zhou [1]; Johan Gustafson [1]; Johan Zetterberg [1]; Mikhail Shipilin [1]; Per-Anders Carlsson [2]; Sebastian Pfaff [1]; Uta Hejral [1]; edvin lundgren [3]

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The surface structure detected during the reaction is sensitive to the composition of the gas phase close to the catalyst surface and the catalytic activity of the sample itself may affect the surface structure. For this reason, we have combined Planar Laser-induced Fluorescence (PLIF) with High Energy Surface X-ray Diffraction (HESXRD) during CO oxidation over a Pd(100) crystal. PLIF compliments the surface structural information observed by HXSXRD with 2D visualization of the gas phase in the vicinity of an active model catalysts. Here in, we present the very first experiment where we combined the two operando techniques of HESXRD and PLIF, where we correlate the sample structure and CO2 distribution on subsecond time resolution. The images of the CO2 gas distribution show a significant different gas composition close to the highly active surface as compared to the rest of the chamber, which is also reflected in the observed surface structure.

Sessions:

New Materials & Energy

23

Structural Characterization of the TP901-1 CI Repressor Protein

Author: Anders Varming[1]

Co-authors: Jens-Christian Poulsen [2]; Karin Hammer [3]; Kim Krighaar Rasmussen [4]; Kristian Frandsen [4]; Leila Lo Leggio [4]; Malene Ringkjøbing Jensen [5]; Mogens Kilstrup [3]; Peter Waaben Thulstrup [4]

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TP901-1 is a temperate bacteriophage of the P335 type that infects Lactococcus lactis bacteria. It has a bi-stable genetic switch making it able to shift between either the lytic or lysogenic life cycle; this is controlled by the regulatory protein called the CI repressor. CI consists of two functional domains connected by a flexible linker, namely an N-terminal domain (NTD) responsible for DNA binding through a helix-turn-helix motif (HTH), and a C-terminal domain (CTD) responsible for the formation of the hexamer.
Here, we present the current state of knowledge on the structure of TP901-1 CI:

- X-ray crystal and SAXS structures of NTD containing CI constructs with and without DNA
- Investigation of the secondary and tertiary structure of the CTD and its subdomains, by CD and NMR spectroscopy and X-ray crystallography revealing a high helical content, which is in clear contrast to the to the CI repressor CTD of the lambda phage

Sessions:

Life Sciences

24

Luminescence endstation at the FinEstBeaMS beamline

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Luminescence experiments at Max IV Lab are going to be performed in one of the branches of FinEstBeaMS beamline, which is developed by a consortium of Finnish and Estonian Universities. The luminescence endstation consisting of an ultra-high vacuum chamber with a close-cycle helium cryogenic system was designed and constructed. To analyze photoluminescence in the UV to near IR range a Shamrock spectrometer equipped with a CCD and several photomultiplier detectors is coupled to an optical fiber, collecting emission from the sample. The registration of the UV luminescence us-ing a UV spectrometer is under development. Upcoming luminescence experiments will include also time-resolved option in single bunch mode and/or utilizing a chopper. The possibility of high-resolution excitation scanning and the option to change the polarization of the incident light by adjusting the undulator phase make this beamline very attractive for the field of luminescence studies under VUV-XUV excitations.

Sessions:

Quantum systems & processes

25

Atom Holographic Imaging and Orbital Characterization by Photoelectron Diffraction

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Photoelectron diffraction provides information on the surrounding atomic configuration, which is recorded as forward focusing peaks (FFPs) at local interatomic directions and diffraction patterns in the photoelectron intensity angular distribution (PIAD). Since PIAD differs by different surrounding atomic arrangement, emitter atom sites can be specified by their characteristic diffraction patterns. By combining this diffraction technique with various spectroscopies (diffraction spectroscopy), the electronic property information of each atomic site structure can be investigated individually. The photoelectron from a localized core level is an excellent probe for element-specific atomic and electronic structure analysis. Here, let us introduce our recent research activities at SPring-8, Japan.

Sessions:

New Materials & Energy

26

Can gas-phase experiments explain the chemistry of radiosensitization?

Author: Eero Itälä[1]

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Nitroimidazoles are imidazole derivatives and have proven to be potent radiosensitizers, compounds that increase the effects of ionizing radiation *e.g.* in radiation therapy. However, despite the promising results on nitroimidazolic compounds in radiosensitization, the exact chemistry of how nitroimidazoles act as radiosensitizers is not fully understood. Combined with clinical studies, gas-phase studies on the fragmentation of three nitroimidaole isomers provide an insight into this matter. The most characteristic feature of the fragmentation following valence ionization (a process commonly related to radiation damage induced *e.g.* by medical X-rays) is the release of cationic or neutral NO, the rate and ratio of which depend greatly on the initial site of the nitro (NO2) group. This indicates that NO production plays an important role in the radiosensitization when nitroimidazoles are considered.

Sessions:

Quantum systems & processes

27

Reactions at Rare Earth Oxide Surfaces

Author: Andreas Schaefer[1]

Co-authors: Benjamin Hagman [1]; Edvin lundgren [2]; Jan Ingo Flege [3]; Jason F. Weaver [4]; Johan Gustafson [5]; Lindsay Richard Merte [5]; Mikhail Shipilin [5]; Uta Hejral [5]; jan Höcker [3]

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This contribution surveys recent results on chemical reactions at rare earth oxide surfaces and nanostructures mainly measured at the MAX-II ring. We studied methanol oxidation on terbia thin films by PES (D1011) and compare the data to earlier results obtained on samaria, praseodymia, and ceria thin films. We found a clear contrast in reactivity of reduced and oxidized terbia films compared to ceria. On Tb₂O₃ methanol mainly desorbs through both molecular and recombinative processes while on TbO₂ nearly half of the adsorbed methanol is transformed into formaldehyde and water (desorbing at 350 K) and CO₂ (600K). Further, results of our recent XPS studies (9.3.2 ALS, Berkeley) on the re-oxidation of CeO_x/Rh(111)

inverse model systems by CO₂ and on the structure of PrO_x/Ru(0001) islands, studied by LEEM intensity-voltage measurements (I311) , are summarized.

Sessions:

New Materials & Energy

29

In situ small angle X-ray scattering of a levitated cellulose nanocrystal droplet

Author: Yingxin Liu[1]

Co-authors: Andreas Fall [1]; Christina Schütz [2]; German Salazar-Alvarez [1]; Lennart Bergström [1]; Michael Agthe [1]

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Aqueous dispersions of cellulose nanocrystals (CNC) produced by acid hydrolysis from plants and bacteria, can form a chiral nematic liquid crystalline phase. In this study, SAXS was applied to explore the time-dependent and evaporation-driven assembly of CNC rods in levitating aqueous droplets. By correlating estimates of the CNC concentration from measurements on the diameter for the shrinking droplet with analysis of the SAXS data, we find that the average spacing between the CNC rods decreases from 47 nm to 1.4 nm, as the volume fraction increases from 1.5 to 38 vol%. The competition between percolation gelation of CNC rods and chiral nematic liquid crystal assembly eventually results in the formation of a hollow CNC sphere. Quantitative exploration of CNC colloidal assembly at high concentrations provides important insight into the competition between gelation, aggregation and self-assembly that can be used in the fabrication of advanced nanocellulose-based materials.

Sessions:

Quantum systems & processes

31

A Versatile Operando Catalysis Flow Reactor for Combining X-Ray Transmission Surface Diffraction with Laser Induced Fluorescence

Author: Uta Hejral[1]

Co-authors: Jakub Drnec [2]; Johan Gustafson [1]; edvin lundgren [3]

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Catalysts are widely employed in fuel cells, vehicle exhaust control systems and chemical industry. Their wide application triggers an economic interest in improving their performance by understanding the interplay between catalyst structure, the surrounding gas phase and catalytic activity.

Transmission Surface Diffraction (TSD) is a novel technique which we are extending to our operando catalysis studies. Unlike conventional (High Energy) Surface X-Ray Diffraction it allows, with high spatial resolution, the study of catalyst structure while ramping the temperature. Planar Laser Induced Fluorescence (PLIF) yields direct information on the gas composition close to the catalyst surface and hence spatially resolves its catalytic activity.

Here we present a novel operando catalysis flow reactor which facilitates the simultaneous use of TSD, PLIF and in-situ Mass Spectrometry and hence the immediate correlation between catalyst structure and catalytic activity.

Sessions:

New Materials & Energy

32

A STRUCTURAL AND FUNCTIONAL INVESTIGATION OF RIBONUCLEOTIDE REDUCTASE CLASS III IN BACILLUS CEREUS

Author: Hedda Johannesen[1]

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Ribonucleotide reductase (RNR) is responsible for the rate-limiting step of DNA synthesis and is therefore a target for anticancer, antibacterial and antiviral agents. The RNRs are divided into three classes based on their radical chemistry. The focus of this project is the strictly anaerobic Class III RNR from the pathogenic bacterium *Bacillus cereus*. It consists of a catalytic unit (NrdD) with a glycyl radical, and a radical initiator unit (NrdG) containing an iron-sulphur cluster. By combining structural and spectroscopic studies, in addition to binding and kinetic studies we hope to solve the X-ray structure of NrdG and understand the activation and re-activation of NrdD by NrdG. This knowledge should give new insight into class III RNR activation, and confirm or contribute to a reviewing of the current reaction mechanism. We are currently establishing purification procedures for NrdD and NrdG followed by crystallisation trial, that will partly be executed at Lund University.

