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Book of Abstracts

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Poster Session 1 / 0

Determination of capture barrier energy of the E-center in Pd/Sb-doped Ge by varying the pulse width

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The capture barrier energy of the E-center deep level defect induced in Pd/Sb-doped Ge by alpha-particle irradiation has been studied. Palladium Schottky barrier diodes (SBDs) fabricated by resistive evaporation technique were successfully characterised by current-voltage (I-V), capacitance-voltage (C-V), conventional and Laplace deep level transient spectroscopy (DLTS). The rectification quality of the Schottky contacts before and after irradiation was confirmed by I-V and C-V. The ideality factor and doping density were determined before and after alpha-particle irradiation to be in the range of 1.23 to 1.46 and 3.55 × 1015 to 5.25 × 1015 cm-3, respectively. The trap thermal emission activation energy and the apparent capture cross section of the E-center were determined from the Arrhenius plot to be 0.37 eV and 1.3 × 10-15 cm2, respectively. Capture barrier energy and true capture cross section of the E-center were also calculated to be 0.052 eV and 2.25 x10-17 cm2, respectively from the experimental findings after varying the pulse width at different temperature range from 145 to 180 K in step of 5 K.

Parallel-Chemistry and Materials / 1

HARPIA: High Resolution Powder X-ray Diffraction beamline at Sirius

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Sirius is a fourth-generation synchrotron light source built at the CNPEM and is forecast to begin operations in 2020. Brazil is transitioning from a second-generation synchrotron source (UVX) to a leading position in the design and operation of the brightest 4th-generation machine in its energy class. This multidisciplinary research infrastructure will bring an advanced facility to the structural characterization of polycrystalline samples – HARPIA beamline. The synchrotron source of HARPIA will be an undulator with an 18 mm period length and importantly, without an energy gap. The beamline will be installed in a low-� straight section of the storage ring to increase the beam size in the horizontal direction. HARPIA's optical design aims to be simple, yet highly effective to provide high photon flux at the sample position, ≈�2.21012 ph/s/100 mA at 20 keV, about 1000 times higher than that of the LNLS at 8 keV. Energy selection will be obtained by the Bruker double-crystal-monochromator. The two sets of Si crystals, (111) and (333), will allow an energy range from 5 to 30 keV. The beam size at the sample position is calculated to be around 0.85 mm (v) x 1.2 mm (h) with a divergence of 25 �rad (v) x 34 �rad (h) at 20 keV. HARPIA's experimental hutch (Fig. 1) will provide high-resolution X-ray diffraction data with a multi-analyser crystal from FMB Oxford having at least 8 modules of Si(111) crystals and NaBr2 scintillators detectors. Moreover, it will allow dynamic experiments using a linear fast detector developed in-house covering 90° in 2theta range to provide second scale temporal resolution.

The 3 co-axial circle heavy-duty diffractometer from the current XRD1 beamline at LNLS will be transferred to the HARPIA experimental hutch. X-ray diffraction measurements will be conducted in Debye-Scherrer geometry (capillary geometry). The diffractometer uses high precision rotary stages (Θ, 2Θ and d axes) and is designed to support heavy detector arrays, such as the two sets of detectors in the aforementioned paragraph.

A storage magazine for samples placed into capillaries allows hundreds of samples to be loaded and measured via the use of a robotic arm which serves as a sample exchanger. The robotic arm allows for the beamline to be programmed and, if necessary, operated remotely providing high levels of efficiency and maximization of the provided beamtime. HARPIA beamline will provide an efficient and user-friendly facility to the structural characterization of polycrystals in a variety of sample environments as well as fast and high-resolution mode detection to Sirius users.

Acknowledgments: FAPESP and CNPEM.

Plenary / **2**

Synchrotron microtomography in palaeontology, a bright future for the South African exceptionnal fossil heritage at the ESRF

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The first application of X-ray synchrotron microtomography in palaeontology was performed in 2000 at the ESRF on the beamline ID19. This topic has been so successful that it has become one of the very visible research topics at the ESRF, making synchrotron microtomography the golden standard for non-destructive imaging of internal structure in fossils, when conventional microtomography reaches its limit. Considering the exceptional fossil record preserved in South Africa, palaeontology became a major collaborative topics between the ESRF and South-Africa during the last decade. More recently, archaeological applications have joined this portfolio. In most of synchrotrons using microtomography, sample size is typically limited to few millimeters in most of the beamlines, with only a handful of them allowing specimens in the decimeter range. Larger specimens are typically imaged with high energy conventional X-ray tomographs, but with severe restrictions in term of resolution and sensitivity. There is a clear lack of solution for high-sensitivity imaging in large fossils.

