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27 NOV

Giuliana Tromba & Christian Dullin

Synchrotron phase contrast CT multi-scale imaging in human sized lungs at Elettra

Background: The lung is a large and complex organ. Disease processes can cause pathological changes at different scales and in different locations within the lung. It is therefore essential to not only identify regions of interest, but also to allow for a hierarchical evaluation. In clinical routine so far High Resolution CT (HRCT) and histological analysis of tissue biopsies is used for this purpose. Taking biopsies is an invasive procedure, which especially in an organ such as the lung which needs to be airtight, can cause risks for the patient such as bleeding and pneumothorax. Therefore, we propose the use of propagation-based local area phase contrast CT (PBI) protocol for patients with non-conclusive clinical HRCT findings.

Methods: To establish PBI protocol in patients, at the SYRMEP beamline of Elettra we performed pilot studies with a human chest phantom equipped with fresh porcine lungs in direct comparison to clinical HRCT and in cascade of higher resolution microCT and histology analysis using a novel vapor-fixation technique.

Results: We demonstrated that with PBI, an isotropic resolution of 67μm was achieved with the same x-ray dose used in clinical HRCT for a resolution of 450x450x900μm. We showed that with that gain in resolution and contrast non-specific findings such as so-called ground glass opacities can be depicted in detail. The novel vapor fixation approach allowed to fix the specimen within the phantom while maintaining the same level of expansion as in the PBI acquisition. This enabled for the first time to supplement the 67μm whole lung scans with 4μm and 0.65μm scans of formalin-fixed and paraffin-embedded (FFPE) lung tissue of the same lung at a defined position. In addition, the FFPE tissue was further processed by histology linking the research pipeline to clinical routine.

Conclusion: The setup of the SYRMEP beamline, with the human chest phantom in combination with the novel vapor fixation approach, enables multi-scale imaging studies in human scaled lungs at clinically relevant dose levels.

Future perspectives: SYRMEP_LS, a new x-ray imaging beamline from a 6T superconducting bending magnet is under construction in the framework of the wide Elettra 2.0 upgrade program. The beamline will be optimized for multiscale applications in the Life Sciences (LS). A medical facility will be realized to make possible applications of lung CT and breast CT on patients. The optics layout and the main characteristics of the new beamline will be presented

28 NOV

Olga Martin

ABSTRACT 8

Different approaches to enhance the treatment effectiveness of microbeam radiotherapy (MRT) in a preclinical breast cancer model

Synchrotron Microbeam Radiotherapy (MRT) leads to extraordinary normal tissue tolerance compared to the ablative effects on the tumour. In addition, MRT induces specific anti-tumour immune responses, and has a potential to not only eradicate local tumours but also to suppress metastatic disease. Also, MRT selectively destroys immature tumour blood vessels, while vasculature in normal tissues is more tolerant. At peak doses of 100-150 Gy MRT provides a time window to enhance delivery of systemic therapy to the tumour. This permeability window increases the effectiveness of chemotherapy and could be combined with other therapeutic agents such as antibodies.

At the IMBL, Australian Synchrotron, we employed a highly aggressive and metastatic triple-negative 4T1.2 mammary carcinoma mouse model to test various daily fractionated radiation schedules involving MRT. We established efficient regimens, i.e., a combination of one session of MRT with two sessions of broad beam irradiation, to effectively control the primary tumour, and studied the impact of an ultrahigh dose-rate. Aiming to enhance the efficacy of MRT and to control both primary and distant tumours, we exploited the MRT-induced vascular permeability to deliver systemic therapies. We extensively explored combinations of MRT fractionated schedules with clinically relevant adjuvant immunotherapy (anti-PD1, anti-CSF-1R) and chemotherapy (doxorubicin). The promising results of this combinatorial study will be presented, with the primary tumour immune response, primary and metastatic tumour growth, and overall survival as the endpoints for comparison.

Authors: Elette Engels, Helen Forrester, Mitzi Klein, Caroline Bell, Robin Anderson, Valentin Djonov, Martin Olga

KEYNOTE TALK

28 NOV

Marie-Christine Zdora

ABSTRACT 12

X-ray speckle-based phase-contrast and dark-field imaging using UMPA at the Australian Synchrotron

X-rays have revolutionised healthcare, industry, and scientific research by visualising the inner structure of opaque objects. Conventional X-ray absorption-based imaging excels in differentiating high- from low-density materials, such as bones and soft tissue, but falls short in distinguishing subtle density differences between soft tissues or micro- and nano-structural features, like lung air sacs. To overcome these limitations, X-ray phase-contrast and dark-field imaging methods, which analyse X-ray phase shifts and small-angle scattering, have been developed.

Here we present the principles and applications of X-ray speckle-based imaging (SBI), a recently established phase-contrast and dark-field imaging method. SBI uses sandpaper as an optical element to scramble the X-rays into a speckle pattern, counterintuitively allowing for encoding the otherwise invisible phase and dark-field signals alongside the conventional absorption channel. These signals are computationally extracted from sample-induced displacements, visibility loss, and intensity loss of the speckle pattern, respectively. SBI's simple setup, using sandpaper, is cost-effective and eliminates the need for precise alignment or high stability of setup components.

The Unified Modulated Pattern Analysis (UMPA), a method for SBI data acquisition and analysis, is particularly flexible and sensitive. UMPA has been widely adopted at synchrotrons such as Diamond (UK), ESRF (France), Elettra (Italy), DESY (Germany), and more recently, the Australian Synchrotron (AS). We present preliminary results from the MCT and IMBL beamlines at AS, showcasing UMPA's capabilities and potential applications. The UMPA processing package has been implemented in the standard MCT processing environment on ASCI, facilitating straightforward reconstruction and real-time monitoring of experimental data. We believe UMPA-SBI has great potential for AS users, with applications in biomedical imaging, materials science, environmental sciences, and other fields.

Authors: Marie-Christine Zdora

Jitraporn (Pimm) Vongsvivut

28 NOV

ABSTRACT 31

Soft-contact piezo-controlled macro ATR-FTIR technique and expansion of beamline's capabilities into battery and catalysis research at Australian Synchrotron

Since 2016, our Infrared Microspectroscopy (IRM) beamline at the ANSTO – Australian Synchrotron has introduced a number of in-house developed synchrotron macro ATR-FTIR accessories, based on hybrid and soft-contact piezo-controlled macro ATR-FTIR devices. With this technique, spatial resolution is further improved by the high refractive index of the ATR crystal, allowing spatially resolved chemical mapping of surfaces at a lateral resolution down to 1-2 µm when coupled to synchrotron-IR radiation [1]. More recently, soft-contact piezo-controlled macro ATR-FTIR device has been re-designed specifically for in-operando monitoring of electrochemical reaction in model batteries. This device known as "piezo-ATR", which is unique only to the Australian Synchrotron, has led to the expansion of user community into the areas of battery and catalysis [2,3].

This presentation aims to provide recent applications based on all macro ATR-FTIR techniques available on the beamline. In addition to battery and catalysis, other key research areas include dairy products [4], microcapsule supplement [5], and bioactive anti-microbial coating [6], as well as industry-based projects involving steel coatings [7], and spider silk/carbon fibres [8].

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Authors: Jitraporn (Pimm) Vongsvivut

KEYNOTE TALK

28 NOV

Ivan Lee

ABSTRACT 35

Automatic Segmentation and Phenotyping of Wheat Root with Synchrotron X-ray Computed Tomography

Root segmentation and phenotyping are crucial for advancing agriculture and environmental sustainability by enabling the detailed study of root systems, which are vital for water and nutrient uptake, stress resilience, and overall plant health. However, current root segmentation methods usually rely heavily on manual annotation, which is time-consuming and often impractical for large datasets.

This report investigates gaps in the literature, addressing the issue of sparse labels for root segmentation, and exploring a general segmentation and phenotyping framework of root structures in Synchrotron X-ray Computed Tomography (CT) 3D images. We employ deep learning algorithms and leverage the high-resolution capabilities of Synchrotron X-ray CT imaging, addressing the complexity of accurately identifying and analyzing root systems in heterogeneous soil environments. By specifically introducing pseudo-labeling strategy, our automatic segmentation framework accurately differentiates root structures from the surrounding soil matrix using the sparse labels. Notably, the pre-trained framework can be applied to segment new root datasets, significantly enhancing precision and efficiency. In addition, we not only improve the quality of segmentation but also facilitate detailed phenotypic analysis, including comprehensive measurements of root length. Furthermore, the proposed framework is designed to adopt multi-GPUs, making it suitable for high-throughput analysis. This is particularly beneficial for research in plant biology, agriculture, environmental sciences, and crop performance. The ability to automatically segment and phenotype roots from large 3D datasets accelerates the research process, providing researchers with precise and reliable data. Our future research will focus on blurry root, thin root segmentation to further enhance our framework capability.

Authors: Ke Sun, Ivan Lee, Hurriyatul Fitriyah, Casey Doolette, Peter Kopittke, Enzo Lombi

Elisabeth Schültke

27 NOV

ABSTRACT 41

Why do we want to establish a canine neurooncology research program at the Australian Synchrotron?

Microbeam radiation therapy (MRT) has recently been shown to be extremely efficient in treating canine malignant brain tumours, a type of cancer notoriously difficult to treat with clinically established therapy options and associated with a bad prognosis (Adam 2022, Eling 2024). Spatial dose fractionation and hypofractionation, descriptors also typical for MRT, are already well established in clinical radiotherapy. Spatial dose fractionation at the millimetre level contributes to normal tissue preservation in clinical radiosurgery. Hypofractionation (increasing single fraction doses beyond 2 Gy) improves the biological effectiveness of cancer treatment.

MRT takes this concept a considerable step further: Spatial dose fractionation is provided at the micrometre range and FLASH dose rates are added in the peak dose zones. The extremely good normal tissue preservation at FLASH dose rates seen in experimental radiotherapy has already caught the attention of the clinical radiation oncology community. Because normal tissue tolerance is the limiting factor in radiation dose prescription in clinical radiotherapy.

Canine and human tumours of the central nervous system, including both the brain and the spinal cord, are very similar in their histology and course of the disease. Furthermore, they are similar in size and depth from surface, two key parameters in radiotherapy planning. Thus, the results from the canine MRT research program will directly feed into planning human MRT trials, both synchrotron-based and at the first compact sources powerful enough to support MRT.

Results from recent treatment simulations and experiments will be presented.

Authors: Elisabeth Schültke, Sam Long, Elette Engels, Michael Lerch, Jason Paino, John Paul Bustillo, James Cayley, Vincent de Rover, Matthew Cameron, Daniel Hausermann, Mitzi Klein, Stephanie Corde, Anatoly Rozenfeld, Moeava Tehei, Olga Martin, Martin Carolan , Marco Petasecca , Bernd Frerker, Abdul Malek Hamada, Guido Hildebrandt

Michael Jones

27 NOV

ABSTRACT 42

Multimodal X-ray Microscopy at XFM

The XFM beamline at the Australian Synchrotron is a world leader in fast, large-scale fluorescence measurements. Due to the nature of the fluorescent measurement and the design of the beamline, many complementary measurements are possible. Some examples include X-ray Absorption Near Edge Spectroscopy (XANES) to map the oxidation state and Scanning X-ray Diffraction Microscopy (SXDM) to obtain high-resolution phase contrast images. In this presentation, we introduce X-ray Backscatter Diffraction Microscopy (XBDM), a powerful technique for rapidly mapping crystallographic textures. We show how this technique can be used to decipher fluid pathways in rocks and to overcome polarisation limitations in XANES measurements. We also present results from recent Scanning Transmission X-ray Microscopy (STXM) and micro X-ray Diffraction (uXRD) mapping experiments and show the current state-of-the-art SXDM results. In concert, these techniques allow for unprecedented views of the sample with the potential to solve long-standing questions in a range of fields.

Authors: Michael Jones, Cameron Kewish, Andrew Langendam, Christoph Schrank, Ioan Sanislav, Daryl Howard, David Paterson

Lucille Chapuis

29 NOV

ABSTRACT 46

MicroCT of sense organs and the central nervous systems in fish, reptiles and crustaceans: a comparative and functional neuroanatomical approach

Bioimaging, or the imaging of biological structures, is changing the field of sensory biology, especially for taxa that are lesser-known, rare and logistically difficult to source. Due to the large difference in X-ray attenuation of mineralised tissues, μCT has been widely used to image hard tissues like bones and teeth. To extend μCT to visualise the nervous system, specimens can be stained prior to μCT scanning using contrast-enhancing staining agents that add density to soft tissues. When integrated with traditional sensory biology approaches, developing an archival, digital repository of morphological information can offer a profound advance in our understanding of whole systems and their function without the issues of surgical intervention and negate the risk of damage and artefactual interpretation. We present some examples of bioimaging the peripheral (sense organ) and central (brain) nervous systems in some fishes, reptiles and invertebrates, covering the work done at the IMBL and MCT beamlines of the Australian Synchrotron. A comparative and functional neuroanatomical approach is taken to improve our understanding of the evolutionary drivers of sensory adaptation and brain plasticity in key taxa.

Authors: Lucille Chapuis, Jenna Crowe-Riddell, Caroline Kerr, Craig Radford, Shaun Collin

Thomas Ray Jones

28 NOV

ABSTRACT 61

Synchrotron Insights: Observing microbially accelerated metal mobility and carbon capture in near-surface environments

Influencing biogeochemical cycling in near-surface environments impacted by human activity has the potential to aid in combating climate change by supporting the green energy transition and accelerating carbon sequestration in soils and mine waste. By leveraging synchrotron-based techniques, such as the XFM beamline at the Australian Synchrotron, we can investigate and observe the complex interactions that govern metal mobility in tailings storage facilities and enhanced rock weathering (ERW) in agricultural soils.

At the Princess Creek Tailings Storage Facility (Tasmania, Australia), we use the XFM beamline to unravel the behavior of copper and cobalt under low pH conditions. These critical metals, essential for renewable energy technologies, undergo dissolution and precipitation influenced by native acidophilic bacteria. Understanding these processes is key to developing sustainable strategies for metal recovery and advancing the circular economy.

Additionally, XFM mapping has been employed to better understand microbially accelerated mineral carbonation (MC) strategies, such as the weathering of ultramafic mine waste and basaltic rock flours in soils (ERW). This has led to the observation of near-surface mineral carbonation processes facilitated by endogenous microbes, which can contribute to reducing the carbon footprints of agricultural and mining activities.

The integration of these studies underscores the importance of synchrotron science in advancing our understanding of near-surface biogeochemical processes that are critical for both climate change mitigation and the development of sustainable resource management practices.

Authors: Thomas Ray Jones, Gordon Southam, Anton Wasson, Andrew Langendam

KEYNOTE TALK

28 NOV

David Jenkins

ABSTRACT 63

3D micro-CT analysis of biochar in microstructure of metallurgical biocoke

The use of renewable biomass is a promising solution to reduce carbon dioxide emissions in steelmaking. Partial substitution of coal with biomass in producing biocoke however affects coke strength, although to different extents depending on the properties of biomass such as type and size. The interaction between biomass derived components (BDC) and reactive maceral derived components (RMDC) in coal determines how well biochar particles are integrated into the coke matrix. It is therefore possible that the quality of bonding at the BDC-RMDC interface influences the strength of biocoke. No studies in literature however quantitively reported such bonding quality. This study aims to develop an image analysis methodology to quantify the quality of BDC-RMDC interface bonding based on 3D micro-computed tomography (micro-CT) images. Bio-coke samples were prepared by blending 95% coking coal and 5% woody biomass and then coked in a pilot oven. The biocoke samples of 20 mm size were imaged at the Image and Medical Beamline in Australian Synchrotron at a resolution of ~9 μm/pixel. An image analysis algorithm was developed to identify the biochar boundary in 3D CT images based on texture and greyscale difference between biochar and the surrounding reactive maceral derived components. Furthermore, using the in-house "onion-skin" analysis codes, the quality of BDC-RMDC interface bonding was quantified by the excess porosity in the vicinity of the biochar surface. This work paves the way for improving the use of biomass in metallurgical cokemaking and linking biocoke microstructure and strength.

Authors: Ai Wang, Salman Khoshk Rish, Lauren North, David R. Jenkins, Arash Tahmasebi

KEYNOTE TALK

29 NOV

Vladimir Golovko

ABSTRACT 68

Atomically precise metal clusters as unique species bridging the gap between atom/ions and bulk-like matter

Synthesis of nanomaterials with precision down to one atom will be illustrated on the example of metal clusters – a class of materials with unique and strongly composition- and size-dependent properties. Selected examples of fundamental studies of such materials as well as selected applications of such species as well-defined active sites in catalysis will be discussed in detail. Specifically, selected studies highlighting unique electronic and structural features of clusters, including studies performed using synchrotron-based techniques will be introduced first. [1-10] Next, catalytic hydrogen production and utilisation of hydrogen using cluster-based catalysts will be briefly presented on several examples. [11-14] Finally, our studies of the catalytic conversion of CO2 to more valuable and more reactive chemicals will be briefly discussed. [15, 16]

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Authors: Vladimir Golovko, Aaron Marshall, Shailendra Sharma, Gregory Metha

Jun Wang

27 NOV

ABSTRACT 75

Real-time grain-scale rotational bursts via Laue X-ray diffraction in Mg-Zn: impact of crystal orientation and autocatalytically coordinated plasticity among neighbouring grains

Metals comprise crystallites/grains. These crystallites rotate while undergoing strain, impacting performance. Understanding this is crucial for advanced engineering applications. Although we understand many of the mechanisms involved, the intermittent nature of grain rotation is not well understood due to the lack of a technique that provides real-time observation with temporal resolution down to 10s' milliseconds.