Sessions:

Life Sciences

33

In Situ Patterning of Ultra Sharp Dopant Densities in Silion

Author: Simon Cooil[1]

Co-authors: Alexei Zakharov [2]; Jill Miwa [3]; Justin Wells [4]; Yuran Niu [5]

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We demonstrate a new method for patterning a buried two-dimensional electron gas (2DEG) in silicon using low kinetic energy electron stimulated desorption (LEESD) of a monohydride resist mask. A buried 2DEG forms as a result of placing a dense and narrow profile of phosphorus dopants beneath the silicon surface; a so-called δ-layer. Such 2-dimensional dopant profiles have previously been studied theoretically, and by angle-resolved photoemission spectroscopy, and have been shown to host a 2DEG with properties desirable for atomic scale devices and quantum computation applications. Here we outline a new patterning method based on low kinetic-energy electron beam lithography, combined with in-situ characterisation, and demonstrate the formation of patterned features with dopant concentrations sufficient to create localised 2DEG states.

Sessions:

Quantum systems & processes

36

Structure determination of engineered GH51 alpha-L-arabinofuranosidase of Thermobacillus xylanilyticus

Author: Tobias Tandrup[1]

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In previous studies, engineered variants of GH51 α-L-arabinofuranosidase of *Thermobacillus xylanilyticus* have been identified and characterized for their improved transglycosylation properties. Therefore, these variants can be used as synthetic tools for the production of branched oligosaccharides, that could lead to different biomedical applications and bioinspired materials. Crystal structures, determined by X-ray diffraction, of two such variants, R69H-L352M and R69H-N216W-L352M, are here described as well as attempts to make complexes with ligands.

Furthermore, the structures are compared to wild-type (PDB 2VRK) and an active site mutant E176Q in complex with an oligosaccharide (PDB 2VRQ) solved in 2008. In addition to the direct effect of the mutated residues, the indirect effect that the mutations have had on the local structure has been analyzed in detail and is discussed in relation to the properties of the enzyme variants.

Sessions:

Life Sciences

37

Fatty acid biosynthesis pathway as target for antibiotic development: structural and biochemical characterization of FabG inhibitors

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The spread of antibiotic-resistance among bacterial pathogens presents one of the major challenges we face today. The problem is particularly serious in the case of Gram-negative bacteria since there are only a few effective antibiotics currently available. Species constituting the ESKAPE group including Pseudomonas aeruginosa, Klebsiella pneumoniae and Acinetobacter baumanni are responsible for most of the nosocomial infections and impose a growing burden on health care systems worldwide. Development of antibacterial compounds that represent a novel mechanism of action is one possible solution, however challenging and requires the participation of academia and industrial partners. Fatty acid biosynthesis in bacteria has been identified as an attractive drug target and several antibiotics (e.g. triclosan, isoniazid) inhibiting this pathway are in use. We have demonstrated the essentiality of the fabG gene in P. aeruginosa furthermore, fabG is an essential gene, hence a promising drug target, in Staphylococcus a., E. coli, Salmonella t., Acinetobacter b. and in M. tuberculosis. In collaboration with the Drug Discovery Unit at the University of Dundee (Scotland) 44 novel inhibitors of P. aeruginosa FabG were identified representing different chemical scaffolds. The strongest inhibitors exhibit binding constants in the lower nM range. Crystal structures of 15 enzyme-ligand complexes show that these compounds bind, unexpectedly, at an allosteric binding site far from the active site, revealing a novel mechanism of action. In order to explore the activity of these inhibitors against the FabG as target from various pathogenic bacteria the study was extended, and several FabG protein structures and the first ligand complex structures were determined using X-ray diffraction data collected at the BioMAX beamline at MAX-IV. In collaboration with the BITS Pilani institute (Hyderabad, India) using these protein-ligand structures as templates compounds were designed that inhibit FabG in more than one species. These inhibitors are characterized regarding their target specific inhibitory effect and their binding mode is investigated by crystallography and presented as valuable starting points for the development of antibiotics.

Sessions:

Life Sciences

38

Combined in-house X-ray scattering and X-ray microtomography of plant structures

Author: Patrik Ahvenainen[1]

Co-authors: Aki Kallonen [1]; Heikki Suhonen [1]; Kirsi Svedström [1]; Lorna J. Gibson [2]; Patrick G. Dixon [2]

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The hierarchical structure of plant materials requires measurements at multiple length scales. X-ray microtomography (XMT) and wide-angle X-ray scattering (WAXS) yield information at micrometer and nanometer scales, respectively. A unique bench-top set-up at the University of Helsinki combines the XMT and WAXS instruments [1].

The localized WAXS connects with 200-µm spatial resolution the sample crystallinity, the average crystallite size and the crystallite orientation to the µm-level structure. It is uniquely suited for certain experiments and a complementary tool for advanced synchrotron studies.

The set-up was recently used to study the microfibril and cell orientation in different tissues of Moso bamboo [2]. Novel quantitative models for the microfibril angle distribution in different tissues were obtained. A new application for this set-up is a project on the wood material used in guitars.

[1] J.-P. Suuronen et al., J. Appl. Cryst. 47 (2014) 471

[2] P. Ahvenainen et al., Plant Meth. 13:5 (2017)

Sessions:

Life Sciences

39

Shedding light on metals in complex systems using X-ray spectroscopy

Author: Graham George[1]

Co-authors: Ingrid Pickering [1]; Natalia Dolgova [1]; Susan Nehzati [1]

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X-ray absorption spectroscopy (XAS) can provide details of the local physical structure and electronic structure of metal ions in a variety of samples. One unique advantage of the method is that it can be used to probe metals in situ in a variety of systems with little or no pre-treatment. As such, XAS has been used to develop an understanding of diverse systems including intermediates of chemical reactions, metalloenzyme active sites, intact biological tissues or organisms, and environmental samples. Despite its success, applications of the method can be limited by spectroscopic lifetime broadening and by lack of access to low concentrations. Recent progress in advanced spectroscopy can overcome both of these limitations, with adequate spectra from concentrations as low as 100 nM. The advantages and limitations of the spectroscopic methods will be discussed, with examples of applications taken from the authors' current research.

Sessions:

Life Sciences

40

In-situ characterization of aerosol nanoparticle production using synchrotron radiation

Author: Sarah McKibbin[1]

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Air borne nanoparticles are the subject of innumerable inquires ranging from the global rise in soot production to applications in smart coatings and catalysis. Aerosol Au nanoparticles have been used to seed growth of III-V nanowires in a technique called Aerotaxy, and has the potential to minimize costs associated with high efficiency nanostructured solar cells[1]. To observe such growth in real time to understand the mechanisms at play would be invaluable.

While small-angle x-ray scattering (SAXS) of synchrotron radiation has been used to study soot aerosols[2], the low concentration of synthesized particles considered here present new challenges. We characterize Au & Pt nanoparticles during spark production in a gas flow by SAXS, a critical step in real-time observation of Aerotaxy. We also discuss the future of in-situ diffraction experiments at MaxIV using a custom built reaction chamber.

[1]M. Heurlin et al., Nature 492, 90–94 (2012).
[2]G. Ferraro, et al.,Energy Fuels 30, 9859–9866 (2016).

Sessions:

New Materials & Energy

44

MedMAX: The biomedical Imaging beamline

Author: Rajmund Mokso[1]

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MedMAX is proposed to be the first MAX IV beamline fully dedicated to full-field imaging in the Fresnel diffraction regime with hard X-rays (12-40 keV). With emphasis on studying processes in biological systems at the micrometer scale, advanced reconstruction routines will be valuable for optimizing the radiation dose on sample. The infrastructure will be set up for in vivo imaging of small animals but applications accross biology and soft matter will all be relevant for this beamline.

Sessions:

Life Sciences

45

Native Oxide Reduction by Zn doping in GaAs Aerotaxy Nanowires

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III-V semiconductor nanowires (NWs) continue to show promising results as components in energy saving devices. Using X-ray Photoelectron Spectroscopy (XPS) we study GaAs NWs grown by the novel aerotaxy growth technique[1]. In aerotaxy the NWs are catalyzed from Au aerosol nanoparticles floating freely in a continuous N2 flow mixed with group III and V precursor gases.

NWs grown using different amount of Zn doping[2] are examined by XPS. Fig 1. shows the As *3d* peak at 350 eV for samples with different doping. The ratio between As-oxide and As-Ga is highest for the lightly doped NWs and lower for the more heavily doped NWs. We suggest that the Zn incorporation reduces the growth of Ga and As surface oxides on the NWs. We also show Atomic Force Microscopy (AFM) measurements and surface roughness analysis of NWs with different doping.

Fig. 1 –XPS core level spectra of As *3d* at 350 eV.

[1] M. Heurlin, et al. Nature 492, 90-94, 2012.

[2] F, Yang, et al., J. Cryst. Growth 414, 181-186, 2015.

Sessions:

New Materials & Energy

46

The Soft X-ray Laser Beamline (SXL) project

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I will present the current status of the scientific case and plans for the Soft X-ray Laser (SXL) beam line at MAXIV and how this can couple to various activities at the MAXIV rings.