The BM18 beamline project at the ESRF, made possible by the development of the EBS new source, aims to tackle these limitations all at once by making possible synchrotron multi-resolution imaging on much larger samples than today, with special emphasis on fossils and natural and cultural heritage specimens. In addition to the other beamlines that were already involved in the thematics (ID19, ID17, BM05) BM18 will be able to image specimens up to 1 m in diameter and 2.5 m vertically. It will cover a pixel size range from 200 µm down to 1 µm, thanks to a 30 cm wide polychromatic beam able to reach 300 keV, tunable in flux, spectrum and geometry through various in-line X-ray optics. The whole beamline is designed for multi-resolution investigations using semi-automatic multi-detector system. The exceptional coherence properties of the ESRF-EBS, coupled with the 38 m of propagation on BM18 will allow phase contrasts imaging capabilities without equivalent worldwide.
BM18 should open tremendous new research capabilities for paleontology, but also for many other research fields, including archaeology, cultural heritage or evolutionary biology. The expected start of first user operations is planned for September 2021.

Parallel-Bio / **3**

Biophysical characterization of Plasmodium falciparum Hsp70-Hsp90 organizing protein (PfHop) reveals a monomer that is char-

acterised by folded segments connected by flexible linkers

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Plasmodium falciparum causes the most lethal form of malaria. The cooperation of heat shock protein (Hsp) 70 and 90 is important for the folding of a select number of cellular proteins that are crucial for cyto-protection and development of the parasites. Hsp70 and Hsp90 are brought into a functional complex that allows substrate exchange by stress-inducible protein 1 (STI1), also known as Hsp70-Hsp90 organizing protein (Hop). P. falciparum Hop (PfHop) co-localizes and occurs in complex with the parasite cytosolic chaperones, PfHsp70-1 and PfHsp90. Here, we characterized the structure of recombinant PfHop using synchrotron radiation circular dichroism (SRCD) and small-angle X-ray scattering. Structurally, PfHop is a monomeric, elongated but folded protein, in agreement with its predicted TPR domain structure. Using SRCD, we established that PfHop is unstable at temperatures higher than 40 ℃. This suggests that PfHop is less stable at elevated temperatures compared to its functional partner, PfHsp70-1, that is reportedly stable at temperatures as high as 80 ℃. These findings contribute to our understanding of the role of the Hop-mediated functional partnership between Hsp70 and Hsp90.

Parallel-Chemistry and Materials / 4

Micro-Raman and X-ray Diffraction stress analysis of residual stresses in fatigue loaded leached Polycrystalline Diamond

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X-ray diffraction and Raman spectroscopy techniques were used to investigate residual stresses in polycrystalline diamond disc samples sintered using the high temperature, high pressure method in the presence of a cobalt solvent/catalyst. The metallic phase primarily aids the formation of diamond to diamond bonds during sintering. During harsh rock drilling applications at elevated temperatures, the same cobalt expands more than the diamond, straining the diamond matrix and leading to premature failure of the component [1]. Since the PCD material formed is virtually a two-phase material comprising of cobalt and diamond, substantial volumes of the metallic phase can be removed through a leaching process without compromising the cohesiveness of the diamond matrix [2]. The leaching process reportedly results in a product with improved thermal stability and overall improved wear resistance. A systematic investigation and evaluation of the average in-plane residual stress fields on fatigue loaded leached PCD disc samples were undertaken. Whilst the Raman results reported a progressive shift of the residual stresses from an average compressive stress state to an average tensile stress state with an increasing number of loading cycles, the X-ray diffraction method recorded compressive stresses throughout. This apparent disagreement in results is likely due to differences in the way the two methods measure the residual stresses. Our results in this regard are presented and discussed in the context of several other reports of similar discrepancies in stress result measurements as reported by the Raman spectroscopy and the X-ray diffraction method.