We have developed a real-time Synchrotron X-ray Laue diffraction technique at the IMBL beamline that can track the real-time rotation of many grains in a polycrystalline magnesium alloy (60 μm grain size) with 64 ms resolution. The tensile sample (500 μm thickness) was subjected to a strain rate of ~3×10-5s-1 when transmitted by a polychromatic X-ray beam (200 μm diameter). We examined 33 grains at the elastic-plastic transition and grouped them based on their initial orientations. We observed the intermittent rotational burst for all grains caused by either slip or tension twinning. In most of the grains with orientation favourable for twinning, this burst is accompanied by a significant intensity drop. We believe the simultaneous grain rotation and intensity drop are caused by twinning. In most grains favourable for basal slip, the misorientation axis indicates that, indeed, basal slip dominates the most significant rotational burst. We also found that the magnitude of the rotational burst is comparable between slip and twin. However, the most significant burst comes from twinning. Importantly, we observed autocatalytically coordinated bursts (caused by either slip or twinning) among all grains in the diffracted volume inside the bulk, regardless of their orientations.

Authors: Jun Wang, Alban de Vaucorbeil, Sitarama R. Kada, Andrew Stevenson, Peter A. Lynch, Matthew R. Barnett

KEYNOTE TALK

Michael Rowe

28 NOV

ABSTRACT 81

Gallium as a Potential Biosignature of Silica-Microbe Interactions in Hot Springs: Preparing for a Future Mars Sample Return Mission

Discovering evidence of life beyond Earth remains a primary aim of astrobiology and is an important driver of planetary exploration. Towards this aim, the LifeSpringsMars mission concept led by Australia has a primary scientific objective of returning samples of what has been interpreted as hot spring silica deposits (home to extremophile life on Earth) from Gusev Crater, Mars. However, since organic biosignatures degrade with time, inorganic geochemical indicators of biological activity may provide important evidence of ancient microbial activity. This study utilises sXRF and XANES on the XFM beamline to investigate the distribution and coordination environment of trace metals associated with microbial textures in terrestrial hot spring silica serving as analogues of the martian silica deposits.

Silicified microbes in hot spring deposits are variably enriched in Ca, Al, Mn, Fe, As, Rb, Cs, Sr, and Ga. Gallium, enriched up to ~1400 ppm compared to a background of 20-30 ppm in most geologic materials, is the most widespread trace metal consistently associated with microbial material in modern to Jurassic (~178-150 Ma) deposits. Gallium XANES results indicate two distinct coordination environments (tetrahedral or octahedral), based on standard comparisons. Tetrahedrally coordinated Ga appears to be associated with silicified microbial textures while octahedrally coordinated Ga is observed in overprinting Fe-rich hydrothermal fluids. The distribution and chemical behaviour of Ga makes it a strong candidate for a novel inorganic biosignature in the search for ancient life.

Authors: Michael Rowe, Kathleen Campbell, Andrew Langendam, Barbara Lyon, Ema Nersezova, Dominique Stallard, Amanda Galar, Diego Guido

Livia Salvati Manni & Patrick Zueblin

27 NOV

ABSTRACT 97

Developing cryo-capabilities at the SAXS/WAXS beamline. The case study of water nanoconfinement in lipidic mesophases

A new cryo-setup was developed to study soft materials at subzero temperature. Maintaining extremely low temperatures (below -100°C) consistently and reliably over long periods is technically demanding, and achieving sub-zero temperature without condensation or ice crystals on the sample holder is difficult. Cryogenic conditions are of potential interest for the characterisation of a wide range of soft materials from pharmaceuticals to food products, and whole cells.

In this case study we investigated the behaviour of lipidic mesophases and the water confined in their water channels. Lipidic mesophases are a class of lipidic materials that can have different complex geometries and have been employed in food,1 as drug delivery systems2 and as biochemical tools for the crystallisation and reconstitution of membrane proteins.3 We have recently shown that they are also ideal nanoconfinement systems to study the behaviour of water, where the nanoconfinement properties the confining matrix can be geometrically tuned. 4,5,6

SAXS can be employed to characterise the geometry and the water channel size of lipidic mesophases, while the WAXS region can be employed to monitor the formation of ice crystals.

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Authors: Livia Salvati Manni, Patrick Züblin , Raffaele Mezzenga

Jiali (Maggie) Zhai

27 NOV

ABSTRACT 100

Inverse cubic structure evolution within ionizable lipid nanoparticles correlates with mRNA transfection in macrophages

mRNA lipid nanoparticle (LNP) technology presents enormous opportunities to prevent and treat various diseases. In a recent study using time-resolved small angle X-ray scattering, we demonstrated that the ionizable lipids ALC-0315 and SM-102 used in mainstream COVID-19 mRNA vaccines manifest pH-responsive formation of inverse lyotropic liquid crystalline mesophases including the cubic and the hexagonal mesophases.1 In this study, we aimed to correlate their pH-responsive structures with mRNA delivery and transfection abilities in macrophage cells.2, 3 Partial phase diagrams of LNPs as a function of ionizable lipid ratio and pH variation examined by small angle X-ray scattering were presented, showing pH-sensitive structural transitions. In terms of biological activities, the pH-dependent mesophase behavior of LNPs during the endosomal acidification process dominates the cell association, where a broader span of structural transition and earlier starting point (higher pH) in the SM-102 ionizable lipid LNPs are more favorable for macrophage MH-S cells compared to the ALC-0315-based LNPs. As a proof-of-concept application, the optimal mRNA@LNPs with desirable pH-dependent phase behavior was demonstrated as a nanocarrier for EGFP mRNA delivery into MH-S cells with a transfection efficiency over 70%. Interestingly, mRNA@LNPs comprising SM-102 lipid showed superior mRNA transfection than the ALC-0315 analogue, which was correlated to the lack of the ability to transform into the cubic phase at an acidic condition (e.g., pH 4).

References:

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Authors: Haitao Yu, Brendan Dyett, Joshua Iscaro, Natalia Martinez, Steven Bozinovski, Calum Drummond, Jiali Zhai

KEYNOTE TALK

29 NOV

Danielle Martin

ABSTRACT 114

Australian Synchrotron: Facility update and new developments

This talk will provide an overview of the Australian Synchrotron and updates at the beamlines. The facility has seen many changes and developments, with new BRIGHT beamlines coming online and with the addition of new beamline capability. I will touch on the projects at the facility, including: the new XFM DMM; progress with the IMBL BCT project; the BioSAXS co-flow; developments in the MEX microprobe; the upcoming MX2 robot and goniometer and PD Mythen III detector upgrades; and various other facility developments that are currently underway.

Authors: Danielle Martin, Helen Brand, Michael James

Alistair Evans

28 NOV

ABSTRACT 139

XFM at the Australian Synchrotron provides fundamental insights into the life history and ecology of Australia's marsupials

The record of trace elements within sequential mineralised tissues is an emerging tool for revealing mammalian life history and ecology. Using the X-Ray Fluorescence Microscopy (XFM) beamline of the Australian Synchrotron, we have undertaken a series of experiments to explore the trace element biology mineralised within the teeth of Australia's most abundant and diverse mammalian lineage – the marsupials.

Our work has uncovered a previously unknown pattern of marsupial tooth development. The long, procumbent incisors of kangaroos, possums and wallabies are ever-growing teeth. Fortunately, the record mineralised within these teeth spans the entire life of these marsupials, making these incisors excellent candidates for chemical analysis.

Much of the work on trace element uptake in the teeth of other mammals, particularly primates, has focused on signals related to birth and weaning. Using XFM mapping of Ca, Zn and Sr, we quantify these signals in the teeth of 5 marsupial species. We find that patterns of Sr uptake are fundamentally different between marsupial and eutherian mammals. As the nutritional requirements of the growing young change compositional variations in marsupial milk are ultimately mineralised into the developing teeth. We also show adult cyclicity in trace element mineralisation and the ecological factors that putatively produce these oscillating patterns, particularly apparent in Sr.

Finally, we apply our findings for extant species to the marsupial megafauna prevalent in Australia until ~40,000 years ago. XFM analysis of incisor teeth from the largest marsupial that ever existed, *Diprotodon optatum*, provides a window into the growth and ecology of this extinct species, including age at weaning.

Authors: William Parker, Graeme Coulson, Marilyn Renfree, Erich Fitzgerald, Justin Adams, Alistair Evans

KEYNOTE TALK

28 NOV

Porun Liu

ABSTRACT 153

In-situ Exploring Transition Metal Electrocatalysts for Energy Conversion Applications

The study of heterogeneous electrochemical processes at electrode interfaces, aimed at converting, storing, and utilizing clean energy, has garnered significant attention in recent research. Developing high-performance inorganic electrocatalysts that can maintain effective electrochemical activity under operando conditions remains a considerable challenge. A deep understanding of the structural, crystallographic, and electronic properties of these activated electrocatalysts during operando conditions is vital for unravelling their mechanisms and assessing their performance. This presentation highlights the application of X-ray Absorption Spectroscopy (XAS) to confirm the presence of monoatomically dispersed transition metals (TM = Mn, Fe, Co, Ni, Cu, Ru) anchored onto high surface area two-dimensional (2D) materials, which serve as electrocatalysts for the Oxygen Reduction Reaction (ORR) and the Hydrogen Evolution Reaction (HER). Furthermore, we showcase in-situ characterizations of transition metal-based electrocatalysts (TM = Bi, Ag, Cr) for the Carbon Dioxide Reduction Reaction (CO2RR), and explore their electrochemical transformations from precursors. The observed enhancements in electrocatalytic activities are attributed to the electronic modulation of the transition metals by the 2D substrates or the chemical environments within the nanoscopic structures.

Authors: Porun Liu

Yameng Fan

27 NOV

ABSTRACT 164

Using Synchrotron Techniques to Study the Structural Evolution and Redox Mechanisms in Cathode Materials for Rechargeable Batteries

Rechargeable batteries are essential for harnessing clean, renewable energy sources such as solar, wind, and tidal power, which are abundantly available in Australia. Improving the lifespan and performance of these batteries largely depends on the intrinsic properties of their electrode materials. Our group employs *in situ* and *ex situ* synchrotron characterization techniques at the Australian Synchrotron—specifically Powder Diffraction, X-ray Absorption Spectroscopy, and Soft X-ray—to track structural changes, monitor redox reactions, and identify intermediate products in electrode materials across various battery systems, including Li/Na-ion batteries, Na-S batteries, and aqueous zinc-ion batteries. This approach enables us to uncover the underlying degradation or functional mechanisms, offering valuable insights to guide the optimization and design of electrode materials for enhanced battery performance. Our findings have been published in high-impact journals such as *Nature Communications, Angewandte Chemie International Edition,* and *Advanced Materials*. This presentation will provide a brief overview of the operating principles, advantages, and challenges of rechargeable batteries, with a primary focus on using in situ and ex situ synchrotron techniques in our group to study and improve oxide and sulfur-based cathodes in diverse battery systems.

Authors: Yameng Fan

29 NOV

Roger Bourne

ABSTRACT 11

Revealing the tissue structural determinants of diffusion-weighted MRI contrast with phase contrast CT microscopy

We investigated correlations between MRI and phase-contrast microCT (MCT) measurements in formalin-fixed human prostate tissue. Contrast in diffusion-weighted MRI is known to depend strongly on local tissue microstructure, however little is known about the specific cellular structural components affecting water mobility – especially in non-neural tissues. Microstructure determination based on histopathology is severely limited by the necessity for tissue processing and thin sectioning for light microscopy. As an alternative, MCT provides a unique tool to non-destructively image tissue microstructure and obtain direct correlations with post-CT MRI measurements. Structural analyses such as tortuosity and porosity are expected to provide direct correlates with apparent diffusion coefficients measured by MRI. In addition, we propose Monte Carlo simulations of particle diffusion in structural meshes derived from MCT data.

Authors: Roger Bourne, Amir Taba, Lorenzo D'Amico, Timur Gureyev, Tim Stait-Gardner, William Price, Geoffrey Watson, Paul Sved, Scott Leslie, Benedicta Arhatari

28 NOV

Samantha Alloo

ABSTRACT 13

X-rays 'flowing' backwards: Enabling the separation of edges and microstructure in dark-field imaging

Speckle-based X-ray imaging (SBXI) is an emerging experimental technique [1,2] sensitive to three complementary imaging modes: attenuation, phase-shift, and dark-field. Radiography relies on attenuation to distinguish bones from soft tissue. Phase-contrast helps visualize weakly attenuating materials, like fat, muscle, and organs. Dark-field contrast is generated by sample microstructures, causing intensity variations smaller than the system's resolution, such as unresolved grains or pores, as well as edges. We have been developing Multimodal Intrinsic Speckle Tracking (MIST), an algorithm to recover attenuation, phase-shift, and dark-field images from SBXI data [1, 2, 3]. MIST is derived from the paraxial Fokker-Planck equation [4, 5], which describes how an X-ray wavefield evolves as it propagates. Traditionally, we have considered X-rays flow in the source-to-detector direction (the 'evolving' perspective), publishing results demonstrating high-resolution image retrieval [3]. Recently, a physically equivalent 'devolving' Fokker-Planck equation, which follows optical flows from the detector back to the source, was revealed [6]. We investigated how these perspectives affect the inverse problem solution and the characteristics of the recovered multimodal images. We re-derived MIST algorithms from the devolving Fokker-Planck equation and compared the recovered images to those obtained with the evolving MIST variants. This talk will present results of this analysis, revealing how microstructure- and edge-induced dark-field contrast can be separated.

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[6] Beltran, M.A. et al. Optica, 10(4):422–429, 2023.

Authors: Samantha Alloo, David Paganin, Kaye Morgan, Konstantin Pavlov

28 NOV

Nick Phillips

ABSTRACT 14

Synchrotron X-ray beam motion by electron source position scanning

High-resolution X-ray imaging is often performed by scanning a probe over a field of view, as for example in nanoprobe X-ray fluorescence microscopy or ptychography. These approaches rely on scanning instrumentation and algorithmic approaches to achieve optimal spatial resolution. Whilst high-performance stages, interferometric systems and the design of advanced instrumentation go some way to provide the desired speed, accuracy, precision and stability, the mechanical performance of these systems remains a limiting factor.

This work describes a new approach for synchrotron X-ray beam scanning without any mechanical motion. Instead, the X-ray beam at the sample plane is scanned by the motion of the X-ray source position within the insertion device, eliminating all mechanical motion. This approach was first proposed in 2014 by de Jonge et al. However, until now the range of electron beam motion thought necessary was deemed impractical, and a demonstration was never realised. Here, we revisit this idea, reposing the concept for a configuration that employs low source-demagnification optics to help limit the required source movement for probe translation at the Swiss Light Source. Source Position Scanning (SPS) is demonstrated for ptychographic data collection and is foreseen to be applicable to other synchrotron imaging methods. The use of electromagnetic optics for beam scanning opens new opportunities for use within instrumentation where scanning stages may not be practical, e.g. furnaces or mK fridges, and possibilities to develop ultra-fast scanning akin to the kilohertz scanning speeds possible in today's electron microscopes.

Authors: Nick Phillips, Ana Diaz, Manuel Guizar-Sicairos, Marie-Christine Zdora, Michael Boege, Andreas Menzel

28 NOV

Saeed Askari

ABSTRACT 15

Superdurable High-Surface-Area Nitrogen-Rich Porous Carbon with Single-Atom Co-N_4 Sites for Enhanced Bifunctional Oxygen Electrocatalysis in Zinc-Air Batteries

Among metal-air batteries, the zinc-air battery (ZAB) stands out due to its market presence and promising performance. ZABs are notable for their high theoretical energy density (1086 Wh/kg), safety, and the abundance of zinc. However, they face challenges with slow kinetics in the Oxygen Evolution Reaction (OER) and Oxygen Reduction Reaction (ORR). In this study, we developed a new electrocatalyst to improve these reactions. We used an innovative synthesis method to create a Co-N-C structure. HAADF-STEM images and FT-EXAFS spectra confirmed the presence of single-atom cobalt sites coordinated with four nitrogen atoms (Co-N_4). Electrochemical tests showed that the catalyst performed exceptionally well, with an ORR half-wave potential of about 0.859 V and an OER onset potential of 1.544 V, demonstrating great stability. The high surface area and 10% nitrogen content of the catalyst contribute to these results. When used in the air cathode of a rechargeable zinc-air battery, the catalyst achieved a peak power density of 178.6 mW/cm^2 and a specific capacity of 799 $mA \cdot h \cdot gZn^{-1}$. The battery also showed long-term stability, lasting through 1600 charge/discharge cycles. Density functional theory calculations revealed the importance of the position and concentration of pyridinic nitrogen in enhancing ORR efficiency, highlighting its crucial role in the Co-N_4 catalyst's performance.