Sessions:

Quantum systems & processes

47

AQP2 interaction with lysosomal sorting protein LIP5

Author: Jennifer Roche[1]

Co-authors: Maria Gourdon [1]; Sabeen Survery [1]; Stefan Kreida [1]; Susanna Horsefield [1]

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Selection of membrane proteins for possible degradation in lysosomes, is an important mechanism for controlling protein expression in the plasma membrane. AQP2 upon phosphorylation is shuttled to the apical membrane. Conversely, down-regulation of the aquaporin commences with ubiquitination with subsequent internalization and lysosomal degradation. Details of this regulation for AQP2 are still yet to be elucidated. The lysosomal trafficking regulator–interacting protein 5 (LIP5) is presumably important for the sorting and degradation and has been shown to interact with the C-terminal tail of aquaporin. The aim is to investigate these proteins by microscale thermophoresis (MST), SAXS and X-ray crystallography.
Using MST, we show that AQP2 interacts with LIP5 with sub-micromolar affinity and the affinity is reduced when AQP2 is phosphorylated. Phosphorylation of Ser256, critical for AQP2 targeting to the apical membrane has approximately 10-fold lower affinity than unphosphorylated AQP2. This illustrates how post-translational modification governs AQP2 trafficking by modulating the affinity to regulatory proteins involved in the trafficking machinery.

Sessions:

Life Sciences

48

Using 3D x-ray diffraction and tomography to follow force-chain evolution in granular materials

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In recent years, significant progress has been made in exploring the mechanics of granular materials, such as sand, using x-ray tomography to reveal local grain kinematics and how the deformation focusses to lead to localised sample failure. However, with such approaches only the displacements and strains can be analysed, but the internal stresses and force transfer mechanisms cannot be resolved. To this end, we have explored the use of grain-resolved x-ray diffraction by 3DXRD to measure the internal strains of individual grains in granular samples undergoing deformation. Recent experimental results from a study on the mechanics of granular materials will be presented for samples of >1000 grains undergoing in-situ confined uniaxial compression. Using a combination of x-ray tomography and 3DXRD with image analysis and a force inference methodology it is possible to follow grain displacements and the inter-granular forces as well as stresses and strains during loading. The results show how the force transfer focusses into preferential pathways, i.e., “force chains”, that redistribute as grains fracture.

Sessions:

Environmental and Earth Sciences

49

Improving Methods for XAS Studies of Metalloproteins at Balder Beamline

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Metalloproteins are most often related to important, biological redox processes. Due to strong scattering from metal centers combined with limited data resolution, the metal coordination is often poorly determined. In addition, the metal centers are subject to photo-reduction in the X-ray beam.

Nevertheless, an accurate description of the redox center in different oxidation and/or coordination states is the key to understand the mechanisms of such a protein and for rational drug design.

In the last ten years XAS (X-ray Absorption Spectroscopy), made up by EXAFS (Extended X-ray Absorption Fine structure Spectroscopy) and XANES (X-ray absorption near edge spectroscopy), has significantly improved the situation. XAS is unique as it probes a specific element –typically a metal. XANES reveals the oxidation state and coordination and both XANES and EXAFS give detailed information of the metal center coordination, typically with standard errors in distances better than 0.01 Å [1-3]. Furthermore, EXAFS and XANES measurements are not limited to the solid state but may be performed on proteins in solutions as well. This opens up for in situ studies and the use of flow cells to ensure oxidation states and to study redox processes and reactions in situ.

The research group at DTU Chemistry in collaboration with beamline scientists at MAX IV is designing the setup for XAS experiments on metalloproteins at the new beamline Balder. This beamline will be of high intensity and low divergence, and thus require lower concentration and measurement time, but at the same time be more challenging in terms of photo-reduction and radiation damage.

The setup includes a microfluidics chip, that prevents radiation damage to the sample, and allows for measurements at room temperature. We have already investigated the flow rates of solutions with different viscosity, and these are in the range of the rate required to avoid radiation damage. In situ UV measurements will also be implemented, to allow measuring at different points on the chip, i.e. along the reaction trajectory.

Acknowledgments

We would like to thank InterReg for their funding of the project.

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Sessions:

Life Sciences

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3D crystallography of kesterite absorber layers

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One of the most promising materials for third generation solar cells is Cu2ZnSnS4 (CZTS) which crystallizes in the kesterite structure [1].
CZTS is a quaternary compound that is thermodynamically stable in a narrow region of the phase diagram Cu2S-SnS2-ZnS [2]. On the other hand high-efficiency CZTS solar cells are off-stoichiometric (Cu-poor, Zn-rich). As a consequence of the thermodynamics and of stoichiometric inhomogeneities, secondary phases which include ternary chalcogenide and binary compounds can form. A new approach to study the structures of CZTS is multigrain crystallography which provides structural characterization of multiphase material at grain scale and atomic scale. Utilizing 3D X-ray diffraction (3DXRD) microscopy, 3D maps of the grains can be generated visualizing their morphology, orientations, and strain [3].
We present the results of simulations using PolyXSim - 3DXRD far-field simulation of polycrystals, which creates 3DXRD diffraction patterns of polycrystalline materials such as the kesterite and its secondary phases. The simulation aims to detect spot overlaps, and to assess the feasibility of the experiment.

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Sessions:

New Materials & Energy

51

Synchrotron photoionization spectroscopy of molecular precursor of functional materials

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Co-authors: Ambra Guarnaccio [1]; Antonio Santagata [2]; Barbara Brena [3]; Carla Puglia [3]; Giovanna Fronzoni [4]; Ieva Bidermane [5]; Johann Lüder [3]; Luca Lozzi [6]; Marcello Coreno [1]; Mauro Stener [4]; Monica de Simone [7]; Oscar Baseggio [4]; Roberta Totani [6]; Teng Zhang [3]

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Synchrotron radiation photoionization and photoexcitation experiments, like X-ray photoemission spectroscopy (XPS) and Near-Edge X-ray Absorption Spectroscopy (NEXAFS), are traditionally used for investigating the electronic structure of matter. Photon flux and energy resolution enable nowadays XPS and NEXAFS studies of gaseous samples over a large energy range and help in overcoming the problem of the intrinsic low signal level attainable from rarefied low-vapor-pressure targets., Such measurements are extremely important to investigate specific effects due to selective excitations of inner-shell electrons. Moreover, in the case of organic molecules precursors of functional materials, they provide a thorough characterization of electronic structures, whose knowledge is of great value for further condensed matter synchrotron radiation studies, which aim at a detailed analysis of intermolecular interactions in functional materials.
Our present study addresses molecular targets such as biphenylene and oligothiophenes. These highly conjugated organic molecules are characterized by a rich photochemistry. In a first step, XPS and NEXAFS data on gaseous samples are shown. By comparison with the results of Density Functional Theory (DFT) calculations, we can identify the characteristic contributions of chemically non-equivalent carbon atoms in the x-ray photoelectron spectra as well as in the core hole absorption spectra of these molecules, and to correctly assign them. The detail of their electronic structure are then used also to explain preliminary results on films of various thicknesses.

Sessions:

New Materials & Energy

52

Establishing the molecular mechanisms of solute-carrier (SLC) transporters: from snapshots to movies

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Crystal structures of small-molecule transporters have shed light on the conformational changes that take place during structural isomerization from outward to inward-facing states. Rather than a simple "rocking"movement of two bundles around a central substrate-binding site, it has become clear that even the most simplistic transporters utilize non rigid-body rearrangements. Here I will present two examples of SLC transporters and their homologues that revel novel refinements to the basic alternating access model currently shown in most textbooks.

Sessions:

Life Sciences

53

Surface and bulk photodegradation in air of PC60BM and PC70BM –comparative study

Author: Vanja Blazinic[1]

Co-authors: Ellen Moons [1]; Leif Ericsson [1]; Rickard Hansson [1]

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The PC60BM and PC70BM are most commonly used electron acceptors in organic solar cells (OSCs). While photoconversion efficiencies have reached commercially viable limit of 10%, overall stability of OSC devices is not sufficiently understood. Here the stability of spin-coated thin films of fullerene derivatives is studied after their exposure to simulated light (AM1.5) and ambient air. Near-edge X-ray absorption spectroscopy (NEXAFS) is used to investigate surface effects of photodegradation, while Fourier Transform Infrared Spectroscopy (FTIR) is used to study the bulk effects of photodegradation in air.

Sessions:

New Materials & Energy

54

t * Infrared Microscopy and nanoscopy at MAX IV.

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Infrared microscopy is under continuous development.
The possibility to couple an infrared spectrometer to an AFM machine has made it possible to go to ~10 nanometer spatial resolution. (Normal IR-microscopy has a spatial resolution from 2 –50 microns, depending on wavelength.)

There are different approaches to this.

One is s-Snom (scattering-scanning optical microscopy) where incident IR-light is focused on the AFM tip apex and the scattered light carrying the optical properties of the sample is collected. The localized light-matter interaction under the AFM tip can provide < 10 mm spatial resolution. By collecting the 2:nd harmonic of the scattered light from the tip an IR spectrum can be obtained.

AFM-IR is a variant where high speed pulsed ir light is focused onto the sample at the AFM tip location. When IR wavelength matches the material absorbance bands rapid thermal expansion occurs. This induces cantilever oscillations which are measured by the AFM. These oscillations can the be Fourier transformed into an IR spectrum.

Infrared tomography combines mid-infrared absorption contrast with computed tomographic data acquisition and reconstruction to enhance chemical and morphological localization by determining a complete infrared spectrum for every voxel.