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Strategy 1 / 5

African Synchrotron Network for Advanced Energy Materials

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New materials for the capture of light and mechanical energy can potentially enable low-cost and innovative renewable sources of energy while eliminating negative effects on the environment that are inherent when non-renewable sources of energy are utilised. Energy materials characterisation with synchrotron x-rays is a vital tool for the development of modern and next generation energy harvesting and storage technologies. The advent of the first African Light Source (AfLS) has the potential to transform the energy materials and related technology industries that underpin a robust and sustainable economy. The ASNAEM project aims to expand the local knowledge base and build capacity in the existing synchrotron community in preparation for the AfLS. It will enable sustainable partnerships that extend beyond the lifetime of the project. In this talk, I will discuss the activities of the ASNAEM project and our vision for synchrotron science at the AfLS.

Parallel-Chemistry and Materials / 6

Complimentary diffraction techniques at Necsa

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Complimentary to using synchrotron light, neutrons as well as laboratory X-rays play invaluable instrumental roles in the study of materials and their characteristics. South Africa, through The South African Nuclear Energy Corporation (Necsa) SOC Limited, offers both neutron and X-ray diffraction capabilities to the scientific and industrial communities. Necsa's X-ray diffraction laboratory houses two commercial diffractometers from Bruker: the D8 Discover (surface strain scanning) and the D8 Advance (surface powder diffraction). The Neutron Diffraction Facility is located at the SAFARI-1 research reactor and consists of the neutron diffractometers MPISI (Materials Probe for Internal Strain Investigations) and PITSI (Powder Instrument for Transition in Structure Investigations). Access

to these instruments is through an active user program and beam time is awarded based on scientific merit. Services are provided at no cost (excluding consumables) under the National System of Innovation and are also available on a commercial basis for proprietary projects.

This presentation will give a brief overview of the instrument technical specifications and focus on typical projects and applications that have been investigated using these instruments. Stress related projects include surface and 2D depth-resolved stress mapping of large engineering samples to thin coatings. Examples of surface as well as bulk material crystallographic texture (preferred orientation) measurements will also be shown. Powder diffraction examples include the study of temperature dependent phase transformations using in-situ sample environments such as a closed-cycle cryostat and vacuum furnace. Room temperature / atmospheric studies and quantitative phase analysis are routinely performed. Student projects and facility visits are encouraged.

Parallel-Paleo / **7**

Image quality in X-ray tomography: the case study of a fossil embedded in rock

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The use of X-ray micro-computed tomography (microCT) in palaeontology, geology, biology and material science and engineering has significantly increased in the last decade. In palaeontology, microCT is now widely used as the best tool to visualise and analyse fossils, which are sometimes still embedded in rock. With the growing use of microCT, the need for high-quality scan data is essential to obtain useful and accurate results, free of image artifacts or noise. However, despite the huge potential and various advances in laboratory microCT hardware, software and skills of users, there remain some issues with regards to image quality. Image quality can vary between different labs or even for different scans at the same lab, due to various reasons. In this paper, we discuss and demonstrate the quantitative effects of the variation of different microCT scanning parameters on the image quality for a fossil embedded in rock, and also demonstrate a simple image quality metric that can be applied to any X-ray tomography scan including synchrotron scans.

Parallel-Chemistry and Materials / **8**

X-ray and Neutron Radiography/Tomography at Necsa: A success story

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Necsa is privileged and in an unique situation within the South African context to host both neutron and X-ray radiography and tomography facilities on its premises at Pelindaba, 35 km West of