Authors: Saeed Askari, Parama Chakraborty Banerjee, Mainak Majumder, Matthew R Hill

Marco Vas

28 NOV

ABSTRACT 17

Structural Expansion upon Cooling in the Skyrmion Hosting Material, Cu_2OSeO_3

The Cu_2OSeO_3 material system has gained interest over the last 10-15 years because it is the only multiferroic insulator to host magnetic skyrmions. This material falls into the B20 class, which crystalises in a non-centrosymmetric cubic P213 space group. Most materials in this class, such as MnSi and $Fe_{1-x}Co_xSi$, despite having different compositions, host magnetic skyrmions.[1] This suggests that the role of the crystal structure might influence the capability of the material to host skyrmions. The skyrmion formation is a result of the four Cu^{2+} sites, which have a 3-down 1-up spin arrangement with Ferromagnetic (FM) and Antiferromagnetic (AFM) super-exchange interactions being present.[2] The lack of inversion symmetry in the corner shared O-Cu_4 tetrahedra result in an appreciable Dzyaloshinskii–Moriya interaction (DMI) between Cu^{2+} sites; this competes with the super-exchange interactions leading to spin canting that underpins the formation of helical/conical spin textures under specific conditions.[3] Due to the system's complex spin and charge interactions, the underlying quantum-mechanical processes behind these phenomena are still not fully understood. Further experiments are required; as such, this project aims to provide details on the roles played by the crystal structure that may enable the magnetic structures observed at different conditions.

I will present high-resolution variable temperature synchrotron pXRD data collected at the Australian Synchrotron that shows a structural anomaly of Cu-Cu interactions lengthening upon cooling the system at similar temperatures where magnetic structures form. I will also show how this anomaly is affected by chemically doping different cations into the crystal structure.

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Authors: Marco Vas, Samuel Yick, Elliot Gilbert, Qinfen Gu, Clemens Ulrich, Tilo Soehnel

28 NOV

Lorenzo D'Amico

ABSTRACT 19

Towards clinical phase-contrast X-ray imaging on the imaging and medical beamline for lung cancer diagnosis

High-resolution computed tomography (HRCT) is the primary modality for assessing pathological alterations within the human lung. However, the spatial resolution achievable with a clinically acceptable dose is approximately 0.5 mm, leading to poor diagnostic outcomes (20 % of the cases) and often requiring further investigations using invasive methods, such as biopsies. In recent decades, propagation-based phase contrast X-ray imaging (PBI) has demonstrated its capabilities for studying lung specimens and small animals in vivo. This phase-sensitive technique can achieve higher resolution at the same low X-ray dose rates as HRCT. Here, we present the first steps toward the clinical application of PBI for imaging human-sized lungs. The current studies were conducted at the Imaging and Medical beamline (IMBL) of the Australian Synchrotron. In the first phase, we imaged a human-torso plastic phantom. This phantom was used to demonstrate that PBI can successfully scan an object the size of the human chest and to optimize the imaging setup (including scan energies and sample-to-detector distances). In the second phase, we applied the optimized parameters to image calf lungs within the rib cage, replicating the tissue composition of the human-chest as closely as possible. In the third phase, we are imaging calf lungs using a human-chest phantom equipped with a mechanical diaphragm to simulate breathing, taking a step closer to real human chest radiography.

Authors: Lorenzo D'Amico, Lucy Costello, Christian Dullin, Kaye Morgan, Martin Donnelley, Giuliana Tromba, Marcus Kitchen, Daniel Hausermann, Chris Hall, Anton Maksimenko

Moshi Geso

29 NOV

ABSTRACT 21

Effect of X-ray FLASH synchrotron-based radiation and nanoparticles on the survival of cultured normal and their tumour derived cells

Irradiation at ultra-high dose rates (FLASH) has demonstrated the ability to protect normal tissue while maintaining tumour control in various in vivo studies. However, only a small number of cell lines have been examined in vitro, which have yielded inconsistent results. If oxygen depletion is responsible for the sparing effect of FLASH, then no protective effect for cells irradiated with low doses in normoxic conditions is expected.

Two primary cell lines (colon epithelial cells & melanocytes) and their cancerous derivatives (Cacao-2 & MM96L cells, respectively) were exposed to either conventional x-ray dose rates (~1 Gy/min) or ultra-high dose rates (FLASH beam > 40 Gy/sec) up to a maximum of 6 Gy. Experiments were repeated in cells pretreated with 1 mM of 15-nm Gold nanoparticles. Cellular responses were determined using clonogenic assays.

Normal cells (skin and colon) showed slightly more sensitivity to the radiation then their cancer derivatives. However, no clear FLASH effects are observed when comparing same cell lines response to conventional and FLASH beams. We attribute this to the experimental conditions where the exposure to the conventional beams required the cells to be transported to the incubator which took about 4 hours. This might have led to some cell proliferation.

A FLASH effect was observed at low doses (6-Gy) under normoxic conditions in these cell lines. The FLASH effect is more obvious in the colon cell line. This might be due to the slow growth of melanocytes. Around 15% dose enhancement was observed with gold-NPs even at FLASH beams.

Authors: Moshi Geso, Rod Lynch, William Patterson, Terrence Piva, Tom French, Masao Nakayama, Helen Forrester

28 NOV

Wengang Huang

ABSTRACT 22

Intermarrying MOF glass and lead halide perovskite for photocatalysis

Metal-organic framework liquid/glass and their nanocomposites have generated considerable interest in an interfacial area between glass, crystal, MOFs and materials engineering. A significant advance in MOF glass composites is their capability to form stable composites with other secondary components, exhibiting highly tuneable properties. These composites usually surpass the performance of their individual components, demonstrating increased porosity, rigidity, optical property, and macroscopic processibility.

One of the most intriguing questions is whether the catalytic properties of the MOF glass can be tuned through functionalisation and nanocomposite interfacial engineering. The answer to this question can help us understand the carrier transfer behaviours within the amorphous glass materials and further design catalysts with various form factors. In this work, we address this open question by fabricating and examining the single atom-functionalised MOF glass and CsPbI3 nanocomposites. We applied a variety of synchrotron characterisations (XAS, in-situ total scattering, in-situ THz-FarIR) to identify the presence of partially amorphous perovskite structures at the interface and built connections with the carrier transfer behaviour and photocatalytic activity of the composite. This information further enables the designing of catalysts for advanced chemical synthesis.

Authors: Wengang Huang, Jingwei Hou

28 NOV

Nicholas Florent

ABSTRACT 25

Measurements of porosity in Martian mineral analogues using Small Angle Neutron Scattering

NASA plans to return humans to the Moon as a step towards preparing for a crewed mission to Mars. Water is a vital resource and In Situ Resource Utilisation of Martian assets is critical to reducing the Earth-departing spacecraft's mass. Recent data shows the regolith of Mars to be basaltic and contain 1-5 wt% of water. It is thus important to understand the regolith's characteristics, particularly its porosity and ability to hold (and release) water. No Martian regolith exists on Earth so two basalts mined from the Manor and Werribee quarries in Victoria, Australia, were used as simulants to develop techniques for understanding porosity characteristics.

The basalt samples were hydrated using a 97% relative humidity or mixed in a 5:1 ratio of basalt to HDO to saturate fully. The total porosity and volume of pores that can be filled with water were determined using Small-Angle Neutron Scattering (SANS) and compared to gas adsorption. We discuss the special steps needed to reduce multiple scattering for these high scattering contrast minerals and we describe a method to calculate pore volumes using the Size Distribution Tool of the Irena software package for Igor Pro.

SANS data shows that approximately 58% of the Manor's pore volume was filled with HDO when exposed to 97% RH, but only 20% of the Werribee's pore volume. When fully saturated, the Manor basalt filled 87% of the pore volume, and the Werribee basalt filled 80%. The implications of these results for future research will be discussed.

Authors: Nicholas Florent, Jitendra Mata, Jan Ilvasky, Saffron Bryant, Gail Iles, Gary Bryant

ORAL PRESENTATION

28 NOV

Denis Korneev

ABSTRACT 28

Synchrotron based micro-CT for precise targeting the areas of interest for biological FIB-SEM

Focused ion beam scanning electron microscopy (FIB-SEM) provides a unique opportunity to collect true 3D datasets at nanometre resolution, but the volume, which can be examined with this method in a reasonable time (a few days session) is strictly limited and rarely exceed 50×50×50 μm, when a typical biological sample (tissue chunk or an organ of a small organism, e.g. insect or fish embryo) has dimensions about 1000×1000×1000 μm.

To make it suitable for FIB-SEM imaging, a biological sample should be stained with heavy metals (typically osmium and uranium) and embedded into resin. A proper staining (osmication) makes the sample completely black, thus any kind of light microscopy cannot be used to target the internal structures.

Using a zebrafish embryo, which was prepared to FIB-SEM (osmicated and resin-embedded), we demonstrated that synchrotron based micro-CT imaging is an ideal method to target the internal structures for FIB-SEM data collection. We successfully targeted some tiny (ventral habenula and Inferior raphe) structures in the brain of the embryo, and imaged them using an oxygen plasma FIB-SEM, collecting large datasets (2500 slices, 6144×4096, isotropic voxel 15 nm) for the targeted areas.

Comparing white beam and monochromatic beam imaging, we found that for such heavy metal-stained samples monochromatic beam does not provide any detectable improvement and white beam should be used as a faster (just a few minutes per sample) imaging method.
The tomograms were processed and analysed in ORS Dragonfly software. To reach the localized areas for FIB-SEM data collection, the face side of the block was precisely trimmed using a ultramicrotome with a diamond knife and a custom sample holder.

Authors: Denis Korneev, Rachel Templin, Sergey Gorelick, Minyu Chan, Georg Ramm

Javad Khosravi farsani

28 NOV

ABSTRACT 29

Acoustic wave assisted synthesis of monolithic MOF superstructures with hierarchical porosity and tunable properties

Charge transfer capability, hierarchical porosity, and stable structure are vital properties and bottle necks in developing metal organic framework (MOF)-based efficient materials for various applications. We are developing a new strategy based on an acousto-microfluidic platform for synthesis of MOF monolithic superstructures with hierarchical micro-meso pores (pore sizes as big as 17nm and more), and improved charge transfer. Due to their comparatively superior stability in aqueous media, capability in bearing high number of defects without structural collapse, and potential real-world applications, we chose zirconium-based MOFs as model for our study. Through a non-classical crystallization phenomenon enabled by our method, monolithic MOF superstructures with high crystallinity and hierarchical porosity in ambient conditions are assembled as quick as 1 minute. In addition, controllable defective nature of the as-synthesized MOF monoliths unlocks light adsorption and better charge transfer capabilities of the as-synthesized MOF superstructures, properties which are in favour of applications where light harvesting is required. The method introduces a new platform for achieving high performance MOFs with tunable desired properties.

As the synthesized MOF monolithic superstructures via our method are in the order of few tens of microns in size, Synchrotron beam (SAXS/WAXS) can enable localized crystallographic analysis of the MOF superstructures synthesized using sound waves, which is not possible using laboratory or other PXRD, XRD methods. The crystallographic data for single monoliths is highly desirable as it can help understand the purity of the crystalline phase in the MOF superstructures. considering the high resolution and localized analysis enabled by synchrotron beam, Synchrotron beam (SAXS/WAXS) is the best option for crystallographic characterization of our synthesized MOF superstructures.

Authors: Javad Khosravi Farsani, Leslie Yeo, Amgad Rezk, Joseph J Richardson

ORAL PRESENTATION

27 NOV

Guanghua Lu

ABSTRACT 30

Impact of iron ore and binder addition on microstructure of ferro-coke for low-carbon blast furnace ironmaking

Coke plays a vital role in traditional blast furnace (BF) ironmaking. As a type of highly reactive coke, ferro-coke produced by poor quality coal and low-grade iron ore can start gasification ($CO2+C=2CO$) at a lower temperature than conventional coke. This results in the conversion of more CO2 to CO, which in turn reduces more iron oxides to metallic iron (CO+ 〖Fe〗_2 O_3→Fe+ 〖CO〗_2). This process not only lowers CO2 emissions but also decreases the reduction agent rate. However, the lower strength of ferro-coke limits its application. To obtain high quality ferro-coke, it is necessary to clarify the correlation between strength and microstructure.

As a non-destructive method of analysis, Micro-CT not only provides high resolution images but also operates with high efficiency, particularly when dealing with large sample volumes. In this study, the prepared ferro-coke samples were imaged at the Imaging and Medical Beamline (IMBL) and white beam (M-CT) of the Australian Synchrotron. The images were imported to GeoDict software to construct 3D structures of each sample, which were then segmented into void (pores) and solid (carbon and mineral) phases according to brightness and contrast. The porosity (void fraction) and pore size distribution were analyzed by counting the number of voxels.

The results show that the increase in iron ore ratio decreased the overall porosity, open pore ratio, and coke strength, but had almost no influence on the pore size distribution. We also found that the type of binder used influences the ferro-coke microstructure, particularly the overall porosity and pore size distribution. These results guided us to further elucidate the microstructural differences from the perspective of coking behaviour.

Authors: Guanghua Lu, Salman Khoshk-Rish, Hannah Lomas, Arash Tahmasebi

James Cayley

28 NOV

ABSTRACT 32

VHEE radiotherapy research at PEER

Very high-energy electrons (VHEE, electrons with energy greater than 50 MeV) are of increasing interest to the field of radiotherapy, due to their ability to penetrate deeply into tissue and reach tumours that are out of reach to clinical electrons of lower energies. Linacs capable of reaching these energies are also capable of exceedingly high dose-rates, well above that of the threshold for FLASH radiotherapy (40 Gy/s), an emerging modality praised for its normal tissue sparing qualities.

While ongoing efforts are being made globally to quantify the exact parameters that deliver a FLASH effect, clearly, dosimetry for ultra-high dose-rate environments is required. The Australian Synchrotron's Pulsed Energetic Electrons for Research (PEER) beamline delivers 100 MeV electrons and has been used to investigate the dose-rate (DR) and dose-per-pulse (DPP) independence of the MOSkin detector, a promising candidate for FLASH dosimetry. Previously, DR independence was established and, more recently, DPP independence was investigated. With up to 28 Gy DPP delivered in 200 ns, corresponding to DRs as high as 1.65×10^8 Gy/s, the MOSkin was shown to remain linear in its response and remains a suitable candidate for quality assurance during FLASH radiotherapy.

Further, recent experiments involving in-vitro cell lines and fresh mice cadavers have been conducted on PEER. The MOSkin was used to verify planned doses, and, in the case of cell experiments, were included in 3D printed phantoms with the sensitive volume located directly behind the cells to allow for quantification of relative doses. The biological results are currently being analysed and will also be presented during this talk.

Authors: James Cayley, Elette Engels, Eugene Tan, Paul Bennetto, Tessa Charles, Dean Cutajar, Jason Paino, Marco Petasecca , Anatoly Rozenfeld, Michael Lerch

Jingwei Wang

28 NOV

ABSTRACT 33

Influence of Acidity in Sulfate-Promoted Pd-Al-MCM-41 Catalysts on Furfural Production from Biomass Pyrolysis

Furfural ($C_5H_4O_2$) is a high-value platform chemical which is traditionally derived from the solvolysis of hemicellulose within lignocellulosic biomass. However, its production from pyrolysis for a high efficiency is far from satisfactory. Herein, we present a series of metal sulfate-promoted MCM-Pd acid catalysts synthesized using both one-pot and impregnation methods. We evaluated various metal sulfate active sites, including $ZnSO_4$, $CuSO_4$, $Fe_2(SO_4)_3$, and $Al_2(SO_4)_3$. The highest furfural selectivity, approximately 70%, was achieved through flash pyrolysis of wet cellulose over the Al-MCM-Pd-$ZnSO_4$ catalyst at 450°C, with an equal mass ratio of catalyst to cellulose. A suitable acidity range, encompassing total acid amount, acid strength, and the Brønsted-to-Lewis acid ratio, was identified as optimal for furfural production. Notably, the Al-MCM-Pd-$ZnSO_4$ catalyst exhibited superior sulfur stability compared to MCM-Pd-$CuSO_4$, MCM-Pd-$Fe_2(SO_4)_3$, and MCM-Pd-$Al_2(SO_4)_3$. CHNS analysis also confirmed minimal sulfur loss in the spent Al-MCM-Pd-$ZnSO_4$ catalyst after five cycles. Additionally, synchrotron S K-edge XAS analysis confirmed the presence of sulfur in the form of "SO_4^{2-}" in the spent catalyst. Advanced in-situ synchrotron high-temperature Pd K-edge XAS, and Pd L3-edge XAS techniques revealed that the active PdO site was reduced to Pd during cellulose pyrolysis. Nevertheless, the catalytic activity and stability were maintained over five cycles in a larger-scale fixed-bed reactor, primarily due to the synergistic effects of $ZnSO_4$, Al_2O_3, PdO, and SiO_2. All these results demonstrate a high practical viability of this heterogenous catalyst for the valorisation of lignocellulosic biomass, an otherwise abundant crop waste across the world.