Sessions:

Life Sciences

55

Synchrotron radiation XPS studies on interfacial thermal oxide on III-V semiconductors prior to high-permittivity oxides grown via Atomic Layer Deposition

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III-V semiconductor substrates such as InAs are characterized by a high carrier mobility, which opens promising perspectives for III-V based transistors for ultrafast (high-frequency) devices, and with significantly lower power dissipation as compared to Si-based technology. For such devices, usually high permittivity (high-k) oxides, such as HfO2 and Al2O3, are deposited onto the semiconductor substrate via atomic layer deposition (ALD). However, the interface between the high-k oxide and the III-V semiconductor substrate plays a crucial role, since high defect densities still hamper device performances. Recently[1] a new passivation approach has been explored, consisting in the removal of the native semiconductor oxide followed by a controlled passivation by thermal oxidation in ultra high vacuum (UHV) conditions prior to the ALD of the high-k oxide.
It has been claimed that this process provides lower interfacial defect densities, Fermi level (FL) unpinning, and lower capacity dispersion. However, the role and the nature of the interfacial thermal oxide deposited in UHV is still controversial, and further characterization is needed. Synchrotron radiation X-ray photoelectron spectroscopy (SR-XPS) is a powerful tool to study such semiconductor-oxide interfaces, since it is compatible with UHV equipment[2,3] and it is surface sensitive. Moreover, SR-XPS is also stoichiometry sensitive, and the high energy resolution allows a thorough chemical analysis of the different oxidation states of the same element.
We present a systematic SR-XPS study of InAs after subsequent processing steps of the passivation procedure, performed *in-situ* under UHV conditions in the SR-XPS chamber: We start with an InAs(100) substrate with native oxide at its surface, considering As3d, In3d, and In4d core levels. The native oxide was completely removed by annealing under a flux of thermally cracked hydrogen; afterwards the sample was heated and passivated under exposure to a controlled flux of O2, it was then taken out from the UHV environment, and an Al2O3 high-k oxide was grown via ALD. In addition to the XPS data, the success of the processing steps was further confirmed by scanning tunneling microscopy and spectroscopy as well as low energy electron diffraction.
We find that native and thermal oxides have a different stoichiometry: the former is formed by a combination of In-oxides and As3+ and As5+ oxides, whereas for the latter only the As3+ and an In2+ oxide components occur. The thin thermal oxide is not stable under ambient conditions and a further oxidation is observed after air exposure, with the occurrence of As5+ and metallic As. The subsequent ALD of Al2O3 results in the nearly complete removal of all As-oxides, as expected from previous studies[3,4].
The XPS analysis at different penetration depths shows that the As3+ component is mostly present at the surface, whereas As5+ is stronger at the interface, suggesting a permeable thermal oxide layer where the further oxidation takes place also in depth. We also observe a shift by ca. -0.2 eV of the binding energy, likely caused by FL unpinning, due to the decrease of the surface state density upon native oxide removal. However, the FL pinning is found to reoccur as soon as the thermal oxidation starts.

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Sessions:

New Materials & Energy

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Ambient Pressure XPS Study of a Surface-Supported Homogeneous Catalyst with Retained Activity

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Co-authors: Ashley Head [1]; Jan Knudsen [2]; Jesper Andersen [2]; Joachim Schnadt [3]; Olesia Snezhkova [1]; shilpi chaudhary [1]

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Immobilisation of homogeneous catalysts is of high interest due to its potential for higher reactor throughput, ease of separation, and catalyst reuse [1]. However, commonly catalysis is still achieved in a solvent-reactant-oxidiser-catalyst liquid mix. Here, we report evidence for catalytic activity of a surface supported heterogenised homogeneous catalyst in a reactant/oxidiser gas mixture.
The focus of our study is the transition metal complex Mn(III)-salen [R,R(-)N,N'Bis(3,5-di-t-butylsalicylidene, 1,2-cyclohexane diaminomanganese(III)chloride] which is highly active for Jacobsen-Katsuki epoxidation of unfunctionalised olefins in the homogeneous phase[2]. Here, the catalyst was deposited on a Au(111) surface to be studied with x-ray photoelectron spectroscopy (XPS) and scanning tunneling microsopy (STM) in UHV and ambient pressure XPS (APXPS) during reaction conditions. We will show that the UHV data can be accurately assigned and molecule-support interactions can be estimated with the help of density functional theory (DFT). Hence, the immobilisation can be understood from the propect of the catalyst's XPS fingerprint.
Propylene(C3H6) is here used to probe the chiral epoxidation reactivity of the surface-deposited Mn(III)-Salen using O gas as oxidiser. Surprisingly, the operando O 1s APXP spectra show CO_2 in the gas phase indicating propylene combustion already at room temperature. This is further confirmed by mass spectra simultaneously acquired with the APXPS data. Indeed, the occurrence of an oxidation reaction in the heterogeneous system shows the feasibility of the approach and the reactivity of the Mn(III)-Salen us further proved with μ-reactor experiments. Hence, we present a proof of concept for employing homogeneous catalysts in a solid-gas environment while retaining some of its catalytic properties.

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Sessions:

New Materials & Energy

57

Neutron studies of new drug leads for the inhibition of cancer-related human carbonic anhydrase IX

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Human carbonic anhydrase IX (HCA IX) expression in aggressive tumors, is an indicator of metastasis and poor cancer patient prognosis. As such, HCA IX has emerged as an important cancer imaging, diagnostic, and therapeutic target. Efforts to develop specific inhibitors for HCA IX are troublesome due to the presence of 14 other HCA isoforms. It has been well established, that ligand (inhibitor) binding to a target protein is mediated through interactions that may include: H-bonding directly and/or through intervening waters, electrostatic interactions with charged or polar amino acid side chains, metal coordination, energetic changes through water displacement, aromatic stacking, or other hydrophobic interactions. Our goal is to apply a powerful combination of X-ray and neutron protein crystallography to the HCA IX system in order to observe the details of ligand binding that involves H atoms. Comparing neutron crystal structures of unbound and drug-complexes of HCA IX with saccharin (a recently identified lead compound, that demonstrates some HCA IX specificity), provides a unique opportunity to directly investigate how saccharin binds through H-bonding, the role of water displacement, and how the making/breaking of H-bonds modulate binding and provides isoform specificity. On the basis of two solved X-ray and neutron derived structures each, we can show the changes in the H-bonding network due to saccharin binding. It is expected this fine structural detail, that is unique to neutron crystallography, can then be used for rational drug design.

Sessions:

Life Sciences

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X-ray phase contrast zoom tomography of biopsies from human peripheral nerves

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An optimal function of the hand and upper as well as lower extremity is deeply de-pendent on the structure and function of the peripheral nerves. Dysfunction, as in dia-betic neuropathy, can be deleterious for the individual patient. A crucial point to eval-uate the mechanisms by which nerves are

affected by a disease is to understand the structure of the nerves in health and disease. By conventional light and electron mi-croscopical techniques it is only possible to achieve a two-dimensional visualization of peripheral nerves. With novel x-ray imaging techniques in Life Science, i.e. the synchrotron technique, it is possible to get a three-dimensional (3D) visualization of nerve fibers in peripheral nerves.
Human nerve biopsies, taken after ethical permission, from the posterior interosseous nerve were harvested in conjunction with surgical treatment of patients with carpal tunnel syndrome. The biopsies were prepared for conventional morphological anal-yses with osmium staining (Thomsen et al Acta Neuropathol., 118(6): 785-91, 2009) and later examined with x-ray phase contrast zoom tomography at the European Syn-chrotron Research Facility (ESRF, Grenoble, France) at the ID16-NI beamline. At Id16-NI a set of KB mirrors focus the beam to a virtual secondary source point, after which the sample can be imaged at different geometric magnification. In order to ex-tract phase information at all spatial frequencies of the sample, tomography is per-formed at four different sample to detector distances for each sample [the so-called zoom tomography imaging mode (Krenkel et al 2015, Scientific Reports | 5:09973 | DOi: 10.1038/srep09973)]. In this particular experiment, our nerve fiber samples were imaged with an isotropic voxel size of 130 nm in the reconstructed tomographic phase contrast volume.
The tomograms clearly revealed the subcomponents of the peripheral nerve, such as details of the myelinated nerve fibers, and blood vessels in the biopsies from healthy subjects. In specimens from patients with type 1 diabetes, fewer myelinated nerve fibers with altered blood vessels could be visualized. Furthermore, through data seg-mentation the 3D structure of healthy myelinated nerve fibers as well as regenerative clusters, i.e. nerve fibers that had been degenerated and then regenerated, could be shown by the technique in the biopsies from healthy subjects and from patients with diabetes, respectively.
We conclude that the synchrotron technique, with visualization of the 3D structure of nerve fibers in biopsies of human peripheral nerves, provides novel insights of the structure of peripheral nerve, which is relevant for finding the mechanisms behind development of diabetic neuropathy.

Sessions:

Life Sciences

59

THz induced anisotropic changes in bovine trypsin

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Abstract:

The use of non-ionizing Terahertz (THz) radiation in today's society is a constantly growing. New emergent technology utilise THz radiation in for instance security screening at airports, and in medical treatment and diagnostics [1]. In contrast to already established diagnostics methods, the THz radiation can for instance screen patients with higher contrast compared to x-rays [2], and has higher resolution compared to for instance MRI and ultrasound [3]. Albeit non-ionizing, studies have shown that THz radiation might still induce changes biomolecules due to collective oscillations [4]. Therefore, it is imperative to study this protein interaction, not only for the sake of potential adverse effects biological systems, but also for the new insight this information provide to protein - light interactions.