Pretoria.
True to the mission of Necsa to engage with stakeholders in the area of radiation sciences, international and national researchers and post graduate students are actively utilizing the imaging facilities through successful User Office beam line applications. Nuclear related areas such as post irradiation examination of nuclear fuel, or the characterization of barriers for nuclear waste within the nuclear fuel cycle, are addressed by this technology. However, the technical expertise of instrument scientists are being development and molded through the utilization of these facilities by researchers and post graduate students from Higher Educational Institutes (HEI's) and research centers, thus contributing to and supporting the National System of Innovation (NSI).
The neutron radiography/tomography facility is currently in an upgrade phase to enhance the versatility of the facility to supply not only a thermal neutron beam but also predominantly fast neutron as well as Gamma-Ray radiation beams. A section of this presentation focusses on the successes and research highlights achieved at the SANRAD facility.
To complement the neutron imaging probe at Necsa, X-ray tomography and micro-focus X-Ray tomography as imaging probes were introduced and implemented in 2007 and 2011 respectively. This facility at Necsa, in concurrence with the µXCT facilities at WITS and SUN, which were established through NRF support in 2011 to address the needs of local researchers in 3D analytical and non-destructive testing research capabilities.. It is generally perceived that the outcome of research conducted at these local µXCT facilities forms the basis of ground work research to be performed before a competitive project proposal can being submitted to a synchrotron facility.
Since the establishment of the µXCT (MIXRAD) facility at Necsa, the available beam time is fully booked as, on average, approximately 35 research projects per annum are being submitted for support. To date, the academic research output comprises of more than 150 publications including post graduate dissertations and thesis's, which spans all scientific fields ranging from palaeosciences to soil, geoscience, civil engineering and biosciences to name a few. This presentation will also highlight the application of µXCT in various research fields to show its versatility but also the important role it plays within the NSI and the South African research community.

Plenary / 9

Structure Property correlation in SOFC & SOEC materials, and the importance of Synchrotron Techniques.

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Solid Oxide Fuel Cells (SOFCs) and Solid Oxide electrolyser cells (SOECs) are exciting electrochemical devices that could provide unique and revolutionary solutions to some of the renewable energy challenges facing society. Central to the design of these devices is the need for a solid electrolyte that is an excellent oxygen ionic conductor whilst simultaneously being and electronic insulator. Additionally the materials needs to be mechanically tough and remain chemically inert in harsh operating environments. The architype materials used as solid electrolyte in most SOFCs include YSZ (Yttrium stabilised Zirconia) and CaSZ (Calcium stabilised Zirconia) with the Y or Ca dopants present at around 8 to 10% level. As the performance characteristics of these materials are not completely satisfactory, there is a definite need for improved alternatives.

Our research has focused on gaining a fundamental understanding of the mechanisms governing the transport properties of these and closely related materials. Typically the cubic forms (Space group Fm-3m) of these materials exhibit higher oxide ion conductivity due to the presence of vacant anionic sites. Our research has included the development of suitable synthesis, preparation and processing methodologies, particularly for the more novel materials, followed by structural, crystallographic, electrochemical and spectroscopic characterisation. Noteworthy, as SOFCs and SOECs have operational temperatures ranging from around 300℃ to 1000℃, we perform XRD, PDF(1), Raman and EIS measurements between ambient to 900℃ or 1000℃. Consideration of the results obtained for the array of distinct materials we have prepared, has highlighted the central role of short range order, as well as the importance of microstructure on the overall transport properties of the materials.

I will present a selection of our results to date, including the results obtained from total scattering experiments performed on ID22 at the ESRF in Grenoble as well as 28-ID-1 at NSLS-II at BNL. Analysis of the data shows structural differences when comparing the structure as perceived on the nano-scale with the bulk average structure. The implications of this for the transport properties of all energy materials is profound, and will be described.

Synchrotron techniques are central to insight into the real structure – property relationships, to this end we have additional experiments planned (beamtime approved) for NSLS-II, Diamond and SSRL. I will also present some of the unique aspects of some of the planned experiments.

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Poster Session 1 / 10

Mechanical,electronic and electrical properties of diamond-like carbon films grown by RF magnetron sputtering