Authors: Jingwei Wang, Lian Zhang

Xiaoran Zheng

28 NOV

ABSTRACT 38

High-Entropy Oxides with Enhanced Functionality for Metal Air Batteries

The metal air battery has the potential to boast extremely high capacity and good environmental characteristics. However, a major challenge lies in finding a suitable air cathode material that balances the oxygen evolution reaction (OER) and oxygen reduction reaction (ORR) during charging and discharging. This limitation results from a lack of fundamental understanding of the OER and ORR mechanisms, which hinders the effective engineering of materials for both applications. The current work investigates the properties and performance of Ce-based high-entropy oxides with varying numbers of metal cations. We synthesized a new MnNiCoFeCeO2 high-entropy oxide composition with unique short-range ordering and significant structural destabilisation of the CeO2 structure leading to unique low-coordinate state Ce, that demonstrated superior performance in OER and ORR. These processes are associated with increasing defect formation, electronic conductivity, and increased entropy. Notably, conventional CeO2 has a cubic structure with Ce having a coordination state of 8, the HEO showed a significant drop to 6.4. This low coordination Ce centres indicated high electron density which contributes to the enhance performance. Thus, this work has enabled the elucidation of the reaction mechanisms of OER and ORR kinetics, marking a significant advancement in the development of this highly stabilized high-entropy oxide

Authors: Xiaoran Zheng, Pramod Koshy, Sajjad Seifi Mofarah

Sitarama Raju Kada

28 NOV

ABSTRACT 40

Development of dynamic loading studies on the Micro-CT beamline

X-ray Micro-Computed Tomography provides an exceptional methodology for non-destructive inspection of internal morphology of materials. When integrated with in-situ dynamic loading capabilities, it offers a unique approach for monitoring damage accumulation during dynamic deformation.

Titanium alloys, such as Ti-6Al4V (Ti64) are extensively used in aerospace applications owing to their lightweight and high specific strength. The inspection of lifespan of the aircraft components during service is crucial for assessing the part's performance under cyclic loading conditions. In this study, we present results obtained from a unique in-situ dynamic Micro-CT technique, to investigate the void nucleation and growth prior to crack initiation during dwell cyclic loading.

On the fly Micro-CT scans were performed during dwell cycle and low-cycle fatigue loading of a cylindrical Ti64 dog bone specimen. Based on an imaging detector with a 9x objective lens and polychromatic X-ray beam, a single tomography dataset could be acquired in about 10 minutes. Individual scans were performed along the sample gauge length (6mm). Based on subsequent data reconstruction and analysis, the onset of void nucleation, void number density and subsequent growth during dwell cycles were reported with a resolution of about 2 microns.

Authors: Sitarama Raju Kada, Jun Wang, Benedicta Arhatari, Andrew Stevenson, Adam Walsh, David Fox, Nicholas Armstrong, Ross Antoniou, Peter Lynch

Ashlyn Austin

28 NOV

ABSTRACT 44

Towards non-lethal fox control: animal odour profiling and synthetic bait development for conditioned odour aversion

Introduced predators, such as the red fox (*Vulpes vulpes*), have severely impacted Australian livestock and native mammals. Poison baits are a widely used control method, although their effectiveness is undermined through reinvasion by foxes from surrounding territories, they can also result in sublethal doses, producing bait-resistant foxes. A promising non-lethal alternative is conditioned odour aversion, a form of classical conditioning whereby aversive behaviours are formed following the consumption of foods containing a nausea-inducing agent and a prey odour.

The goal of this project is to develop a novel synthetic bait formulation that offers a sustained release of a synthetic prey odour mimic (e.g., sheep). The volatile organic compounds (VOCs) that contribute to the characteristic odour profile of sheep was determined using gas chromatography mass spectrometry to assess for differences between ages, sexes, and breeds. Subsequently, baits were formulated as gelled emulsions, consisting of an oleogel dispersed within a continuous agarose scaffold. The synthetic bait formulations were loaded with the synthetic sheep odour mimic (comprising VOCs) in the oleogel phase and an aversion agent in the aqueous phase. As the synthetic odour was encapsulated in the oleogel, understanding the structure of the oleogel was essential in correlating the odour release to the specific formulation and optimising the odour release profile and bait longevity. Towards this goal, we used a variety of techniques including synchrotron SAXS/WAXS and diffusing-wave spectroscopy to characterise the crystallinity and particle size of the oleogel within the baits and interpret the effects of incorporating a synthetic odour.

Authors: Ashlyn Austin, Anton Blencowe, Todd Gillam, Marta Krasowska, Adrian Manning

Michael Lerch /James Cayley

28 NOV

ABSTRACT 45

Pushing canine radiotherapy towards clinical standards on IMBL

Introduction
In synchrotron radiotherapy, the patient must be vertically translated through the synchrotron beam to fully cover the target volume whilst shaping the field to conform to the target. Currently, no existing clinical system performs both dynamic motion of the patient and dynamic shaping of an X-ray beam. Therefore, we developed a new dynamic treatment delivery system to achieve this in radiotherapy treatments on the Imaging and Medical Beamline (IMBL).

Method
An industrial robotic manipulator was used for patient positioning, boasting sub-millimetre accuracies during motion up to 150 mm/s. For field shaping, a novel dynamic collimator developed on IMBL for synchrotron radiotherapy was utilised. A real-time event-handling system was used to synchronise the motions of the two moving systems. Mock treatments were delivered, and the positional and temporal accuracy of the treatment delivery system was assessed. Finally, geometric treatment margins for the system were determined.

Results
The position of the ball-bearing relative to the treatment fields were small horizontally (<0.1 mm) but large vertically (<1.06mm), changing with delivery speed. Clinically comparable treatment margins up to 2.3 mm were calculated.

Conclusion
We have implemented the first robotic treatment delivery system for synchrotron radiotherapy. The largest errors were observed in the direction of motion of the patient through the beam but can be reduced. Our treatment system offers treatment capabilities and accuracy similar to what is found in current clinical radiotherapy practice, and is ready to support the treatment of large animals on IMBL.

Authors: Micah Barnes, Nader Afshar, Taran Batty, Tom Fiala, Matthew Cameron, Daniel Hausermann, Nick Hardcastle, Michael Lerch

Bernt Johannessen

29 NOV

ABSTRACT 48

The XAS Beamline - an update for 2025

In recent years, the XAS Beamline has experienced a significant increase in demand for beamtime, driven by a growing user community focused on advanced materials, catalysis, and energy storage research.

To meet these evolving needs and align with the capabilities of the new Medium Energy XAS Beamline, we are implementing strategic changes to our user program at XAS. This presentation will outline the current status of the XAS Beamline, detail the upcoming modifications to our operational framework, and discuss how these adjustments will enhance research outcomes and streamline user access.

Our goal is to ensure that the XAS Beamline remains an accessible and critical resource for cutting-edge scientific investigations.

Authors: Bernt Johannessen, Jessica Hamilton

Vaishnavi Krishnamurthi

27 NOV

ABSTRACT 51

Structural evolution of liquid metals and alloys

Liquid metal systems are a new and exciting frontier in chemistry. Room temperature liquid metals (RTLMs) are a subset of pure liquid metals and their alloys, which remain fluidic at room temperature and have great potential in electronic, catalytic, and biomedical applications. However, their complete utilization is hindered due to the lack of analytical techniques which can prove their bulk-liquid chemical processes. The main obstacle to studying these systems is the presence of their metallic bonds, which renders them opaque to most traditional solvent characterization techniques and fails to provide atomic-level insights. Studying the nanoscale structures of bulk liquid metals can provide valuable information on their properties and potential use in different liquid metal applications. Neutron scattering techniques like small angle neutron scattering (SANS) have matured significantly in recent years and can now resolve atomic structures, clusters, and covalent associations within soft matter systems. This talk will highlight the various investigations carried out on liquid metals and alloys, specifically, gallium and several gallium-based eutectic and hypo/hyper eutectic alloys with In, Sn and Cu as the dopants at varying concentrations to probe the nanoscale structures of these systems and develop structure-property relationships for RTLM systems using SANS and molecular dynamics (MD) simulations. Using a defined shape model at a length scale between 6 Å and 1570 Å, crucial knowledge of particle-particle interaction and its effect on the atomic structure is obtained that will help develop the fundamental understanding of solvation dynamics in liquid metals and alloys.

Authors: Vaishnavi Krishnamurthi, Jitendra Mata, Jitendra Mata, Pierre Vaillant, Andrew Christofferson, Gary Bryant, Aaron Elbourne, Torben Daeneke

Elette Engels

28 NOV

ABSTRACT 52

Veterinary microbeam radiation therapy trials at the Australian Synchrotron

Radiotherapy is used in half of all cancer cases, however, curative doses are limited by healthy tissue tolerances. Synchrotron Microbeam Radiation Therapy (MRT) distributes radiation doses spatially to produce extraordinary normal tissue preservation that conventional beams cannot achieve. MRT uses 50µm high-dose "peaks" separated by low-dose 400µm "valleys," which is well-tolerated by healthy tissue, but disrupts tumours and creates a novel transient permeability window for chemotherapy delivery.

To demonstrate the efficacy of MRT and evaluate MRT-facilitated chemotherapy delivery, we commenced the first veterinarian trials on spontaneous canine osteosarcoma at the Australian Synchrotron IMBL. We further developed treatment protocols for future veterinary and clinical trials, including soft-tissue sarcoma and brain cancer.

Dogs were recruited from veterinarian clinics in Melbourne, Australia for the world's-first osteosarcoma trial using MRT. Biopsy, collection of blood and urine, and contrast-enhanced imaging with CT and MRI were performed 3 days before MRT. A 2cmx2cm MRT array with 100Gy peak doses was delivered at 100Gy/s to partially irradiate these tumours. The treatment planning system was also used to compare future whole-tumour irradiations. Chemotherapy (carboplatin) was administered 30mins after MRT to utilize the selective permeability window. Fluids and images were collected again post-MRT, and histological analysis occurred after routine limb amputation.

We treated (40 ± 13)cm3 osteosarcomas in the distal tibia and radius, with (3.9 ± 0.2)Gy valley doses and (130 ± 2)Gy peak doses with 100Gy delivered to (99.3± 0.1)% of the in-field tumour. No skin toxicity was observed, and tumour volume reduced 2 months post-MRT. We further developed methods for future whole-tumour and brain MRT treatments. This work will enhance Australian veterinarian and clinical radiation research.

Authors: Elette Engels, Olga Martin, Stewart Ryan, Mitzi Klein, Stephanie Corde, Elisabeth Schultke, Michael Lerch, Arthur House, Daniel Hausermann, Valentin Djonov

Evan Robertson

28 NOV

ABSTRACT 53

Astrochemistry goes Chiral: Spectroscopic and powder diffraction studies of propylene oxide and vinyl oxirane

Astrochemistry has been proposed as a source of the homochirality found in life, where sugars and proteins are found as either “left-handed” or “right-handed”, but not both. Thus, the recent detection of propylene oxide in a molecular cloud within Sagittarius B2 has great significance as it is presently the only chiral molecule to be directly observed in interstellar space. We report gas and solid phase experiments spanning the electromagnetic spectrum to learn more about propylene oxide and its analogue vinyloxirane, another candidate for interstellar detection.

The first high-resolution infrared measurements of propylene oxide open a window into the rotational energy levels of low lying vibrational states that could be populated in space and produce absorption lines known as “vibrational satellites” in radioastronomy surveys. In the laboratory microwave spectrum of vinyloxirane a previously unobserved gauche conformer has been identified and further analysis of the anti conformer enhances the prospect that vinyloxirane could be the second chiral molecule to be detected in space.

X-ray powder diffraction experiments have revealed the crystalline phase behaviour of racemic propylene oxide and vinyloxirane at low temperatures. Structure determination finds unit cells with equal proportions of “left and right-handed” enantiomers. Complimentary studies on the THz beamline have revealed the far-IR and mid-IR spectral signatures of these molecular ices, both amorphous and crystalline. Intriguingly, crystalline propylene oxide is coloured despite a molecular structure with only single bonds, while double or triple bonds are generally considered essential for absorption of visible light.

Authors: Evan Robertson, Afnan Alasmari, Qinfen Gu, Dominique Appadoo, Courtney Ennis, Chris Medcraft

Elette Engels

28 NOV

ABSTRACT 56

Personalising synchrotron breast-CT: patient-specific simulation, dosimetry, and imaging in preparation for clinical trials at the Australian Synchrotron

Breast screening is an important stage of cancer detection and intervention. Current conventional techniques such as planar mammography and digital breast tomosynthesis involve painful breast compression and images are subject to low sensitivity and image quality, particularly for patients with high breast density. The ANSTO Australian Synchrotron is approaching clinical trials using phase contrast-based breast computed tomography (bCT) at the Imaging and Medical Beam Line (IMBL). This technique can achieve exceptional image quality and a full CT scan using the same radiation dose of a single planar mammography. This work summarises steps towards personalisation of bCT dosimetry and imaging in anticipation of the various breast sizes and composition expected in the clinical trial.

Geant4 simulations of a realistic breast model were calibrated with experimental dose measurements taken at the IMBL. After validating the model, total breast dose and mean glandular dose (MGD) was calculated for different beam energies, and breast density and size. Once MGD was calculated, these were implemented for real bCT acquisitions at the IMBL for different breast sizes. To further investigate the relationship between image quality and MGD, a novel anthropomorphic phantom that allows modification of breast density and size was used for bCT, and the image quality was compared with commercial breast phantoms and conventional CT and MRI.

The MGD simulations and the anthropomorphic phantoms have already contributed in the upcoming clincial trial for quality assurance. The results found that patient breast diameter has the greatest impact on MGD and image quality, rather than breast density. We determined that the synchrotron bCT produces significantly better images than a conventional clinical CT with less radiation dose.

Authors: Elette Engels, Tavjot Kaur Matharu, Matthew Cameron, Yakov Nesterets, Lorenzo D'Amico, Amir Entezam, Michael Lerch, Chris Hall, Anton Maksimenko, Timur Gureyev, Daniel Hausermann

Ying Ying How

28 NOV

ABSTRACT 67

In vivo 4D x-ray dark-field lung imaging in mice

X-ray dark-field imaging is useful in visualising the health of lungs since the many tiny air sacs, or alveoli, cannot be individually resolved, but do create a strong dark-field signal. However, achieving time-resolved tomographic (i.e. 4D) x-ray dark-field imaging is challenging since dark-field imaging has typically required multiple sample exposures, while scanning the position of crystals or gratings, to extract the signal.

Here, we present the first *in vivo* 4D x-ray dark-field lung imaging in mice, performed at the Australian Synchrotron Imaging and Medical Beamline. This is achieved by synchronizing the data acquisition process of a single-exposure grid-based imaging approach [1-3] with the breath cycle of the mice. The short data acquisition time per dark-field projection has made this approach more feasible for 4D x-ray dark-field imaging since it minimizes any motion blur, the total time required, and the radiation dose imposed on the sample. Images were captured of both healthy and diseased mice, specifically models of cystic fibrosis and lung cancer, where a change in the size of the alveoli is expected.

The results demonstrate that the 4D x-ray dark-field signal reveals how the size of the alveoli from different parts of the lungs changes throughout a breath cycle, with examples shown across different models. By quantifying the dark-field signal and relating it to other physical properties of the alveoli, this technique could be used to perform functional lung imaging that allows the assessment of both global and regional lung conditions where the size or expansion of the alveoli is affected.

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[3] How and Morgan, 2022, Opt. Express, 30(7).

Authors: Ying Ying How, Michelle Croughan, Nikki Reyne, Patricia Cmielewski, Marie-Liesse Asselin-Labat, Daniel Batey, Lucy Costello, Ronan Smith, Jannis Ahlers, Marcus Kitchen, David Paganin, Martin Donnelley, Kaye Morgan

29 NOV

James Pollock

ABSTRACT 70

Clinically Relevant Phase-Contrast CT Optimisation of Large Animal Imaging with Synchrotron Radiation

Many lung diseases and abnormalities require precise visualization for effective diagnosis and treatment. Infants, particularly those born pre-term, may experience further complications due to lungs being among the last organs to develop in-utero. A majority of conditions, such as emphysema, bronchopulmonary dysplasia and hypoxia, may be readily diagnosed through volume reconstruction methods such as CT reconstruction. However, exposure to ionising radiation introduces long-term risk, especially for high resolution scans. Phase contrast X-ray techniques, by exploiting the phase information of X-rays, may allow safe improvements to image resolution via modifications to the imaging system. In particular, propagation-based phase-contrast imaging requires minimal adaption of existing medical systems and has already been demonstrated to allow large dose reductions over absorption X-ray imaging. Herein, optimization of propagation-based phase contrast CT for paediatric imaging is demonstrated in large animal lamb models using monochromatic radiation at the Australian synchrotron. Optimisations of image quality and radiation dose were performed for beam energy and propagation distance, with optimal conditions used to test image quality at very low dose. Noise-limited spatial resolution was measured using Fourier ring correlation to assess the dominant effect of Poisson noise on resolution in very low flux scenarios, while dosimetry was performed through Monte Carlo simulations. The resulting CT images demonstrate superior resolution to existing high resolution CT systems while preserving dose to be within or less than current Australian Radiation Protection and Nuclear Safety Agency (ARPANSA) guidelines for infant chest CT exposure (<2.5mSv effective dose).