In this study, the crystal structure of bovine trypsin was obtained via a so called time-resolved x-ray crystallography experiment. Here, the proteins were excited with 0.5 THz radiation, for 25 ms, and subsequently studied with 14 KeV x-rays for 3 ms, in a 50 % duty cycle (no THz radiation at half of

the readout). This high resolution data (1.15 Å) show the structural anisotropy in individual atoms, represented by for instance the calculation of individual B-factors, and how the anisotropy might be altered by the THz radiation. This study also provides a good platform for developing statistical tools, to detect and validate structural differences.

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Sessions:

Life Sciences

60

Generation of isolated attosecond pulses for XUV-XUV pump-probe experiments using a two-color laser field

Author: Jasper Peschel[1]

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High-order Harmonic Generation (HHG) is a nonlinear process that enables the generation of sub-femtosecond pulses in the extreme ultraviolet (XUV) or even soft X-ray regime from infrared laser pulses. At the Intense XUV Beamline at the Lund Laser Centre low repetition rate high-flux harmonics are generated with photon energies up to 60 eV. Through tight focusing, the beam is intense enough to induce multiphoton processes in atoms [1] and molecules. The detection of the resulting electrons and ions is based on velocity-map-imaging and time-of-flight spectroscopy [2]. In order to take advantage of the temporal resolution, a split-and-delay unit was recently developed [4] which opens up the possibility to do pump-probe experiments for studying electron dynamics in molecules on the attosecond time-scale.

So far, the light source creates an attosecond pulse train (APT). To investigate dynamics in molecules more closely, the generation of an intense isolated attosecond pulse (IAP) is beneficial. A recent approach to generate intense IAPs without a carrier envelope phase stable laser pulse is to mix a mulitcycle two-color (TC) laser fields [4]. A supplementary wavelength of 1300 nm is added to the existing driving laser field of 800 nm which leads to a continuous harmonic spectrum and the suppression of the APT.
I will present a theoretical investigation of TC HHG based on the strong-field approximation (SFA), as well as a first experimental attempt to generate the supplementary 1300 nm field. Future planning includes working on optical parametric amplifier (OPA) for efficient generation of the supplementary field, as well as the implementation of the TC scheme at the intense XUV beamline.

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Sessions:

Quantum systems & processes

61

Studies of the interaction between hAQP5 and PIP

Author: Veronika Nesverova[1]

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Human aquaporin 5 (AQP5) is a membrane-bound water channel that maintains water balance in lacrimal and salivary glands. A defect in this protein's trafficking from intracellular storage vesicles to the apical membrane is thought to play a role in development of Sjögren's syndrome - a chronic autoimmune disease. Prolactin-inducible protein (PIP) is a cytoplasmic protein, which was found to contribute to the pathogenesis of this disease. An interaction between the AQP5 C-terminus and PIP was suggested but further biochemical or structural data are still unavailable. This project aims to study the proposed interaction. Both proteins were overexpressed in the yeast Pichia pastoris and purified using column chromatography.

Microscale thermophoresis (MST) is a method which measures a movement of molecules along a temperature gradient created by an IR laser. This way changes in size, charge and hydration shell of molecules are detected using covalently bound dyes or fluorescent fusion proteins. By titrating a concentration of a ligand against a fixed concentration of a labelled molecule it is possible to construct a binding curve. All experiments are performed in a solution loaded in a capillary.

In this study PIP was labeled with red fluorescent dye which binds to lysine residues. The non-labeled AQP5 was titrated. Each MST experiment was performed in triplicates. PIP bound to the full-length AQP5 with a KD of 0.6 uM. As a negative control truncated AQP5, which was completely lacking the C-terminus, was used. In this case the KD shifted to approximately 7 uM which may correspond to non-specific binding.

Sessions:

Life Sciences

62

A synchrotron journey inside the Earth

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Our lives as surface dwelling creatures are profoundly affected by processes originating deep in our planet, yet it would be easier for us to reach Mars or Venus than to visit even the base of the thin crust on which we live. Fortunately, seismic waves do penetrate the Earth's interior and since more than one hundred years we have known its structure. However, more detailed knowledge had to wait another fifty years for technical developments that would allow us to visit the Earth's interior in the laboratory. Whatever randomness led our universe to possess both diamonds and the predilection of accelerated electrons to give off X-rays was a lucky break for us indeed. Both are indispensable to probing the nature of materials at high pressure, which constitutes the vast majority of solid matter in our solar system and the known universe. Our group has been fortunate to have been part of many exciting developments and discoveries at the interface where high pressure meets synchrotron radiation, revealing secrets about the world beneath our feet. The presentation will showcase recent achievements and provide a tantalising glimpse of discoveries yet to come.

Sessions:

Environmental and Earth Sciences

63

Transformed, not lost - Increasing the Information Content of X-ray Crystal Diffraction by including Continuous Diffraction

Authors: Julia Lieske[1]; Oleksandr Yefanov[1]

Co-authors: Alke Meents [1]; Henry Chapman [1]; Kartik Ayyer [1]; Maximilian Cerv [1]; Stefan Kreida [2]; Susanna Törnroth-Horsefield [2]

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Imperfections in crystal packing decrease the resolution, resulting in fading of Bragg peaks in the higher resolution rings. However, rather than disappearing altogether, the diffraction can be transformed into clouds of intensity known as continuous diffraction, extending well beyond the last Bragg peaks. Although continuous diffraction is normally disregarded in data treatment, it does contain structural information. This was recently shown for Photosystem II for which combining Bragg peak data at 4.5 Å with the intensities of continuous diffraction improved the resolution to 3.5 Å [1].
Here we present further investigations of continuous diffraction information content from crystals of Aquaporin 2, using synchrotron as well as SFX data. We also present the concept of on-chip crystallisation as an alternative to liquid microjet set-up for XFEL, where crystals are grown on a flat silicon chip that is then raster scanned with femtosecond XFEL pulses.

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Sessions:

Life Sciences

64

First Combined Scattering and Fluorescence Scanning Transmission Microscopy at the NanoMAX Beam Line at MAX IV

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Materials with the approximate stoichiometry Cu_2ZnSnS_4 with the crystal structure of the mineral kesterite are currently being investigated as promising materials for thin film solar cell fabrication. Direct imaging, along with chemical analysis, can crucially contribute to assess the quality of the process.
This poster presents the results from the obtained fluorescence and scattering maps from a sample of kesterite precursors produced by pulsed laser deposition (PLD). The obtained chemical information was compared with energy dispersive spectroscope (EDS) measurements previously made on the same sample.
The results presented in Figure 1 (top) suggest that the differences in the scattering signal may be due to the boundaries of a droplet with nonuniform Cu and Zn distribution as seen in the respective fluorescence maps. In other regions of the sample, this combined scanning technique returned maps with no fluorescence-scattering correlation as Figure 1 (bottom) suggesting a possible morphological change at the surface that could be explained for example by a crack in the material's surface.

Sessions:

New Materials & Energy

65

First Combined Scattering and Fluorescence Scanning Transmission Microscopy at the NanoMAX Beam Line at MAX IV

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Materials with the approximate stoichiometry Cu_2ZnSnS_4 with the crystal structure of the mineral kesterite are currently being investigated as promising materials for thin film solar cell fabrication. Direct imaging, along with chemical analysis, can crucially contribute to assess the quality of the process.
A pulsed layer deposited (PLD) sample of kesterite precursors was previously imaged with a scanning electron microscope (SEM) and electron dispersive spectroscopy (EDS), revealing in particular the presence of surface irregularities. In order to possibly observe finer details and analyze the chemical composition, we acquired fluorescence and scattering maps of such sample at the NanoMAX beam line at MAX-IV, currently in commissioning. This experiment was part of the beam line development.
In this talk we report the outcome of this experiment. We show both fluorescence and scattering maps from features that were highlighted. We present an analysis of the acquired data and a comparison with the previously obtained results from SEM and EDS. Perspectives for cheap, third generation solar cells will also be presented.

Sessions:

New Materials & Energy

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MECHANICAL TESTING USING NEUTRON AND X-RAY TOMOGRAPHY TO CHARACTERIZE BONE-IMPLANT INTERFACE

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Keywords: neutron and X-ray tomography, in-situ loading, digital volume correlation, bone

INTRODUCTION: Metal implants are used for many orthopaedic conditions, e.g. in artificial joints or fracture fixation. The long-term stability of an implant requires new bone formation, which grows towards the implant and integrates it with the surrounding bone. High-resolution imaging combined with mechanical testing are of interest when evaluating bone-implant constructs and in improving their stability. X-ray tomography is commonly used to image bone, but causes artefacts in the immediate surrounding of a metallic implant. On the contrary, neutrons interact weakly with metal, and thus represent an interesting alternative to image the bone-implant interface [1]. However, neutron tomography has hardly been explored for bone. By applying a mechanical loading and simultaneously acquiring tomographic images, we can investigate the mechanical response of the bone-implant interface. DVC tracks texture between a first image (reference image) and a second deformed image, and enables to calculate the internal displacement fields, and subsequently the internal strain fields of the bone close to the screw. We have been investigating the potential of neutron and X-ray tomography to image the bone-implant interface and characterize its mechanical response by identifying damage and fracture during in situ pull-out.