Authors: James Pollock, Kaye Morgan, Linda Croton, Emily Pryor, Kelly Crossley, Chris Hall, Daniel Hausermann, Anton Maksimenko, Stuart Hooper, Marcus Kitchen

Kang Hui Lim

29 NOV

ABSTRACT 71

Stable and Active PtZnx Intermetallic Single Atomic Catalyst by One-pot Amorphous Silicalite-1 Confinement Strategy for Alkane Dehydrogenation

Propane dehydrogenation (PDH) reaction is one of the most efficient and selective processes for the production of propylene and hydrogen. Platinum alloyed with non-noble metals has proven to give higher activity and selectivity. In our work, we developed the use of PtZn alloy-embedded embryonic zeolites to improve accessibility (i.e., shorter diffusion path length) and to prevent deep hydrogenation to carbon (i.e., improves selectivity). A modified one-pot synthesis strategy was employed to synthesize amorphous embryonic silicalite-1 zeolites containing PtZn intermetallic compounds. Interestingly, we further found an optimal loading of Zn (i.e., 5 times more; PtZn20) for best catalytic performance to be in excess of the stoichiometric ratio for Pt1Zn1 single atomic site formation in PtZn4 alloy. Specifically, propane conversion increased by two-fold with ca. 98% propylene selectivity for 0.3PtZn20 catalyst compared to the stoichiometrically optimal 0.3PtZn4 catalyst. Scanning transmission electron microscope (STEM) and X-ray Adsorption Spectroscopy (XPS) reveal the presence of well-defined PtZn alloy and positively charged Zn species assigned to ZnOx-Si in PtZn20 sample. X-ray adsorption spectroscopy completed in ANSTO reveals excess zinc do not form nanoclusters, and the excess zinc atoms promote higher concentrations of PtZn intermetallic, which is more conducive for catalytic reactions.

Authors: Kang Hui Lim, Claudia Li, Sibudjing Kawi

ORAL PRESENTATION

28 NOV

Christina Loidolt

ABSTRACT 73

Insights into U-REE-Cu-Au skarn occurrences in the eastern Mount Isa Inlier from garnet geochemistry and geochronology

Complex U-REE-Cu-Au skarn occurrences in the Mount Isa Inlier, Australia, are suggestive of a larger mineralising system. U-REE mineralisation hosted in uraninite-apatite-allanite assemblages are intimately associated with skarn garnet, but the nature of that relationship is ambiguous. Although our understanding of individual skarns has improved, the processes controlling trace element enrichments are contentious. Previous and ongoing research on garnets related to mineralisation in other deposits demonstrates that garnet records information which is key to understanding the evolution of those deposits.

Detailed studies of garnet mineral geochemistry and U-Pb geochronology using EPMA, LA-ICP-MS and Synchrotron XFM indicate two main events of garnet formation associated with U-REE mineralisation between ca. 1750-1500 Ma. Formation of garnet-dominated skarn (Group A) and initial U-REE mineralisation is associated with the ca. 1750-1700 Ma, syn-tectonic intrusion of the Burstall granite. Synchrotron XFM element maps of garnet reveal two phases of garnet growth associated with Cu-Au mineralisation and U-REE remobilisation between ca. 1550-1500 Ma – a pre-mineralisation group (B) and syn-mineralisation group (C).

Group A garnet generally forms inclusion- and fracture-rich crystals with well-developed concentric zonation of Fe, Ti, Y and Zr. Group B garnet mainly forms concentrically zoned (Fe, Ti, Zr, Y) rims around vugs in older garnet skarn. Group C garnets are characterized by higher Fe, Mn, Ti, Nd, Y, Zr, U, Th and Rb than group B garnet and are associated with Cu-Au-U-REE mineralisation hosted in allanite-sulfide-feldspar-epidote assemblages. This assemblage occurs in vugs rimmed by group B garnet as well as in veins cross-cutting older skarn lithologies. This study illustrates the ability of garnet to record important stages of mineralisation in complex multi-element skarn deposits.

Authors: Christina Loidolt, John Mavrogenes, Andrew Langendam

Achini Herath

28 NOV

ABSTRACT 74

SYNCHROTRON FTIR MICROSCOPY REVEALS DISTINCT POLYPHENOL ACCUMULATION PATTERNS IN PIGMENTED RICE GRAIN ULTRASTRUCTURE

Polyphenols in pigmented rice grains contribute significantly to their nutritional value, but their precise localisation within the grain ultrastructure remains unclear. Here, we show that synchrotron-based Fourier Transform Infrared (FTIR) microscopy can non-destructively map polyphenolic biomolecule distribution in pigmented rice grains with unprecedented spatial resolution. Using machine learning, we identified distinct accumulation patterns of polyphenols, primarily localised in the top pericarp tissue layer, separate from lipid-associated polyphenols in the aleurone tissues. Integration of prominent polyphenolic-based functional groups, including C=C and C=O stretching vibrations of flavones (1350-1380 cm-1) and C=C stretching vibrations of flavanone ring B (1560-1620 cm-1), confirmed this localisation pattern. Cluster imaging further identified four distinct biomolecular clusters in rice tissues, with the topmost cluster rich in polyphenolic-based functional groups. This high-resolution imaging technique provides new insights into the biochemical variations within different grain tissues, advancing our understanding of rice grain composition. Our findings lay the foundation for future studies exploring polyphenol localisation patterns across various pigmented rice varieties, potentially informing breeding strategies for enhanced nutritional quality.

Authors: Achini Herath, Annaleise Klein, Kaiyang Tu, Vito M. Butardo Jr

28 NOV

Jannis Ahlers

ABSTRACT 76

Reference-free single-exposure dark-field imaging at IMBL

Dark-field imaging is a burgeoning technique which measures the scattering of X-rays from microstructure in an object that is below the resolution limit of the imaging system. The ability to characterise the microstructure of large samples has made dark-field imaging a promising candidate for a variety of applications, such as medical imaging and security scanning. Since imaging potentially moving samples at low dose and high throughput are common requirements in such applications, minimising the exposure time needed for a dark-field reconstruction is an important goal of dark-field imaging techniques.

A number of techniques have been developed that allow for dark-field imaging. These often rely on sensitive optics and require scanning or reference images and therefore several exposures. Recent work modelling dark-field effects in X-ray propagation has enabled dark-field reconstruction in simple propagation-based imaging (PBI), by deconvolving the effects of attenuation and scattering using images taken at two distances or two energies.

In this work we present the development of single-exposure dual-energy imaging on the Imaging and Medical Beamline (IMBL), and its application to dynamic PBI dark–field imaging. The IMBL has a double-crystal monochromator that passes higher harmonics of the set energy, as well as a photon-counting Eiger2 detector with two energy thresholds. The careful choice of beamline parameters, such as wiggler field, filtration, and monochromator energy, allows for an even flux of first and third harmonic photons that can separately and simultaneously be imaged by the Eiger2. We discuss challenges and limitations in the realisation of this experimental setup, and present results of using such single-exposure dual-energy imaging to reconstruct dark-field images of dynamically changing samples.

Authors: Jannis Ahlers, Konstantin Pavlov, Marcus Kitchen, Stephanie Harker, Emily Pryor, James Pollock, Michelle Croughan, Ying Ying How, Marie-Christine Zdora, Lucy Costello, Dylan O'Connell, Chris Hall, Kaye Morgan

Marcus Kitchen

27 NOV

ABSTRACT 78

Dark-field X-ray imaging from near-field X-ray speckle

Dark-field X-ray imaging uses partially coherent radiation to reveal regions of materials that produce ultra-small-angle X-ray scatter (USAXS). Porous and particulate matter can provide strong USAXS signals that, for example, can be used to detect powdered narcotics for customs inspections or to improve diagnostic capabilities of lung diseases [1]. Reconstruction of a dark-field image typically requires multiple images of the object to be collected under different optical configurations, which increases radiation exposure and makes dynamic imaging difficult or impossible. Dark-field imaging also normally requires the use of X-ray optical elements placed before or after the sample, which require highly stable mounting systems. Here we show a new method for dark-field imaging that can be performed from a single phase-contrast X-ray image that requires no optical elements. This technique uses near-field Fresnel diffraction, whereby porous and particulate media are readily revealed by characteristic near-field speckle patterns [2]. We demonstrate its use for imaging the tissues of mice to clearly reveal the presence of tissues that produce USAXS including the lungs and bones. We demonstrate that this dark-field imaging can be achieved using synchrotron radiation or polychromatic radiation from a microfocus X-ray source. Our results indicate that the dark-field signal can provide information about the number of particles/pores in projection if the resolution is sufficiently high with respect to the scattering feature size.

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[2] Kitchen et al. "X-ray specks: low dose in vivo imaging of lung structure and function." Physics in Medicine and Biology 60(18), 7259-7276 (2015).

Author: Marcus Kitchen, Jayan Gunasekera, James Pollock, Stuart Hooper

Brendan Dyett

27 NOV

ABSTRACT 80

Coupling Surface Interactions with Colloidal Transport to Understand Antibiotic Delivery with Self-Assembled Lipid Nanocarriers

Low discovery rates for new antibiotics, commercial disincentives to invest and inappropriate use of existing drugs has created a perfect storm of antimicrobial resistance (AMR). This 'silent pandemic' of AMR looms as an immense, global threat to human health. In tandem, many potential novel drug candidates are not progressed due to elevated hydrophobicity which may result in poor intracellular internalization and undesirable serum protein binding. With a reducing arsenal of effective antibiotics, enabling technology platforms which improve the outcome of treatments, such as repurposing existing bioactive agents is a prospective option. Self-assembled lipid nanoparticles, such as cubosomes, have emerged as promising nanocarriers (NCs) capable of amplifying the therapeutic outcome.

Here, the performance of several antibiotic classes encapsulated within the lipid-based cubosomes are examined. The findings demonstrate that encapsulation affords significant improvements in drug concentration:inhibition outcomes and assists in other therapeutic challenges associated with internalization, enzyme degradation and protein binding. Here we demonstrate the utilisation of scattering and surface sensitive techniques, particularly total internal reflection fluorescence microscopy to reveal dynamics in interactions and uptake of cubosomes. The rationale in optimized drug selection and nanocarrier choice is contextualized by surface interactions and multiscale transport modelling which agrees with experimental inhibition results. We emphasize that currently side-lined compounds became active and revealed a significant increase in inhibition against the pathogenic gram-negative strain, Pseudomonas aeruginosa. The results demonstrate that lipid nanocarrier encapsulation may alleviate a range of challenges faced by antibiotic therapies and increase the range of antibiotics available to treat bacterial infections.

Authors: Brendan Dyett

Shatabdi Chakraborty

27 NOV

ABSTRACT 82

Defining the host-viral roles of the multifunctional rabies virus phosphoprotein

Rabies virus (RABV) is the causative agent of rabies, a severe neurological disease with no therapeutic options for symptomatic infection. After invading a cell, the rabies virus interacts extensively with host proteins to replicate inside the host and circumvent antiviral defense mechanisms. As the RNA of this virus only encodes five proteins, many of the host-viral interactions are mediated by the multifunctional phosphoprotein (P-protein). The functional diversity of P-protein is in part due to discrete functions of the individual domains but also through the expression of five P-protein isoforms (P1-P5), that differ through N-terminal truncations. These isoforms have distinct phenotypes whereby they show differing organelle localization and interact with different cellular components. The cytosolic P1 is important for viral replication as a cofactor for the RNA polymerase (L-protein) and for binding and inhibiting the antiviral transcription factor, STAT1. P3, however, lacks the regions for binding L-protein, and has gained new functions absent in P1, including microtubule association and accumulation in nucleolus. We have also found that P3 binds RNA, whereas P1 does not. Both P1 and P3 have been shown to undergo liquid-liquid phase separation (LLPS), however it is unclear how this property impacts RNA binding. The focus of this study is to characterize the structure of P1 and P3, phase separated and not phase separated, and their interactions with RNA. We have combined NMR spectroscopy, small angle X-ray scattering (SAXS), light microscopy and mass spectrometry together with cell-based assays to uncover the structural and functional differences of P1 and P3.

Authors: Shatabdi Chakraborty, Ashish Sethi, Stephen Rawlinson, Gregory Moseley, Paul Gooley

Lucy Costello

29 NOV

ABSTRACT 83

Lung Cancer Zoomed In: How the IMBL Is Helping Us Take A Closer Look at Cancer

Lung cancer is the leading cause of cancer death in Australia. It is the fifth most common cancer diagnosed and is responsible for almost one in five cancer deaths.

Currently, the path for a patient to be diagnosed is a chest X-ray to look for obvious abnormalities, followed by a chest Computed Tomography (CT) scan to gain a better understanding of the pathology. Unfortunately, a medical CT does not provide sufficient information to properly visualise tumours, often resulting in a poor prognosis for the patient.

Because of this, the idea of "zooming-in" to a suspicious area of a patient and taking a Region of Interest (ROI) image was formed. We couple this with Phase Contrast (PC) which looks at how the x-rays are refracted (or how they have shifted in phase) to get more information or contrast from the patient's soft tissue. The lungs create strong phase contrast effects which means that the once-apparently homogenous soft tissue, as observed in a conventional medical image (X-ray and CT), is now revealed with greater visible detail.

PC-CT imaging has primarily been used as a research tool in small animal studies. In this project we extend to large scale pre-clinical models and introduce ROI-CT imaging. This technique is not widely used and has numerous challenges. We understand that medical imaging is an invaluable non-invasive tool used in diagnostics to enable a detailed, deeper look inside the body. With this technique, prognosis could be improved given sufficient sensitivity and spatial resolution in ROI-CT imaging.

Authors: Lucy Costello, Lorenzo D'Amico, Martin Donnelley, Daniel Hausermann, Marcus Kitchen, Kaye Morgan, Ronan Smith

ORAL PRESENTATION

Shane Usher

28 NOV

ABSTRACT 85

Characterising the platy morphology of talc in copper ore flotation: insights from synchrotron micro-CT

Rising copper demand has necessitated the mining of low-grade ores, which are much more complex in morphology and minerology. But low-grade copper deposits contain a high amount of complex gangue (impurity) minerals with relatively low copper content. As a result, future beneficiation of low-grade copper ores will necessitate a thorough understanding of these complex gangue minerals to better understand how to effectively separate them and enhance the copper grade. Talc ($Mg_3Si_4O_{10}(OH)_2$) is one of the few gangue minerals whose mineralogical properties, particularly platy morphology, must be fully understood because it imparts a level of hydrophobicity, causing it to float into the concentrate in a flotation circuit, lowering the copper grade and influencing subsequent smelting processes.

Hence, this study aims to obtain a microscopic understanding and quantification of talc morphology by using synchrotron X-ray micro-CT, which presents a significant challenge to the mineral processing of copper to meet the high demand for copper. Synchrotron X-ray micro-CT has received less attention in mineral flotation; however, this project has the potential to fill that gap and pave the way for its widespread use in mineral processing of low-grade ores. Mining operators would be able to sustainably separate talc from copper ore and improve the copper grade because they would have a thorough understanding of the floatability of talc. This would pave the way for an environmental method of separating talc in low-grade copper ores in Australia and globally.

Authors: Daniel Dodoo, Nathan Webster, Shane Usher, Andrew Stevenson, Nick Owen, Liza Forbes, Peter Scales, Anthony Stickland

Robert Komljenovic

29 NOV

ABSTRACT 87

In-Situ Piezo-Polymer & Ruddlesden–Popper perovskite Crystallisation via Megahertz Frequency Electro-Acoustic Waves

This project outlines the *in-situ* characterisation of the preferential crystallisation of piezoelectric-polymers (PVDF & Nylon-11) under the influence of high frequency (MHz) sound waves. Recently, we have uncovered an unconventional low-energy method for uniquely synthesizing polymeric films. In this novel concept, the nanoelectromechanical energy from a miniature (mm) piezoelectric chip is directly coupled into a polymer during its crystallization to produce highly orientated films. Although a variety of standard laboratory techniques (XRD, NMR, PFM & others) confirm the concept, *in-situ* Synchrotron SAXS/WAXS & THz-IR (particularly GIWAXS) experiments crucially uncovered the mechanism of this novel sono-crystallisation process, to resolve the crystal phase both spatially and temporarily. Specifically, GIWAXS proves the quality of the preferential orientation of individual domains critical for evaluating the piezoelectric quality of the polymeric films, illustrated from Bragg peaks arising from the polymeric GIWAXS experimental patterns.