MATERIALS AND METHODS: Metal screws were implanted transversely in rats'tibiae and osseointegrated during 4-6 weeks. Animals were sacrificed and tibiae with screws were dissected.

Comparison of neutron and X-ray tomography. One sample was imaged unloaded with 5 different tomography setups using either X-rays or neutron radiation (Table 1). Microstructural parameters were measured in a same ROI in the trabecular bone and the bone ingrowth around the implant was quantified if possible (no artefacts).

Loading under neutron or X-ray tomography. The screws were pulled-out in displacement control using a custom made loading device, under neutron and X-rays radiation. In both experiments, a first scan was acquired at sample contact with a preloading of 5N, and subsequent scans were realized every 0.2mm increments (0.05mm with X-rays) until rupture (Figure 2A). Two samples were loaded under neutron imaging at ICON, SINQ, PSI [2] (flux 3.107 neutrons cm-2 s-1, 27 µm voxel size, 5h scan) and 11 samples under synchrotron radiation at TOMCAT beamline, SLS, PSI, Switzerland (30 keV, 3.6 µm voxel size, 45s scan). The screw was masked on the unloaded scans using ImageJ to quantify the bone ingrowth around the implant. DVC was applied between the loaded steps using the in-house code TomoWarp2 [3].

RESULTS:

Comparison of neutron and X-ray tomography. Despite using relatively high energy, the metal implant induced artefacts in the X-rays images close to the metal screw, which was not observed in the neutron images, thus allowing analysis of bone ingrowth (Figure 1). The microstructure quantification away from the implant agreed well among all imaging techniques, except for the neutron low-resolution scan, where the detailed trabeculae structure was difficult to visualize.

Loading under neutron or X-ray tomography. DVC was successfully applied to the neutron images, with vertical displacements begin consistent with the experimental applied displacements. DVC identified localized shear strains and positive volumetric strains at the crack zones, coherent with a crack opening (Figure 2B). The DVC analysis applied on the synchrotron images are promising (Figure 2C), however still limited by the artefacts close to the implant.

DISCUSSION: No image artefacts were observed in the neutron images close to the interface, and despite the drawbacks with lower flux, longer acquisition times and lower resolution, DVC enabled identification of the fracture directions through high strain localizations. X-ray based imaging were fast and enabled high resolution. However, the metallic implant induced artefacts that limited the analysis of the bone-implant interface. These images are still being improved. This study provides a proof-of-concept that neutron tomography can be used to image and quantify bone microstructure, with advantages especially when studying bone-implant interfaces when the implants are made of metals. These studies needs to be extended, for instance testing more samples, before damage and fracture mechanisms can be accurately identified.

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ACKNOWLEDGEMENTS: Swedish Foundation for Strategic Research. Swiss spallation neutron source SINQ, Paul Scherrer Institut, Villigen, Switzerland and TOMCAT beamline, SLS/PSI, Switzerland for experimental time. Mea Pelkonen for help with surgeries and sample preparation.

Table 1 - Scanning parameters applied to a same sample

Figure 1 - Comparison of X-rays and Neutron Tomography of a sample

Figure 2 - (A) Schematic of the loading experiments. (B) 3D-views of one sample's tibial plateau with neutron tomographic images (cracks highlighted in white arrows) and DVC results for the first two loading steps. (C) X-rays scan cut and DVC results. Despite the artefacts, the crack can be highlighted by localized shear and volumetric strains (white arrows).

Sessions:

Life Sciences

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Revealing Novel Physical Phenomena in Functional Materials with Coherence and Nanobeam X-ray Scattering

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The functional properties of emerging polar materials, including complex oxide ferroelectrics and multiferroics, depend on complex features in the structure and dielectric polarization and nanometer length scales. In ferroelectric/dielectric heteroepitaxial superlattices, intriguing physical properties arise from the pattern and phase transformations of spontaneously formed striped nanodomain patterns. X-ray nanobeam diffraction and coherent scattering methods reveal an optically induced transformation of the domain pattern, show that confinement effects can be used to manipulate the distribution of domain walls, and provide evidence for thermally driven equilibrium fluctuations. Precise structural studies of oxide and semiconductor crystals require detailed consideration of the optical phenomena underpinning nanobeam diffraction. Studies of oxide nanosheets and semiconductor heterostructures illustrate different regimes of sample parameters in which simulations can employ kinematic or dynamical diffraction methods. Further developments of these approaches

have the potential to impact the synthesis of novel materials and the manipulation of their properties using nanoscale engineering.

Sessions:

New Materials & Energy

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Kinematic and Dynamical Diffraction Methods in the Simulation of X-ray Nanobeam Diffraction

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X-ray nanobeam methods now permit the formation of intense x-ray beams with spot sizes of tens of nanometers. The optical instrumentation used to focus these beams, including Fresnel zone plates, introduces a beam convergence of on the order of 0.1-0.3 degrees with a very high degree of optical coherence. This convergence presents a challenge in the analysis of x-ray nanobeam diffraction patterns because the convergence angle can be larger than the angles associated with the characteristic widths of x-ray reflections or the separations of scattering features in reciprocal space. We show that optical simulation methods incorporated kinematic and dynamical diffraction effects can be used to simulate these diffraction patterns. Applications of the simulation methods to nanodiffraction studies of complex oxide sheets illustrates how effects associated with mosaicity and crystal rotation can be separated from variations in the lattice parameter. Using such simulations to interpret nanodiffraction patterns acquired from semiconductor heterostructures reveals that the electrodes used to define quantum devices produce nanoscale strain distributions of sufficiently large magnitude to perturb the device characteristics.

Sessions:

New Materials & Energy

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Exploring hydrogenases - Using a combination of chemical and biological tools

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Hydrogenases are enzymes involved in hydrogen metabolism, catalyzing the interconversion between H2 and protons. The remarkable catalytic efficiency of these enzymes, in combination with the unique nature of their co-factors, has attracted the attention of the bioinorganic chemistry community. Moreover, their biotechnological potential has resulted in intense studies of the enzyme in the context of biological H2-production.

In the case of [FeFe] hydrogenases, the reaction occurs at the H-cluster featuring a, in biology unique, dinuclear [2Fe] subsite.1 Synthetic chemistry has long been a powerful tool in studies of this cluster, via the preparation of biomimetic model compounds. In 2013 we described how such synthetic complexes can be introduced into the enzyme itself under in vitro conditions, allowing the manipulation of the enzyme using synthetic chemistry.2, 3 More recently we discovered how this concept can be extended to in vivo conditions, and the apo-enzyme activated using synthetic compounds inside living cells.4

Here I will present how our semi-synthetic approach can be used to generate both active "native" hydrogenases, as well as "artificial"hydrogenases incorporating modified cofactors resulting in enzymes with new catalytic and spectroscopic properties. Moreover, I will highlight some of the key unresolved questions concerning the biosynthesis of the H-cluster and the catalytic mechanism of the enzyme.

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Sessions:

Life Sciences

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Structure of the SnO_2(110)-(4×1) surface

Author: Lindsay Richard Merte[1]

Co-authors: Andreas Schaefer [2]; Bjørk Hammer [3]; Chris Nicklin [4]; Chu Zhang [5]; Geoff Thornton [6]; Johan Gustafson [1]; Jonathan Rawle [4]; Katariina Pussi [7]; Mathias Jørgensen [3]; Mikhail Shipilin [1]; Robert Lindsay [8]; edvin lundgren [9]

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Using surface X-ray diffraction (SXRD) supported by quantitative low-energy electron diffraction (LEED) and density functional theory (DFT) calculations, we have determined the structure of the (4×1) reconstruction formed by sputtering and annealing of the SnO_2(110) surface. The dominant components of the SXRD pattern indicate a structure based on a quasi-hexagonal Sn monolayer.

A systematic DFT search using an evolutionary algorithm yielded a globally-optimal structure composed of Sn_3O_3 clusters atop a stoichiometric $SnO_2(110)$ slab. The structure, which does not incorporate in-plane oxygen vacancies as was once believed, is confirmed by SXRD and LEED measurements, as well as previously published scanning tunneling microscopy images.

Sessions:

New Materials & Energy

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Opportunities and challenges in soft X-ray spectroscopy and microscopy studies of materials for organic photovoltaics

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After two decades of research, organic photovoltaics has now reached record efficiencies above 10%, strongly competitive processing costs and shorter energy payback times. To break through as a reliable technology, these advantages need to be accompanied by an acceptable durability. Enhancing the stability of OPV modules, which are continuously exposed to external factors such as light, heat, in-diffusing oxygen and humidity, is the next critical issue. Materials with a good thermal and photochemical stability are therefore required to achieve organic solar cells with long lifetimes.
Probing the distribution of donor and acceptor molecules in the active layer of polymer solar cells requires high-resolution methods that provide chemical contrast. A combination of the synchrotron-based soft X-ray technique near-edge X-ray absorption fine structure (NEXAFS) spectroscopy and scanning transmission X-ray microscopy (STXM) can map surface composition and local composition in lateral phase-separated domains, as well as identify molecular signatures of degradation. Here we illustrate, by way of selected results, the relevance of these complementary techniques to the field of organic photovoltaics. We focus here on the active layer materials in polymer solar cells. In particular, we have studied the composition and electronic structure of the fullerene derivative PC60BM, the conjugated polymer TQ1, and blends of those.
We demonstrate firstly that the determination of local composition from X-ray absorption spectra requires cautious use of fitting techniques. Furthermore, we show that drop-like clusters of PC70BM formed during the transfer of spin-coated polymer:PC70BM blend films onto Cu-grids lead to an underestimation of PC70BM/polymer concentration ratios. Finally, we show that the selective degradation of one of the components can impair the accurate determination of local blend composition.