Authors: Robert Komljenovic, Leslie Yeo, Amgad Rezk

27 NOV

Kang Hui Lim

ABSTRACT 90

Engineering Catalyst and Process Design for Carbon-neutral Methane Pyrolysis Hydrogen Production

Catalytic methane decomposition offers an attractive and sustainable solution to producing highly demanded COx-free hydrogen while utilizing greenhouse gas methane. Concurrently, carbon solids in the form of carbon nanotubes (CNTs) have significant industry value with applications in energy storage devices and fuel cells. We introduce state-of-the-art innovations developed for low-temperature catalytic methane decomposition (i.e., < 600 oC) in anticipation of integrating with an H2-permeable membrane for simultaneous H2 extraction and enhanced equilibrium catalytic conversions. Catalyst-induced control of CNTs favoring base-growth mechanism allows facile recovery of metal-free CNTs and hence grants regenerability and reusability of metal-based catalysts for catalytic methane decomposition. We have explored phyllosilicates-derived Ni catalysts for enhanced metal-support interactions and micropore-confinement strategy to entrapped Ni nanoparticles within the support framework during CNT growth. Here we report the use of Ni-based dendritic fibrous nanosilica (DFNS) or KCC-1 catalysts which combine both strong metal-support interactions via silica sacrificial template for phyllosilicates and spatial separation via morphology control (i.e., fibrous morphology) to induce base-growth CNTs. Our results are characterized by TEM-EDX, SEM, FTIR, XPS, Raman and XAS. We also introduce Ni-based catalysts exsolved from layered double hydroxide (LDH) structures for catalytic methane decomposition due to the unique lamellar flake structures that allow for enhanced mass transfer diffusion and provide insights on the importance of tuning the electronic and physical structure of active sites to optimally control the rate of parasitic amorphous carbon formation and its transformation to crystalline CNTs, thereby exposing sufficient active sites for prolonged active catalytic methane decomposition.

Authors: Kang Hui Lim, Claudia Li, Guoqiang Song, Sibudjing Kawi

Rosemary Young

29 NOV

ABSTRACT 94

Cutting Edge Chemical Crystallography

A range of new techniques for collecting and analysing chemical crystallography data have been developed on the MX beamlines of the Australian Synchrotron.

High-pressure single crystal diffraction experiments can now we routinely carried out at room temperature. Areas of further development underway include improved methods of data analysis with CrysalisPro, a new goniometer head to improve sample centering between runs, low-temperature high-pressure experiments, and the ability to carry out high-pressure experiments on the MX2 beamline. All these developments will allow data acquisition on a larger range of samples and in a greater number of conditions, as well as streamline the data collection and data analysis process.

Photo-crystallography utilizing high-powered and narrow bandwidth LEDs (26 wavelengths from 265-1050 nm are available) is now offered on both MX1 and MX2. This is ideal for studying irreversible and long-lived (>30 sec at 100K) photochemical processes, and automated data collection and software control of the LEDs make these experiments straight-forward to carry out. New developments in light sources and software will soon enable the study of short-lived and transient processes down to 50 millisecond timescales.

Other new developments include cold-mounting, improved automated variable temperature, automatic data solution with CXASAP, and automated variable position experiments. We hope that all these developments will allow members of the supramolecular community to carry out even more novel research and analysis.

Authors: Rosie Young, Stephanie Boer

Andreas Moll

29 NOV

ABSTRACT 95

The Source behind the Source - Scientific Computing at the Australian Synchrotron

After 15 years of uninterrupted operation with the original beamlines, the Australian Synchrotron is currently entering an exciting new phase with the addition of 8 new beamlines. This created an opportunity for the Scientific Computing team to redesign the whole software stack from the ground up.

This presentation will take you on a journey of Scientific Computing at the Australian Synchrotron. You will learn how we employ modern, industry standard tools and architectures in a research environment in order to handle the large data throughput of modern detectors and provide the robustness our users expect from us. A particular focus will be on our use of web interfaces to control experiments and cloud technologies, running on-premises, across our whole stack from hardware control to data processing on GPUs.

Authors: Andreas Moll

Qinfen Gu

29 NOV

ABSTRACT 96

Unlocking the potential of zeolites in visible-light photocatalysis with carbon

Zeolites are widely used thermal catalysts, but rarely used in photocatalysis because their wide bandgaps prevent zeolites from using visible or even ultraviolet light. Here we report a carbon-substituting strategy that successfully turns zeolites into visible-light photocatalysts via controlled calcination of organic templates hosted in zeolites, by which the carbon-containing moieties (R) are incorporated into zeolite framework in the form of SiO_3R and/or $SiO_x(OH)_{3-x}R$ (x=1, 2) by carbon-for-oxygen atom substitution. This brings zeolites desired semiconductor properties, especially a significantly reduced bandgap (e.g., ΔE_g = 1.33-1.59 eV for CHA zeolites), for stable visible-light photocatalysis under ambient conditions, as proved by our experimental characterizations and DFT calculations and demonstrated by effective formaldehyde degradation, bacterial inactivation, and CO_2 reduction. This carbon-substituting strategy can be generally applied to other zeolite types, and thus would open a new avenue for developing next generation zeolite-based visible-light-driven photocatalysts combining merits of unique porous structure and intriguing photocatalytic properties.

Authors: Qinfen Gu

27 NOV

Andrew Stevenson

ABSTRACT 98

Technical details on and experiences of the MCT beamline multilayer monochromator

The micro-computed tomography (MCT) beamline was the first of the 8 new BRIGHT beamlines to become operational. One of the key X-ray optical components in the MCT photon-delivery system is a double-multilayer monochromator (DMM), used to select monochromatic X-ray beams with an energy in the range 8 to 40 keV. This DMM was the first such monochromator to be installed at the Australian Synchrotron, with all of the existing hard X-ray beamlines employing a double-crystal monochromator (DCM) based on perfect Si single crystals (all in Bragg geometry, with the exception of the Laue geometry used on IMBL).

Now that MCT has been operating successfully with users for just over two years, it is timely to report on the operation and characteristics of the DMM. Some technical details and key learnings will be shared, including performance aspects related to stability, energy calibration and flux delivery. These findings are also timely given that three other BRIGHT beamlines have or will have a DMM (BioSAXS, which is now operating; MX3 and Nano, which are to follow). In addition, the existing XFM beamline has recently had a DMM installed as part of an upgrade.

Authors: Andrew Stevenson, Benedicta Arhatari, Adam Walsh

Sampa Sarkar

27 NOV

ABSTRACT 101

High-throughput Lipid Nanoparticle Development in Biomedical Applications

The increasing use of lipid nanoparticles as drug and vaccine delivery systems was topically exemplified via the global deployment of the LNP-based mRNA COVID vaccines in late 2020. While liposomes are most commonly used in lipid-based drug delivery, there has been increasing research interest in the design of more complex non-lamellar lipid nanoparticles, including cubosomes which have a unique porous internal nanostructure of cubic symmetry. FDA-approved lipid nanoparticle-based formulations include Doxil®, a liposomal formulation of the chemotherapy drug doxorubicin and Onpattro®, a lipid nanoparticle formulation of siRNA used in the treatment of hereditary transthyretin-mediated amyloidosis.

High-throughput formulation and characterisation techniques (including synchrotron and neutron-based techniques) enabling the rapid exploration of various lipid compositions, particle morphologies and manufacturing processes in the nanoparticle design phase will be discussed. The integration of high-throughput techniques in lipid nanoparticle development streamlines the experimental process allowing for the identification of formulations that offer desirable drug delivery characteristics such as high encapsulation efficiency and controlled drug release. Molecular engineering principles used in the rational design of peptide drugs will be described via the synthesis of potent, ultrashort antimicrobial peptide fragments with enhanced antimicrobial activity. In silico modelling is used as a complementary technique to optimize lipid-drug interactions and guide the rational design of lipid carriers with improved performance.

The creation of combinatorial libraries of lipid nanomaterials can accelerate the identification of promising formulations and facilitate a more systematic understanding of the biological fate and behaviour of nanoparticles in vivo, ultimately advancing the field of nanomedicine.

Authors: Charlotte Conn, Brendan Dyett, Sampa Sarkar, Priscila Cardoso, Tu Le, Celine Valery, Calum Drummond

28 NOV

Brittany Kerr

ABSTRACT 102

In Situ XAS Insights into Acid-Stable Mixed Silver-Bismuth Oxides for Water Oxidation Catalysis

The rational design of effective catalyst materials relies on high quality theoretical and experimental research that focuses on understanding the structure vs function relationship of said materials. X-ray Absorption Spectroscopy (XAS) is well suited to the study of catalytic materials as it is capable of effectively analysing amorphous, disordered, complex catalytic systems. While ex situ XAS can probe the structure of a catalysts ground, active, and depleted states, it often misses transient structural changes that occur under operational conditions. In situ XAS measures the structure of materials under operational conditions, offering real-time insights into the dynamic structure of a catalyst. Here, we investigate the structural evolution of a bismuth-stabilised Ag/BiOx acid water oxidation catalyst via both ex situ and in situ XAS studies. Ex situ analysis revealed the catalyst is composed of a nanocomposite of AgOx and Bi2O3, with the AgOx phase transitioning from an initial, disordered phase to a more crystalline Ag2O3 phase after electrochemical testing while the BiOx remained largely unchanged. In situ XAS indicated the AgOx phase transitions from the initial disordered phase, through Ag2O3, into a third identified phase. The existence of this third AgOx phase is not supported by the ex situ studies and is therefore likely a result of photodamage. This work highlights the importance of in situ XAS studies whilst also stressing the importance of evaluating data for beam-induced effects.

Authors: Brittany Kerr, Rosalie Hocking, Darcy Simondson-Tammer, Bernt Johannessen, Daniel Eldridge, Alexandr Simonov

Andrew Clulow

28 NOV

ABSTRACT 105

BioSAXS – The Future of Solution Scattering at the Australian Synchrotron

This presentation will showcase the capabilities of the BioSAXS beamline, which came into operation in late 2023 as part of the BRIGHT suite of beamlines currently under construction at the ANSTO Australian Synchrotron. BioSAXS is a high-flux small angle X-ray scattering beamline dedicated to the characterisation of solutions and dispersions, with a particular focus on characterising biological macromolecules. The high flux of the beamline is generated by combining a short superconducting undulator with a double multilayer monochromator. Photon flux on the order of 1014 photons/second has been measured at the sample position, which will facilitate time-resolved studies down to the millisecond timescale and strong signal-to-noise for dilute samples.

To mitigate beam-induced radiation damage, the beamline will be home to a new coflow sample autoloader. The coflow operates on the principles that a laminar flow of sample injected into a flowing sheath fluid reduces radiation damage by keeping the sample away from the static capillary walls where flow is slowest and the tendency for sample to burn onto the internal capillary walls is greatest. The coflow will allow measurements of samples from well plates either by direct injection into a capillary mounted in the beam (batch mode) or by first subjecting the sample to Size Exclusion Chromatography (SEC mode) using an onboard HPLC pump and UV-visible spectrometer.

Over time, a range of other sample environments will be made available for users allowing for highly automated measurements including: temperature control; monitoring structural changes during chemical reactions in flowthrough; applying shear; the application of magnetic fields; and the beamline will have the flexibility to incorporate user-designed sample environments.

Authors: Andrew Clulow, Lester Barnsley, Taran Batty, Tom Caradoc-Davies, Michelle Chan, Gonzalo Conesa-Zamora, Sergio Costantin, Emily Griffin, Navid Hamedi, Adrian Hawley, Simon Humphrey, Brian Jensen, Christina Kamma-Lorger, Justin Kimpton, Nigel Kirby, Richard Krah, Michael Kusel, Thanh Le, Cynthia Leung, Zhaolin Liu, Christina Magoulas, Sam Marrable, Tony Mazonowicz, Stephen Mudie, Mia Oldfield, Clinton Roy, Tim Ryan, Vesna Samardzic-Boban, Nick Sarris, Ashish Sethi, Becky Siriweera, Steve Truban, Sudharshan Venkatesan, Elvis Wang, Annmaree Warrender, Jason Wirthensohn

Tam Greaves

28 NOV

ABSTRACT 107

Solvent effects of protic ionic liquids on proteins

Currently buffered aqueous salt solutions are used as solvents for proteins. However, these are limited in their ability to control protein solubility and stability, which adversely affects protein activity, folding-unfolding transitions, aggregation and crystallisation. Therefore, there is a need for new solvents which can control protein and biomolecule solubility and stability.

Protic ionic liquids (PILs) are cost efficient "designer" solvents which can be tailored to have properties suitable for a broad range of applications. Certain aqueous PIL solutions have beneficial properties, including stabilising biomolecules, suppressing aggregation and enhancing protein crystal growth. However, there is a lack of systematic and consistent studies, so structure-property relationships are not possible, which prevents solvent design for specific protein applications.

Here, I will discuss our ongoing work into designing PIL solvents for proteins, which includes developing and adapting characterisation methods for use with proteins in PIL solutions. This has largely involved using Synchrotron small angle X-ray scattering (SAXS) and crystallographic studies using the MX2 beamline. We have been able to identify changes to protein structures, aggregation and folding and relate it to PIL structure and concentration. We have also been able to identify specific ionic interactions of PILs, cations and anions, with the protein surface. These findings will contribute towards being able to produce designer solvents for specific biomolecule applications.

Authors: Stuart Brown, Hank Qi Han, Ashish Sethi, Calum Drummond, Tamar Greaves

Mohammed Abdelbassit

28 NOV

ABSTRACT 108

Synthesis and XANES characterization of novel transition metal oxide clusters

A key structural feature observed in stannate clusters is the formation of MSn6-octahedra filled with various transition metals. These octahedra can either be isolated or connected to form one-dimensional endless chains through shared corners and edges of the [MSn6]-octahedra [1]. We have also reported new clusters of Fe(Fe3-xMnx)Si2Sn7O16 (x = 0…3) and FeMn3Ge2Sn7O16 which exhibit an alternating octahedra of stannide and oxide layers as well as bridging units of SiO44– and GeO44–, respectively [2,3].

A group of novel cluster compounds Ir3Sn12In3O14, RuSn6In6O16 and Ru4Sn20In2O21 have recently been discovered, which exhibit new types of structures with In+ and In+3 sites. Only RuSn6In6O16 contains highly ordered Sn/In sites with an alternating discrete Ru(Sn)6 octahedra incapsulated in oxoindate channels of InO6 and InO7 polyhedra. Ru4Sn20In2O21 show the formation of isolated and condensed clusters RuSn6 clusters in the same compound for the first time. So far, only either isolated or condensed clusters could be found in a compound. Ru4Sn20In2O21 could be seen as a combination of Ru3Sn15O14 and a (hypothetical) RuSn6[SnO3]O4. Ir3Sn12In3O14 crystallizes in the Ru3Sn15O14 structure type.
The presentation will summarize the synthesis and XANES characterization including Ru, Ir, Sn and In L3-edge spectra of these interesting novel materials.

References:

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Authors: Mohammed S. Abdelbassit, Samuel Yick, Tilo Söhnel

Christoph Schrank

28 NOV

ABSTRACT 112

Mapping nano-porosity in cm-sized samples of deep crustal rocks with scanning small-angle X-ray scattering

Exposed deep crustal rocks have very low porosities and are thus essentially impermeable. However, widespread field evidence suggests that large amounts of fluids move through the deep crust, especially in ductile shear zones. Ductile shear zones are the deep roots of fault zones dissecting the crust and contain very dense, fine-grained, crystal-plastically deformed rock called mylonite. Given the very low macro- and micro-porosity of mylonites, it is hypothesized that transient nano-pores serve as principal fluid pathways in ductile shear zones.

However, it is very difficult to measure nano-porosity non-destructively in sufficiently large mylonite samples with imaging techniques such as X-ray tomography and electron-beam microscopy. Here, we present how transmission small-angle X-ray scattering (SAXS) complemented with X-ray Fluorescence Microscopy (XFM), both conducted at the Australian Synchrotron, and supplementary scanning-electron microscopy were used successfully to map nano-porosity in centimetre-sized mylonite samples for the first time. The experimental and data processing approaches are described, followed by a discussion of the results and their far-reaching implication for mechanisms of deep-crustal fluid transfer.

Authors: Christoph Schrank, Nicole Bishop, Michael Jones, Alfons Berger, Marco Herwegh, David Paterson, Livia Salvati Manni, Nigel Kirby

Andrew Marshall

28 NOV

ABSTRACT 116

Probing protein structure in the context of biomolecular condensation

Molecular compartmentalisation is a central pillar of life. Spontaneous demixing of proteins and nucleic acids from solution via liquid-liquid phase separation has been identified as a key mechanism underlying the formation of dynamic membraneless compartments in the cell. *Biomolecular condensates* facilitate concentration of specific molecules at specific sites in response to specific environmental conditions.

RNA-binding proteins are over-represented as drivers of condensate formation, and are often composed of both ordered (stable 3-dimensional fold) domains and intrinsically disordered (sample many conformations) regions (IDRs). Stable folded structures of proteins are generally well understood and are confidently predicted from their amino acid sequence. However, relationships between IDR composition, structure, material state and function are poorly understood.

Using small-angle scattering techniques, X-ray crystallography, in vitro biophysical and cell-based assays, we aim to characterise both folded domains and IDRs to describe composition-structure-material relationships. Our model system is a family of abundant RNA-binding proteins in mammalian cells (DBHS proteins) that form condensates for regulating transcription, RNA-processing and DNA repair. DBHS proteins have a conserved core folded dimerisation domain, with extended intrinsically disordered regions at each terminus that are diverse in length and amino acid composition. We show that the IDRs of these proteins are central to their ability to undergo liquid demixing by phase separation in vitro and in the cell nucleus. We hypothesise that differential dimerisation of DBHS partners provides an avenue for tuning condensate formation and material properties in the cell, and provides a unique opportunity for investigating IDR composition-function relationships.