Sessions:

Quantum systems & processes

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Galectin-3: Studying molecular recognition in search of inhibitors exhibiting high affinity and selectivity

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Galectin-3 belongs to the lectin family that recognizes carbohydrates. It has a highly conserved carbohydrate recognition domain (CRD) of 130 residues, which is responsible for binding to beta-galactosides. Galectin-3 has been shown to be involved in cancer, angiogenesis and stroke. Its involvement in these diseases makes it a wonderful drug target. Natural ligands of galectin-3 always have a galactose residue. Among attempts to develop small and more drug-like molecules, 3C-substitution of galactose and 3,3'-di-substitution of thiodigalactoside have proven to be successful. In particular, high-affinity small-molecule inhibitors with low uM to nM affinities have been discovered by appending aromatic amido groups or 4-amido-1,2,3-triazolyl groups at one C-3 carbon in mono or both C-3 carbons in dithio-galactoside. . Galectin-3 favors a disaccharide or a larger oligosaccharide over a monosaccharide in terms of binding efficiency. In our present work we have solved very high resolution(0.96-1.1 Angstrom) X-ray structures of Gal3CRD with novel set of inhibitors based on galactose but having several modifications. Only preliminary inhibitor data has been used here as further analysis is required for depicting the role of water network in the ligand binding and the thermodynamics associated with it.

Sessions:

Life Sciences

73

Latest results and features of McXtrace 1.4

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McXtrace [1][2] is a Monte Carlo Ray tracing package for performing simulations of any kind of X-ray optical instrumentation or scattering experiment. We present the latest results obtained using the new release McXtrace version 1.4.

Some highlights of simulations using McXtrace include:

- McXtrace in space - simulations of an X-ray telescope satellite ATHENA [3]. McXtrace is being adopted as the general tool for simulating X-ray optics of the European Space Agency.
- Ray tracing integrated with the Simex platform [4] for XFEL simulations The SimEX platform is general platform for performing Source-to-End simulations at X-ray Free Electron laser facilites supported by the EU under the EUCALL initiative. We show that McXtrace may interoperate with the SimEX platform, creating a versatile tool with which to explore the new possibilities created by the FEL X-ray sources.
- A full beamline description of the DanMAX beamline at the MaxIV synchrotron. McXtrace is used to simulate the DanMAX beamline while it is being designed, not only supporting design choices, but in parallel also building a virtual facility. (See image)

Exciting new features in the latest release of McXtrace include:

- A new (python based) GUI
- New device model examples:
- A new polyphase/polycrystal sample model.
- Mirror with heatbump.
- Synchrotron source models / interfaces to other source codes.
- Generalized reflectivity library.
- Grid scan capabalities

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Sessions:

New Materials & Energy

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Real-time Study of Atomic Layer Deposition of HfO2 on Si(111) Surfaces by operando APXPS

Authors: Fabrice Bournel[1]; Jean-Jacques Gallet[1]; Joachim Schnadt[2]; Payam Shayesteh[3]

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In this study in situ and operando studies of atomic layer deposition (ALD) aim to address the lack of knowledge about ALD surface chemistry. We have carried out Ambient pressure x-ray photoelectron spectroscopy (APXPS) at high temporal resolution to study of the ALD growth of HfO2 on the clean, oxidized, and native Si(111) surfaces from tetra¬kis¬(di¬methyl¬amido)¬hafnium and water precursors. We observed clear cyclic shifts between different species during the different half-cycles. We also observed that HfO2 grows faster on the oxidized Si(111) than the bare surface. An interesting, but readily explainable contrast is observed in comparison to the ALD of HfO2 on InAs(001): the native oxide layer on Si(111) is not removed by interaction with the metal precursors. This difference arises from the higher stability of SiO2 in comparison to the native oxide on InAs. Further, we report the results of a post mortem atomic force micros-copy and transmission electron micros¬copy analysis.

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BioMAX - Macromolecular Crystallography at MAX IV Laboratory

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BioMAX is the first macromolecular crystallography beamline at the 3 GeV ring of MAX IV Laboratory, which will begin user operations in early 2017. It is a state-of-the-art resource accommodating multiple cutting edge experimental possibilities. The design goal for BioMAX was to create a stable and reliable beamline that is user friendly.

The beam focus is 20 x 5 μm^2 at the sample position with a flux of 2 x 10^{13} ph/s at 500 mA ring current. Alternatively, using aperture overfilling it is possible to obtain a stable 5x5 μm^2 beam at the sample position. Beam defocusing creates a practically parallel beam, which can be used to resolve extremely large unit cells (> 1000 Å) at high resolution.

BioMAX has been equipped with an MD3-microdiffractometer, an Eiger 16M detector for extremely fast data acquisitions and an ISARA sample changer for operation with up to 400 cryo-cooled samples at the same time. The commissioning and initial user operation is being performed in parallel and a first user call has been reviewed recently, which will enable a number of important scientific projects to be operated before summer 2017.

Sessions:

Life Sciences

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The long range periodicity of the Pd(100)-(√5×√5)R27°-PdO(101)

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Co-authors: Chu Zhang [2]; Johan Gustafson [1]; Lindsay Richard Merte [1]; Uta Hejral [1]; edvin lundgren [3]

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Structural studies of ultrathin PdO layers have been lately the focus of numerous research works [1, and references therein] as this oxide forms on Pd under sufficiently oxygen-rich conditions in the processes of, e.g. catalytic CO oxidation [2] or methane combustion [3]. In particular, the formation of the surface oxide on a Pd(100) single crystal surface acting as a model catalyst accompanied by the increase in the CO oxidation reaction rate has been repeatedly reported suggesting a high reactivity of this phase [4, 5, 6].

Determination of the atomic structure of the surface oxide was firstly attempted more than 30 years ago by Orent and Bader [7], who came to the conclusion that the oxide layer is similar to the (001) crystallographic plane of bulk PdO. This model has been refined later in several publications [8, 9, 10] showing that a layer similar to (101) crystallographic plane of bulk PdO is forming on the surface comprising coordinatively unsaturated Pd atoms, which play an important role during a catalytic reaction.
In the current contribution, the long-range periodicity of the surface oxide structure is studied in detail under UHV conditions as well as during CO oxidation at semi-realistic pressures. The relatively periodic stripes of distorted periodicity constantly observed in STM images of this structure are discussed and related to the incommensurability of the surface oxide and the substrate along the [011] crystallographic direction. This mismatch causes the accumulation of lateral stress, which

is released in the long range by shifting of the surface oxide atomic lattice. The fine splitting and shifting of the superstructure diffraction features obtained in High-Energy Surface X-Ray Diffraction (HESXRD) experiments are analyzed and attributed to the presence of a larger coincidence unit cell of the surface structure. A qualitative model of this unit cell is suggested and the influence of its internal structure on the diffraction pattern is discussed.

The authors would like to acknowledge the Röntgen-Ångström collaboration "Catalysis on the atomic scale" and the financial support by the Swedish research council (VR).

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Sessions:

New Materials & Energy

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Microdynamic studies using synchrotron radiation in acute respiratory failure

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Acute respiratory failure or acute respiratory distress syndrome (ARDS) is a common condition with 40% mortality. In fact, about 15% of the beds in intensive care units (ICU's) in developed countries are occupied with patients with ARDS. These patients need ventilator treatment, which is lifesaving but, on the other hand, is harming the lungs and is contributing to the high mortality in this condition. We have used synchrotron radiation computed tomography in order to examine the underlying causes of ventilator induced lung injury in experimental set-ups and data from these studies will be presented. These findings may help us to improve ventilator treatment and ultimately, we hope, to reduce the high mortality in ARDS.

Sessions:

Life Sciences

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Catalytic reaction on a stepped surface: CO oxidation with pre-adsorbed O on Rh(553)

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In contrast to the perfectly flat surfaces often studied in surface science, real catalysts consist of active metal nanoparticles on oxide supports. These nanoparticles expose edges with under-coordinated atoms, which will affect the interaction between the reactants and the surface, and hence the catalytic activity. To study the effect of such defects in a controlled way, we have combined XPS and DFT and investigated the reaction between CO and O on a stepped Rh(553) surface and compare with previous results from flat Rh(111).

The under-coordinated atoms at the steps are expected to show a higher reactivity, that is tendency to bind to other atoms, which is often assumed to lead to higher catalytic activity. Our results indeed shows that the CO oxidation reaction is faster on the stepped surface, but the reaction is not happening on the step edges, but rather on the terraces close to the steps. The reason for the higher activity is probably in-plane relaxations enabled by the step.

Sessions:

New Materials & Energy

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Johansson crystal: manufacturing process and characterization

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“Balder” is a hard x-ray XAFS beamline at the brand new Swedish 4th generation, first of its kind, synchrotron: MAX IV Laboratory. It was designed for a broad energy range (2.4 –~50 keV), high flux (> 10 to the power of 13 ph/s), quick scanning (>1 Hz repetition rate for full EXAFS [Extended X-ray Absorption Fine Structure]) and simultaneous high-resolution emission detection compatible with various sample set-ups.

A high energy resolution X-ray Emission Spectrometer paves the way towards site-selective XAFS [X-ray Absorption Fine Structure] —disentangling spectra of individual species in a mixture. In such applications, high incoming flux is necessary to detect weak satellite lines and/or to work with low elemental concentrations. Balder will use its high flux source for XES but will have to tackle

the overload problem and this tasks, high flux fluorescence detection and high resolution emission spectroscopy, can be solved with one instrument.

The central part of the spectrometer are the crystal analyzers which in order to cover all the emission lines, would be of various orientations. This project includes grinding, lapping, polishing, metrology measurements, special surface treatment, bending, assembling and testing with x-rays. The crystals will be of the Johansson type, i.e. ground to a radius equal to the Rowland circle diameter and bent down to one half of this radius. In order to bend a crystal, it has to be sufficiently thin. A safe thickness-to-radius ratio for silicon crystals is usually taken as 5000. We therefore aim at a thickness of 300 to 400 μm.

This poster is presenting part of the manufacturing process and the surface metrology results.

Sessions:

New Materials & Energy

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In-situ oxidation of Cu(100) by CO2

Authors: Benjamin Hagman[1]; Johan Gustafson[2]

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In the light of the increasing CO2 in the atmosphere and its relation to global warming, an interest to achieve a carbon-neutral society has risen. A promising approach for this is to recycle CO2 instead of releasing it into the atmosphere. Due to the inertness of CO2, this is a rather difficult task, but already today, industrial production of methanol is performed over Cu based catalysts with CO2 as the main source of carbon. However, as for many other catalytic reactions, the fundamental knowledge about this process is limited. In order to fill this gap, we are studying the interaction between Cu surfaces and different relevant gases. More specifically, the present contribution will discuss the interaction of CO2 with Cu(100). We see a change in the oxygen uptake from CO2 dissociation which comes in conjunction with a saturation of oxygen being 4-fold coordinated to Cu atoms.

We will present a combined (AP)XPS and DFT study of dissociative adsorption of CO2 on Cu(100) and compare the resulting structures with those formed by exposure to O2. We have followed the evolution of the O 1s signal in situ as the surface was exposed to 300 mTorr CO2 at sample temperatures of 100℃ and 200℃. There is a distinct continuous shift towards higher binding energy, as the oxygen coverage increases, which can be nicely analyzed to show how the component at higher binding energy starts to grow and eventually takes over. We assume that the difference in binding energy comes from a change in adsorption site for the surface oxygen. If Cu(100) is exposed to O2 a c(2x2) structure will form at low exposure. At a coverage of ~0.3 ML, however, this structure becomes unstable and the surface will gradually reconstruct into a $(2\sqrt{2}x\sqrt{2})R45^\circ$ missing-row structure, where every forth Cu row in either [010] or [001] direction is removed from the surface layer. This structure is complete at a coverage of 0.5 ML. For XPS, it has previously been found that the O 1s peak, corresponding to chemisorbed O, shifts gradually towards higher binding energy with increasing oxygen coverage. This was interpreted as different adsorption geometries of the oxygen

in the reconstructed and unreconstructed surface. By comparing the trend with oxidation with CO2 and O2, we believe that the origin of the growth of the higher binding energy component is that the oxygen atoms changes from being 4-fold to 3-fold coordinated to Cu atoms, in agreement with a transition from c(2x2) to the missing row structure.

For the adsorption process, we see a decrees in oxygen uptake as the coverage approaches 0.25 ML. This appears in conjunction with the saturation of the low binding energy component, which could mean a structural dependence on the decrease of uptake. We will also present a preliminary DFT study which suggest that CO2 can dissociate up to an oxygen coverage of 0.25 ML. B. Eren, et. al., observe a similar phenomenon, at room temperature, as they saw that at ~1/3 ML the surface gets poisoned by the atomic oxygen.

Sessions:

New Materials & Energy

81

Structural basis for a novel immune deficiency

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The protein FP functions as an essential positive regulator of the innate immune system providing first line of defense against pathogens and participating in the maintenance of tissue homeostasis. The oligomeric nature of FP has challenged structural analysis so far. We describe here a novel FP deficiency (E244K) caused by a single point mutation which results in a very low level of FP activity and is lethal to patients expressing this variant. Recombinant FP E244K is monomeric and we have compared this to a monomeric unit excised from oligomeric FP, which is also partially dysfunctional but still binds to the so-called convertase, a giant proteolytic enzyme assembled upon detection of pathogens and dying host cells. The crystal structure of a FP-convertase complex determined from diffraction data obtained exclusively with microfocus synchrotron radiation suggests that the major contact between FP and the AP convertase is mediated by a single FP thrombospondin repeat and a small region in one subunit of the convertase. Synchrotron small angle X-ray scattering clearly reveals that FP E244K is trapped in a compact conformation preventing its oligomerization. Our studies demonstrate how access to state of the art synchrotron radiation can be essential for a detailed comprehension of pathogenesis.

Sessions:

Life Sciences

82

MicroMAX –A new tool for Structural Biology

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Synchrotron radiation has revolutionised structural biology and allowed important scientific questions to be solved, illustrated by several Nobel prizes awarded to achievements partly based on the use of synchrotron radiation. The possibility to determine macromolecular structures using smaller and smaller crystals has played a key role in this development but the success is based on a combination of many developments such as better storage rings, more powerful computers, new detectors and improved analysis software. This rapid but constant evolution has been challenged by the advent of X-ray free electron lasers (XFELs) and new ways of collecting crystallographic data from a large number of microcrystals using a range of methods commonly referred to as "serial crystallography" .

The proposed MicroMAX beamline will offer new possibilities in macromolecular crystallography by exploiting the unique properties of the MAX IV 3 GeV ring providing a brilliant X-ray beam with 1-10 m size that is energy tuneable in the range 5 –30 keV and has an energy bandwidth of either 10-4 or a few percent. This will be combined with a flexible experiment setup providing both a high performant goniometer and the full portfolio of new sample delivery techniques and serial crystallography data collection methods.

The MicroMAX performance and possibilities will allow new scientific questions to be tackled in important areas such as membrane protein biology. MicroMAX will also allow time-resolved studies down to the microsecond timescale.

Sessions:

Life Sciences

83

Materials science of and physical phenomena in clays; Overview of X-ray studies and related investigations

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In this presentation I will give an overview of physical phenomena as they manifest themselves in soft and complex clay materials, and how this can be studied by means of X-ray scattering techniques in complementary with other techniques. At NTNU we have performed studies of clayey materials in this context for about 20 years, and here I will focus on our own results during this time in relation to the works of many other groups worldwide. At the end I will point out future directions in this area. The topics that will be covered in this presentation are: Molecular interactions with clay materials [1,2,3,4], consequential self-assembly of clay particles in bulk saline water, including isotropic to nematic transitions in colloidal clay platelet systems, as controlled by clay concentration, water salinity, gravity or magnetic fields [5,6,7,8,9], self-assembly of clay colloidal nano-platelets at oil-water interfaces [10], self-assembly of clay colloidal nano-platelets in bulk oil, as controlled by clay concentration or electric fields [11,12], self-assembly of clay colloidal nano-platelets at oil-oil interfaces, as controlled by clay concentration or induced electro-hydrodynamics or dielectrophoresis [13,14]. From nano to macro: These nano-scale functional phenomena have several significant macroscopic consequences in various directions [15,16,17,18].

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Sessions:

Environmental and Earth Sciences

85

Amyloid-like protein fibrillation - a highly dynamic and complex process

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Amyloid-like protein aggregation into fibrillar structures is associated with a variety of neurodegenerative disorders, such as Parkinson's and Alzheimer's disease. It is becoming increasingly evident that the pathology is caused by oligomeric species, formed transiently during the fibrillation process, rather than by the mature fibrils, thus calling for a thorough molecular investigation of these oligomers in order to elucidate the mechanism of their cytotoxicity. The inherently transient nature of these species however hampers this endeavour greatly, as isolation of different components interferes with the overall equilibrium in solution, ultimately causing structural rearrangements. This issue can be circumvented by studying undisturbed fibrillating systems *in vitro* using small angle X-ray scattering (SAXS), coupled with subsequent chemometrics-based decomposition of the data. In conjunction with orthogonal techniques, this approach indeed allows us to identify the species present in solution over time, as well as to extract structural information, revealing just how dynamic the process of amyloid-like protein fibrillation really is.

Sessions:

Life Sciences

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A handle on nonisomorphism: from multi-crystal datasets to serial crystallography

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Datasets measured from different crystals (e.g. in Serial Crystallography) are affected by both random and systematic errors.
Datasets differing systematically are called non-isomorphous, and current crystallographic procedures are far from being able to capture and analyse the various sources of systematic error. It is therefore desirable to develop methods that can separate random and systematic
effects on data, in order to e.g. separate datasets corresponding to different conformations, or different composition of complexes.
The talk presents a novel type of data analysis which positions datasets within a low-dimensional space whose axes are associated with the types of systematic differences between the datasets.

Reference: Diederichs, K. (2017) Acta Cryst. D73, https://doi.org/10.1107/S2059798317000699 (in the press)

Sessions:

Life Sciences