Authors: Andrew Marshall, Heidar Koning, Anthony Duff, Ashish Sethi, Andrew Whitten, Archa Fox, Charles Bond

28 NOV

Matthew Evans

ABSTRACT 117

Synergy in the s-Block: Alkali Metal Magnesiates for Small Molecule Activation

Organoalkali reagents provide access to an array of reactive nucleophiles and are used extensively in academic chemical research and in industry. Accessing heavier derivatives of these species by pairing an alkali metal with an alkaline earth or p-block element has become a core facet of main-group chemistry. In this regard, alkali metal magnesiates have attracted considerable interest within the realm of small-molecule activation. These synergistic combinations can be used to enable reactivity not previously accessible by related monometallic magnesium systems. We recently reported that a potassium/magnesium bimetallic promotes the reductive capture of dinitrogen through a transient 'anionic' magnesium(I) radical intermediate – the first example of nitrogen activation facilitated by a molecular magnesium complex. We have also investigated the role of alkali metals in the chemistry of magnesium(II) hydride complexes through simple coordination processes. This presentation will discuss our recent breakthroughs in the convenient synthesis of these mixed magnesium/s-block systems, their role in the activation of small molecule substrates (i.e. CO and N_2), and the use of the MX1 and MX2 beamlines at the Australian Synchrotron to characterise a number of these highly challenging reaction products.

Authors: Matthew Evans, Cameron Jones, Rahul Mondal, Dat T. Nguyen, Jeremy Mullin

Praveena Thirunavukkarasu

27 NOV

ABSTRACT 118

Insights Into The Molecular Recognition Mechanism Of A Headless Lipid By Natural Killer T cells

Natural Killer T (NKT) cells are a specialised subset of T cells that recognise lipid antigens via their T cell receptors (TCRs), when presented by the antigen-presenting molecule, CD1d. In the absence of foreign lipids, NKT cells display self-reactivity to CD1d-bound self-lipids, in conditions like autoimmunity, tumour immunity and graft-versus-host disease. Identifying the nature of self-lipids is a central aspect of understanding NKT cell self-reactivity. Using a high throughput lipidomics approach, we have identified CD1d-bound self-lipids from mammalian cells, which lacked the polar sugar head group that is normally involved in NKT TCR binding. Our X-ray crystallography studies of an NKT TCR binding of CD1d-presenting headless lipid antigens revealed the TCR adopted a parallel docking topology positioning itself atop the F'-pocket of CD1d. Surprisingly, the majority of the intermolecular interactions in the complex were formed between CD1d and TCR itself with minimal interactions in contacting the lipid. The absence of the sugar headgroup abolished key interactions it normally displays with the NKT TCR but, nevertheless, the overall conserved docking pattern was maintained. Of note, the NKT TCR bound the CD1d-headless lipid with micromolar affinities as measured by SPR. Collectively, this study provides the first detailed insights into how a CD1d presenting a headless antigen is structurally recognised by the NKT TCR. Our data provides a proof of concept that small naturally occurring headless lipids could function as CD1d ligands in activating NKT cells.

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Authors: Praveena Thirunavukkarasu, Tan-Yun Cheng, Srinath Govindarajan, Catarina F. Almeida, Daniel G. Pellicci, Wellington C Arkins, Ildiko van Rhijn, Koen Venken, Dirk Elewaut, Dale I. Godfrey, Branch Moody, Jamie Rossjohn

27 NOV

Vigneshwar Hari

ABSTRACT 119

Characterisation of trace Sr distribution in hypoeutectic Al-Ni alloy using the XFM beamline

Al-Ni alloys have a suitable combination of properties for use as a brazing filler material. The eutectic temperature of the Al-Ni system is however quite high at 640°C. Sr was added to Al-Ni alloy, as it was hypothesised to reduce the eutectic temperature like in Al-Si alloy. It was found that 300 ppm Sr added to Al-5.3wt%Ni alloy did not significantly affect the eutectic temperature and slightly modified the eutectic morphology. However, characterising the location of Sr in the microstructure proved difficult using standard laboratory methods like EDS. The Australian Synchrotron XFM beamline was used to macroscopically image Sr distribution in the sample. It showed that Sr strongly segregated away from both the primary Al and eutectic Al/Al3Ni, and mainly aggregated at grain boundaries, with trace amount found in the eutectic. This data proved useful in hypothesising the mechanisms under which Sr segregation affected the final microstructure of Al-5.3Ni-0.03Sr.

Authors: Vigneshwar Hari, Kazuhiro Nogita, Xin Fu Tan, Stuart McDonald, Dongdong Qu

Yang Cao

29 NOV

ABSTRACT 120

High-Energy X-ray Diffraction Tomography at the Australian Synchrotron

Diffraction tomography is an advanced X-ray imaging technique that combines the x-ray diffraction with the computed tomography data acquisition approach. By utilizing crystallinity information such as cell parameters and orientation, diffraction tomography constructs crystallographic properties of materials in three dimensions, offering insights into grain position, size, shape, and orientation with high precision. Operating with high-energy x-ray, this technique is particularly valuable for studying thick, dense, and complex materials, making it indispensable for fields such as energy storage, catalysis, metallurgy, and mineralogy. The Australian Synchrotron's upcoming BRIGHT beamlines, ADS-1 and ADS-2, will bring this advanced technique to the facility, enabling researchers to investigate complex material behaviors with exceptional spatial precision under real-world conditions. These new capabilities will facilitate studies of phase transitions, crystalline formation, and stress-strain analysis, providing a deeper understanding of material properties. The presentation will delve into this specific capability of ADS beamline, focusing on how high-energy x-ray diffraction tomography will contribute to science and engineering community.

Authors: Yang Cao, Justin Kimpton, Josie Auckett

Alaa Bazeed

28 NOV

ABSTRACT 122

Microstructural and morphological analysis of poly(lactic-co-glycolic acid) organogels for in situ forming implants

Poly(lactic-co-glycolic acid) (PLGA) has been among the most used polymers in biomedical applications, including drug delivery, tissue engineering and sutures, due to its biocompatibility and biodegradability. One of the main clinically approved drug delivery applications of PLGA is in medical implants, including injectable, in situ forming implants (ISFIs), which offer sustained release of therapeutics. ISFIs typically consist of a polymer such as PLGA dissolved in a water-miscible organic solvent that is exchanged upon injection resulting in precipitation of the polymer and entrapment of the therapeutic. Changes of the PLGA composition (monomer ratio) are often used to control the physical properties, degradation, and release characteristics of ISFIs. However, the effect of PLGA microstructure (monomer sequence) on the formulation and release of therapeutics from ISFI has yet to be studied. Therefore, we prepared PLGA with a fixed lactide to glycolide mole ratio (1:1) via ring-opening polymerisation in bulk and solution. While solution synthesised PLGA formed a traditional liquid injectable ISFI, bulk synthesised PLGA formed novel, thixotropic organogels in various solvents. To interpret this behaviour, the morphology and underlying microstructure of the PLGA was characterised using a range of techniques including nuclear magnetic resonance spectroscopy and synchrotron small- and wide-angle X-ray scattering (SAXS/WAXS). In addition, the thermal characteristics and viscoelastic behaviour of the organogels were characterised using differential scanning calorimetry and rheometry.

Authors: Alaa Bazeed, Anton Blencowe, Andrew Clulow, Michael Wiese, Larisa Bobrovskaya

Dom Appadoo

29 NOV

ABSTRACT 124

Capabilities of the THz Beamline: THz synchrotron spectroscopy from Astrophysics to Material Science

THz synchrotron spectroscopy has become an important tool in the identification and quantification of molecular species; it is a routinely used technique as it is well established that synchrotron radiation offers a considerable S/N advantage over conventional thermal sources. The brightness advantage is perfectly suited for high-resolution gas-phase spectroscopy where spectral features have narrow line-widths, and at the Australian Synchrotron, this advantage is limited to energies lying below 1500 cm-1; on the other hand, a flux advantage is observed for energies below 350 cm-1 which facilitates the study of homogeneous condensed-phase samples.The THz/Far-IR beamline at the Australian Synchrotron is a multi-disciplinary facility catering for a diverse research community both at national and international levels, and offering a suite of instruments to accommodate the requirements: multipass vacuum chambers operating from room temperature down to cryogenic temperatures for gaseous samples, and cryostats and an ATR to study condensed-phase samples. In this paper, some gas phase as well as some condensed phase applications and capabilities of the THz/Far-IR beamline will be presented.

Authors: Dom Appadoo, Ruth Plathe

ORAL PRESENTATION

29 NOV

Moshi Geso

ABSTRACT 125

Characterization of Alanine and Presage Dosimeters Using Ultra-High Dose Rate Synchrotron-Generated X-Rays and Electrons

Many dosimeters including the commonly used ionisation chamber are not suitable for measuring ultra-high dose rate beams or FLASH. There is some potential radiobiological advantages in tumours treated with FLASH.

Alanine pellets are considered dose rate independent dosimeters. Composed of an amine acid group and a carboxylic acid group attached centrally to a carbon atom which carries a methyl group side chain. When exposed to ionising radiation, free radicals are formed in groups with one group showing in an electron paramagnetic resonance analysis a large dominant peak. This peak correlates to the exposing dose i.e. the level of energy deposited in the palette.

Our alanine dosimeters were exposed to various doses of low energy x-rays from the IMBL and high energy (100 MeV) electrons at the Australian Synchrotron. Both beams were of ultra-high dose rate, >1000s Gy/sec, in the FLASH radiotherapy range. The pellets were scanned at the National Physics Laboratory (NPL) in UK. These alanine dosimeters were independent of dose rate. Alanine dosimeters measured the nominated synchrotron x-ray doses within 0.5%.

The alanine dose measurements for electrons from a LINAC showed excellent agreement but deviated from the 100 MeV synchrotron beams significantly. We attribute this over-estimation of dose to the loss of electrons over their collision energy losses leading to shifting some electrons in the lower energy alanine states to the high energy causing the peak swallowing. Measurements were conducted to determine a correction factor for electrons similar to that of x-rays

Authors: Moshi Geso, Supaporn Sriswan, William Patterson, Rod Lynch, Pradip Deb, Eugene Tan, Tessa Charles, Ricky O'Brien

Sampa Sarkar

27 NOV

ABSTRACT 133

Prospective Subunit Nanovaccine against Mycobacterium tuberculosis Infection - Cubosome Lipid Nanocarriers of Cord Factor, Trehalose 6,6′ Dimycolate

An improved vaccine is urgently needed to replace the now more than 100-year-old Bacillus Calmette–Guérin (BCG) vaccine against tuberculosis (TB) disease, which represents a significant burden on global public health. Mycolic acid, or cord factor trehalose 6,6′ dimycolate (TDM), a lipid component abundant in the cell wall of the pathogen Mycobacterium tuberculosis (MTB), has been shown to have strong immunostimulatory activity but remains underexplored due to its high toxicity and poor solubility. Herein, we employed a novel strategy to encapsulate TDM within a cubosome lipid nanocarrier as a potential subunit nanovaccine candidate against TB. This strategy not only increased the solubility and reduced the toxicity of TDM but also elicited a protective immune response to control MTB growth in macrophages. Both pre-treatment and concurrent treatment of the TDM encapsulated in lipid monoolein (MO) cubosomes (MO–TDM) (1 mol %) induced a strong proinflammatory cytokine response in MTB-infected macrophages, due to epigenetic changes at the promoters of tumor necrosis factor alpha (TNF-α) and interleukin 6 (IL-6) in comparison to the untreated control. Furthermore, treatment with MO–TDM (1 mol %) cubosomes significantly improved antigen processing and presentation capabilities of MTB-infected macrophages to CD4 T cells. The ability of MO–TDM (1 mol %) cubosomes to induce a robust innate and adaptive response in vitro was further supported by a mathematical modeling study predicting the vaccine efficacy in vivo. Overall, these results indicate a strong immunostimulatory effect of TDM when delivered through the lipid nanocarrier, suggesting its potential as a novel TB vaccine.

Authors: Sampa Sarkar

Paul Di Pasquale

27 NOV

ABSTRACT 136

Precision Measurement of Absolute Absorption and Phase Fine Structure Spectra of the Copper K-edge Using Holographic Spectroscopy

Precision spectroscopic techniques provide a powerful mechanism for the structural analysis of complex molecular structures and materials. X-ray absorption fine structure (XAFS) offers a simple and effective medium of analysis by means of structural analysis. However, XAFS encounters experimental limitations with the low signal-to-noise ratio associated with weakly absorbing samples. Measuring the phase interactions has its own advantages in the x-ray regime as the interactions are several orders of magnitude more sensitive than absorption, this will allow us to overcome the issues associated with thin films and biological samples.

Recently we have been showcasing a method of measuring the absorption and phase spectra simultaneously. By applying an extension of Fourier transform holography, we have been able to obtain very high-quality spectra of copper and iron on a relative scale. These results not only demonstrated the promising new capability of combining imaging and spectroscopy, but also highlight several inconsistencies in alternative methods of phase spectroscopy. In collaborations with the beamline scientists at the Australian Synchrotron SAXS/WAXS beamline, we have made further development to the experimental methodology, allowing us to reconstruct the absorption and phase fine structure spectra of the copper K-edge on an absolute scale. The results allow for a novel structural probing tool for low-absorbing samples.

Authors: Paul Di Pasquale, Tony Kirk, Pierce Bowman, Minh Hong Dao, Jake Rogers, Nigel Kirby, Pablo Mota-Santiago, David Hoxley, Christopher Thomas Chantler, Nicholas Tran, Daniel Sier, Chanh Tran

Marta Krasowska

28 NOV

ABSTRACT 137

Isolating the Interface of an Emulsion using X-Ray Scattering and Tensiometry to Understand Protein-Modulated Alkylglyceride Crystallisation

Dairy proteins and mono- and diglycerides (MDG) are often used in unison to tailor the properties of dairy-based emulsions. However, there are significant gaps in our understanding of how proteins affect lipid crystallisation at the oil-water interface. We have used a unique combination of interfacially-sensitive techniques to elucidate the impact of dairy proteins on interfacial MDG crystal formation.

The formation temperature of interfacial MDG crystals was assessed through interfacial tension studies via drop shape analysis. Small and Wide-Angle X-ray Scattering measurements were performed on isolated oil-water interfaces, allowing for in-situ interrogation of MDG crystal structure and concentration at and near the interface.

Dairy proteins are seen to reduce the temperature at which MDG crystals form at the oil-water interface. The displacement of proteins upon interfacial crystal formation was also clearly observed in interfacial tension measurements. For the first time, lipid crystals formed at the oil-water interface have been characterised using X-ray scattering. All scattering studies showed no change to the MDG crystal structures at the oil-water interface in the presence of adsorbed proteins. The results demonstrate that informed selection of emulsifier components is critical to controlling interfacial crystallisation with concomitant impact on emulsion stability.

Authors: Stephanie MacWilliams, Andrew Clulow, Nigel Kirby, Reinhard Miller, Ben Boyd, Gilles Graeme, David Beattie, Marta Krasowska

ORAL PRESENTATION

27 NOV

Jayan Gunasekera

ABSTRACT 143

Micro-structure Quantification Using Two-Dimensional Near-Field X-ray Speckle Imaging

In propagation-based phase contrast X-ray imaging, enhanced image contrast occurs when the scattered wavefield propagates over a sufficient distance. This effect is particularly noticeable in lung tissue images, where increasing propagation distance improves contrast, causing the lungs to appear grainy due to near-field speckles (NFS). These speckles, originating from lung alveoli—small air sacs—provide valuable morphological information about the lungs [1]. Analysing these speckles enables quantitative assessment of micro-scale lung structures, potentially facilitating earlier detection of diseases such as pneumonia, cystic fibrosis, pulmonary fibrosis, bronchopulmonary dysplasia, and emphysema [2]. Current attenuation-based imaging systems often miss these diseases due to low contrast and poor resolution, leading to late diagnoses when treatment is less effective.

Our study explored NFS behaviour using the Autocorrelation Function (ACF) with varying propagation distances and sample thicknesses. The central peak width of the ACF accurately estimates speckle size [3]. Using a step-wedge with PMMA microspheres, we found that speckle size increases with distance and thickness, though it initially decreases before increasing, indicating an X-ray beam "focusing" effect. Simulations confirmed this effect. Additionally, phase vortices were observed with increasing propagation distances in our simulations. Preliminary results suggest that ACF decay rate might provide insights into the short-range ordering of tightly packed microstructures within the sample.

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Authors: Jayan Gunasekera, Marcus Kitchen, Konstantin Pavlov

Riya Joseph

27 NOV

ABSTRACT 145

Structural studies of recently identified Bacteroides fragilis Cholesterol-Dependent Cytolysin Like (CDCL) proteins.

Bacteroides fragilis are gram-negative anaerobic bacteria that are found in the human gut. Although generally commensal, they can become pathogenic under conditions of impaired intestinal barrier function, leading to various diseases.

B. fragilis bacteria are shown to produce a novel class of pore forming proteins termed as Cholesterol Dependent Cytolysin Like proteins (CDCLs). These pore-forming proteins produced by *B. fragilis* play a crucial role in their survival within the intestinal environment by helping them target competing microorganisms.

We are currently investigating the structure and pore-forming activity of two CDCL proteins (Bf long and Bf short) from *B. fragilis*. These proteins when proteolytically activated at their target membrane, forms a two-component beta-barrel pore comprising of approximately 30 monomers. Interestingly, *B. fragilis* also produces a surface lipoprotein named Bacteroides CDCL immunity protein (BcdI) that protects it from its own toxins (CDCLs).

We employ a diverse array of structural biology techniques, including X-ray crystallography to determine monomer structures, small-angle X-ray scattering (SAXS) for solution-state analysis, and cryo-electron microscopy to investigate the pore complex of these proteins. Progress towards these aims, including X-ray crystallography and SAXS of soluble forms of BcdI and CDCLs will be discussed. These findings, along with our ongoing research, contribute to our understanding of the pore formation mechanism and regulation of Bf CDCLs, shedding light on how *B. fragilis* utilises these virulence factors to its advantage.

Authors: Riya Joseph, Michelle Christie, Bronte Johnstone , Hunter Abrahamsen, Craig Morton, Rodney Tweten , Michael Parker

Nigel Kirby

28 NOV

ABSTRACT 146

Grazing Incidence Scattering at the Australian Synchrotron

Grazing incidence X-ray scattering is a sensitive technique for determining the structure of solids to depths of tens to hundreds of nanometers from smooth, flat surfaces. Grazing incidence wide angle X-ray scattering (GIWAXS) yields diffraction information at length scales down to Angstoms. GI-SAXS can resolve structures up to ~100 nm. Both techniques have been available to SAXS/WAXS Users since 2009, undergoing steady development during the beamline's first decade of operations.

The major endstation upgrade conducted in 2018 started a step-change in grazing development that has continued for the last 5 years. The three key hardware upgrades were:

- the addition of an in-vacuum sample handling chamber, dramatically improving signal:noise
- an in-vacuum hexapod, enabling high throughput batch mode by moving virtual rotation centres throughout a 2-dimensional stack of up to 80 samples
- a Pilatus3-2M detector, increasing angular range by 40% to better serve User requirements.

Arguably the most important advances for grazing incidence experiments have come through software. The automated sample alignment and data acquisition code was initially moved to python in 2018, adding iteration loops and data analysis to increase robustness and convergence range. The code has been continuously improved and expanded to improve reliability, ease of use, and provide optional features for tailored data acquisition. The recent addition of Full geometric fitting of sample rotation scans was can determine and correct longitudinal positioning errors. This assists measuring samples down to 4 mm length for high resolution GIWAXS and improves rotation alignment accuracy to a few millidegrees.

This presentation will describe the instrumentation, sample environments and methodology, and illustrate the capability with some example data.

Authors: Nigel Kirby, Pablo Mota-Santiago, Livia Salvati Manni, Izabela Milogrodzka, Stephen Mudie

Livia Salvati Manni

27 NOV

ABSTRACT 149

Lipidic drug delivery systems can be responsive to the human microbiome

Lipid mesophases are biocompatible nanomaterials offering selective and 'smart' drug-release properties. Recent studies have focussed on understanding how they are influenced by physiological environments and external stimuli [1]. In this study explores how representative members of the human microbiome can influence the nanostructure and the drug release of these systems.

Four bacterial strains that are commonly present within targeted routes of administration were mixed with monoolein lipidic mesophases. The effects on lipid mesophase structure and release were examined using SAXS, CPLM and fluorescence measurements. The effects on bacteria were observed with growth studies and RNA sequencing.

Of the strains tested, only S. aureus caused a phase transition upon incubation to inverse hexagonal phase after 8 h. The changes to the mesophase nanostructure were influenced by different components present in the supernatant at different size fractions, where both cellular debris >10 nm and biomacromolecules such as enzymes play a role.

As a consequence of the S. aureus exposure, a reduced rate of hydrophilic dye release from bulk monoolein cubic phase was observed over 8 h. This transformation was consistent with an increase in oleic acid content by lipolysis of monoolein by lipase [2]. Hence the respiration of bacteria can change the way drugs are released from a lipidic matrix. This research demonstrates the influence that bacteria can have on the structure and drug release properties of monoolein liquid-crystalline drug-delivery systems.

References:

[1] W.-K. Fong, et al., J Colloid Interface Sci 484 (2016) 320–339.
[2] L. Salvati Manni, et al., J Colloid Interface Sci 588 (2021) 767–775.

Authors: Livia Salvati Manni, Jonathan Caukwell, Wye-Khay Fong

28 NOV

Santosh Panjikar

ABSTRACT 151

ASWEBRICK: a secured server of Auto-Rickshaw

Auto-Rickshaw (AR) is an automated crystal structure determination system deployed at the Australian Synchrotron, utilizing Docker and Kubernetes technology for high-throughput job execution. It integrates various macromolecular crystallographic programs to form a pipeline for efficient structure determination, offering experimental and molecular replacement phasing protocols.

The Fragment Screening Pipeline, developed for drug discovery at the MX Beamlines, streamlines the process from sample setup to data analysis and ligand evaluation. With the need to analyze a large number of datasets (>100), off-site data analysis becomes essential to supplement on-site evaluations during beamtime.

Recognizing this need, ASWEBRICK has been developed as a secured Auto-Rickshaw server to enable off-site data analysis. This platform will enhance productivity for MX users by providing access to Auto-Rickshaw functionalities from their home laboratories. The security framework ensures data integrity and user privacy, with a frontend for user interaction and a backend for data analysis and result hosting.

ASWEBRICK's implementation signifies a significant advancement in supporting drug discovery efforts, offering a secure and accessible platform for MX community members to accelerate their research endeavours.

Authors: Santosh Panjikar

Qi (Hank) Han

27 NOV

ABSTRACT 155

Ion binding and interactions of ionic liquids with proteins

Ions are important for modulating protein properties, including solubility and stability, through specific ion effects. Ionic liquids (ILs) are designer salts with versatile ion combinations which have great potential to control protein stability, conformation changes, crystallization and aggregation. The protein phase separation and metal ion (e.g., Ca2+)-binding sites in eukaryotes have been extensively studied [1], however, with some simple protein models, current understanding of specific ion effects on protein properties, interactions and ion binding is limited. There is a need for understanding the IL effect on proteins and developing ILs to control protein behaviours.

This presentation explores using small angle X-ray scattering, protein crystallography and spectroscopies to understand the IL effect on model proteins, with a focus on lysozyme and green fluorescence (GFP) [2, 3]. In particular, this work unveils the molecular mechanisms underlying the interaction and ion binding between the ILs and protein, providing unprecedented insights into the interfacial phenomena associated with protein ion binding. We emphasize the specific ion binding can induce more flexible loop regions in the protein, while the ion binding in bulk phase can be more dynamic in solution and protein behaviour depend on the net effect of nonspecific interactions and specific ion binding. Overall, anions showed to have specific binding to the protein surface via direct electrostatic interactions with the charged side chains, and hydrogen bonding with polar and aromatic residues. These findings provide new insights into interfacial behaviour of proteins, protein-IL binding interaction and using ILs to modulate protein solution behaviours.

References:

[1] Chem Rev 103 (2003) 773-788.
[2] J Colloid Interface Sci 650 (2023) 1393-1405.
[3] Int J Biol Macromol (2023) 127456.

Authors: Hank Qi Han, Tamar Greaves, Calum Drummond

27 NOV

Kiersten Kneisel

ABSTRACT 157

Facile dissociation of molecular nitrogen on crystalline lanthanide surfaces

Due to its potential as an energy carrier, ammonia is an emerging pathway to decarbonise hard-to-abate industries (heavy industry and heavy-duty transport). While still maintaining fertiliser production for agricultural sectors, ammonia is entering new markets as a carbon-free fuel, energy storage medium, and transportation vector for hydrogen. However, the current ammonia production process requires high temperatures and pressures, accounting for ~2% global energy consumption and ~1.3% of CO2 emissions. The scientific problem is the inefficiency of the critical nitrogen-hydrogen reaction in the Haber-Bosch process, resulting in low conversion (~15%) per pass through the synthesis reactor. The dissociation of the strong triple molecular nitrogen (N2) bond is one of the rate-limiting steps in the Haber-Bosch process. In recent years, it has been shown the N2 bond can be broken with surprising ease by lanthanides, which spontaneously form lanthanide nitrides under ambient conditions. This opens a pathway for a potential new and more efficient catalyst for the ammonia synthesis.

We explore this reaction by combining experimental data with various computational techniques. Experimental results from an in-situ study conducted at the Australian Synchrotron on incrementally nitrided gadolinium and samarium thin films using x-ray photoelectron spectroscopy (surface sensitive) and near edge x-ray absorption spectroscopy (bulk sensitive) will be discussed. These results are compared with density functional theory density of states and Anderson impurity model calculations. The resulting preliminary model of lanthanide nitride formation is an important step towards developing a microscopic understanding of the catalysis and ultimately a low energy ammonia production process.

Authors: Kiersten Kneisel, Jay Chan, Caitlin Casey-Stevens, Anna Garden, William Holmes-Hewett, Ben Ruck, Franck Natali, H. J. Trodahl

POSTERS

Abstract #	Title	Presenter
7	Exploiting cancer metabolism: a structural focus on mitochondrial malic enzyme inhibitors	Ben Krinkel
9	Micro-Computed Tomography beamline: density measurement imaging	Benedicta Arhatari
16	Megapixel laboratory XFM on the CSIRO Maia Mapper	Nick Phillips
18	Removing carbon contamination on the SXR beamline	Lars Thomsen
23	Intermarrying MOF glass and lead halide perovskite for photocatalysis	Wengang Huang
24	Tracking the Mobilization and Speciation of Nickel during Enhanced Leaching of Mine Tailings: A Holistic Synchrotron-based Approach	Zhen Wang
26	An Integrated Approach to Structural Characterisation of DNA Aptamers Bound to Small-Molecule Targets	Bruce Chilton
27	Metal-organic Framework Confined Polyoxometalate Catalysed Oxidation Reaction: Understanding the active site and mechanistic studies using X-ray Absorption Spectroscopy and In Situ Spectroscopic Kinetics	Paramita Koley
34	IMBL's photon counting imager	Chris Hall
36	Comparison of Naturally Weathered Polysiloxane and Polyurethane Coatings using Synchrotron IRM, XFM and GiSAXS/GiWAXS	Ashleigh Farnsworth
37	Novel Dynamic X-ray Imaging Techniques for Respiratory Research	Ronan Smith
39	Focusing high energy x-rays using a CRA	Daniel Hausermann

POSTERS

Abstract #	Title	Presenter
43	Angiopep2-Functionalized Lipid Cubosomes for Blood-Brain Barrier Crossing and Glioblastoma Treatment	Xudong Cai
47	Advancements in Synchrotron-based Micro-CT Imaging of Fast, Dynamic Multiphase Flow in Porous Media	Eric Sonny Mathew
49	Exploring the effect of Mechanical Milling on Rare Earth Alkaline Earth Doped Manganites	Mark Appletree
50	The rapid attenuated total reflectance infrared spectroscopy assessment of changes in E. coli following exposure to Synchrotron sourced Terahertz radiation	Zoltan Vilagosh
54	Characterising the behaviour of glucose mono-esters at an isolated oil-water interface	Jessica Frahn
57	Chevrel Phase Materials as Cathodes in Rechargeable Magnesium Ion Batteries	Ryan Silk
58	X-ray tomographic imaging of catalytic hollow fiber zeolite membranes	Claudia Li
59	Optimizing Lipid Cubosomes for Alzheimer's Drug Delivery: Impact of Lipid Composition and Stabilizers	Lucrezia Guarneri
60	Influence of recycled plastic addition on microstructure formation of metallurgical coke	Jangho Jo
64	Updates and Developments at the Australian Synchrotron Powder Diffraction beamline	Liam Tan
65	Using the x-ray dark field to reveal subpixel microstructure of bones and teeth affected by cystic fibrosis.	Michelle Croughan

POSTERS

Abstract #	Title	Presenter
66	Valorizing Waste: Flexible Bioplastic Blends and Biocomposites for Sustainable Packaging Application	Jumana Alshehhi
69	Ultra-thin Ionic Liquid Films on Surfaces	Sowbarnika Senthilkumar
72	Synchrotron Imaging to Visualize Leaching Process	Quan Zheng
77	Unlocking New Horizons in Material Science: Recent Progress and Development of ADS Beamline in Australia Synchrotron	Yang Cao
79	Quasi-freestanding AA-stacked bilayer graphene induced by calcium intercalation of the graphene-silicon carbide interface	Anton Tadich
84	Investigation of Fracture Development in Defected Rock Samples Under Coupled Static Stress and Dynamic Loads	Haojun Wang
86	Developing the 100 MeV Pulsed Energetic Electrons for Research (PEER) End-station	Eugene Tan
88	High Entropy Alloys Enable Durable and Efficient Lithium-Mediated CO2 Redox Reactions	Liang Sun
89	In-Situ Piezo-Polymer & Ruddlesden–Popper perovskite Crystallisation via Megahertz Frequency Electro-Acoustic Waves	Robert Komljenovic
91	Using 1.0 THz to 20.0 THz spectroscopy for assessment of cosmetic foundation products	Negin Foroughimehr
92	Anti-sintering PtCu Single-atom Alloy Catalysts with Boron Doping	Kang Hui Lim

POSTERS

Abstract #	Title	Presenter
93	Synchrotron Infrared Microscopy Study of Novel Pectin Methacrylate Hydrogel	Nisha Arunachalam
99	Bringing AI to Infrared Microscopy (IRM) beamline image analysis using QUASAR	Keith Bambery
103	MEX2 present capabilities	Bruce Cowie
104	BioSAXS – The Future of Solution Scattering at the Australian Synchrotron	Andrew Clulow
106	A multi analytical investigation of materials and previous conservation interventions used in Tutankhamun's Painted Wooden Bed	Mohamed Moustafa
109	More Flux, Please! The Double Multilayer Monochromator at XFM	Daryl Howard
110	MEX-1 Present Capabilities	Pria Ramkissoon
113	Developments in Medium Energy X-ray Absorption Spectroscopy Beamline (MEX2): Advances in Sample Preparation and Multi-Edge Scanning	Negin Foroughimehr
115	High specification machining process parameters optimisation	Abdul Md Mazid
121	Preservation and destruction of silicified microbes in fossilised hot spring deposits as evidenced by trace metal distributions	Barbara Lyon
123	Integration of Rheology-SAXS Technique at the Australian Synchrotron	Izabela Milogrodzka

POSTERS

Abstract #	Title	Presenter
124	Capabilities of the THz Beamline: THz synchrotron spectroscopy from Astrophysics to Material Science	Dominique Appadoo
128	High accuracy and camera-length independent beam centre determination and the use of radiation-resistant calibrants at the SAXS/WAXS beamline, part of ANSTO	Pablo Mota Santiago
129	Alternative approach to Multimodal Intrinsic Speckle Tracking to reconstruct phase and fast varying dark-field images	Jayvan Liu
130	Non-Ionic Surfactants are Affected by Salts too!	Yang Guo
131	Unravelling the structure and function of SCFbxo36 complex in context of prostate cancer	Preeti Preeti
132	Highly stable Fe-based oxygen carriers for Intensified methane dry reforming with CO2 splitting	Alfred Appiagyei
134	Progress in parametric optimisation of machining Ti-alloys	Abdul Md Mazid
135	Precision Measurement of Absolute Absorption and Phase Fine Structure Spectra of the Iron K-edge Using Holographic Spectroscopy	Pierce Bowman
138	Unravelling the structure and function of SCFbxo36 complex in context of prostate cancer	Preeti Preeti
140	A simplified approach to spot welded joint stress analysis	Neamul Khandoker
141	Interaction of small polar molecules with cell membranes	Dilek Sezer

POSTERS

Abstract #	Title	Presenter
142	The comparative study of Toad tympanic membrane and cornea using temperature variation at 2.0 to 20 THz	Zoltan Vilagosh
147	Crystallographic fragment screen of the SARS-Cov2 main protease at the Australian synchrotron	Gautham Balaji
148	The changes in infrared spectra of Melanoma and COS-7 fibroblast cells following THz exposure	Zoltan Vilagosh
150	Investigating the Impact of Ionizable Lipids on mRNA Delivery: Structural Transformations and Endosomal Escape Mechanisms in Lipid Nanoparticle Systems	Ravindu Fernando
152	Conversion of Epitaxial Graphene to 2D diamane on Silicon Carbide	Michael Reynolds
154	Development of Lipid Nanoparticle Compositions for Mesophase and Stability in Organ-Specific Therapeutic Delivery	Han Nguyen
156	Protein-Nanoparticle Interactions within Ionic Liquids and Deep Eutectic Solvents	Zachary Candiloro
158	Optimizing Phase Transitions and Magnetic Properties in Fe/Cr-Doped $SrMo1\text{-}xM_xO_4$ for Advanced Solid Oxide Fuel Cells	Muneerah Almohareb
159	Structural Characterization of Protein Aggregates in Biopharmaceutical Formulations Using Biological Small Angle X-ray Scattering (Bio-SAXS)	Vinodya Karunadhika
160	The nanoscale lattice deformations in two-dimensional materials	Dong Hyeon Kim
161	Near-field probing of nonlocal vibrational strong coupling enabled by surface lattice resonance	Yeonjeong Koo