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Diamond-like carbon (DLC) thin film is an amorphous carbon consisting of sp3 bonded and sp2 bonded carbon, and in addition contain up to several tens atomic percent of hydrogen. it can be used as protective anti –reflecting coatings for basic silicon solar cells to enhance the cell efficiency. On the other hand, it can be changed the opto-electronic and mechanical properties that depend on the sp3/sp2 fraction. Therefore in the work the opto -mechanical properties of DLC thin films by in situ control of the nucleation and growth of DLC thin films. Thus DLC thin films have been deposited on Si substrates using unbalanced RF magnetron sputtering at a constant power density of 4.4 W/cm2 and various substrate bias voltages in the range -25 to -100 V. Raman spectroscopy has been used to determine the sp3 fractions from the area ratios of the D-peak and G-peak (ID/IG). The results show that these ratio vary between (1.15-0.87) corresponding to sp3/sp2 ratio in the range (1.18-1.33). In addition, the hydrogen content were determined photoluminescence background in the range of (33.15-18.00) .The Tauc-gap and cluster size were determined by an empirical approach based the direct measurement in the range of (1.51-157eV) and (9.90-9.04 Å),respectively. The sheet resistivity were determined by using the expression of the Van der Pauw method in the range of (0.95-131× 102Ωcm). The elastics constant of DLC thin films were determined by surface Brillouin scattering and the optimum was determined at -100V. The thicknesses and the densities of the films have been determined to be (91-132 nm) and (2.20-2.35) using X-ray reflectivity, respectively.

Poster Session 1 / 12

The Search for an Improved SOFC Electrolyte Material: Stabilizing the Fm3¯m Phase of Bismuth Oxide to Lower Temperatures

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SOFCs have emerged as a leading candidate in the search for an efficient and environmentally friendly source of electrical energy.[1-7] SOFCs are, however, marred by a variety of limitations[1,4,6] which have prevented the widespread commercialization of this technology. Most of these limitations stem from the high operating temperature (typically 800-1000 ℃) that is associated with these cells – a feature dictated by the electrolyte material. As such, there exists a need for an improved electrolyte; a material that will display high oxide ion conduction at substantially lower temperatures. One such candidate is the Fm¯3m-structured δ-polymorph of Bi2O3 – the highest known oxide ion conductor. Normally only stable within a high and narrow temperature range (730-824 ℃),[1] this cubic polymorph has been exclusively studied in this work with the primary aim of stabilizing the δ-polymorph structure to lower temperatures by means of yttrium doping. These attempts have been successful; various YxBi2-xO3 members have been found to display the Fm¯3m structure at room temperature. Detailed structural analyses, enabled by synchrotron-based experiments, coupled with ionic conductivity and thermal expansion studies enable the establishment of preliminary material-specific structure-property relationships that allow for the overall suitability of these materials as SOFC electrolytes to be assessed.

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Poster Session 1 / 13

Exploring air exposure as a major pitfall in producing LiFePO4

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Lithium ion batteries convert chemical energy into electrical energy and the process is reversible making them suitable for energy storage systems.(1) Having efficient and long term storage devices allows for increased use of sustainable energy sources. The cathode material remains the largest focus area for the improvement of the battery performance (2) and any structural changes of the cathode material can affect this performance. Lithium iron phosphate (LiFePO4) forms part of the Pmna space group. All materials were synthesised using a hydrothermal methodology, using in-house developed Teflon bombs. Of interest were the effects due to different air exposure times, purging the sample with nitrogen before closing these teflon bombs and investigating the reproducibility of the synthetic method. The structural differences and phase purity due to these reaction variables were investigated; characterization techniques used include powder X-ray diffraction (PXRD) (coupled with Rietveld refinement analyses) and Mössbauer spectroscopy. The strong structure-property correlation that exists for these materials opens the door to future electrochemical measurements to be made.

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Poster Session 1 / 14

Exploring structure-property relationships in NASICON-type Sn-doped LiTi2(PO4)3

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NASICON-type materials such as rhombohedral LiTi2(PO4)3 (LTP), belonging to the R-3c space group, have been studied as potential solid-state electrolytes because of their thermal and chemical stability, as well high ionic diffusion attributed to their 3D framework consisting of TiO6 octahedra, corner-linked to PO4 tetrahedra, allowing for fast transportation of Li+ cations. [1] However, the room-temperature conductivity of LTP is not practical for use in Lithium ion batteries (LIBs) as it is approximately 4×10-7 S cm-1. [2] Research around this class of materials has been focused on ways to increase their conductivities, including tuning the bottleneck size by substituting Ti4+ with other cations such as Zr4+ and Hf4+, and increasing Li+ concentration by lattice site substitution with M3+ cations as in Al-doped LTP. [3, 4] In the former case, substitutions in the framework with cations of larger ionic radii increase the lattice constants a and c, resulting in a bigger bottleneck size, thus higher conductivity of the mobile cations, Li+.

In this work, we explore the possibility of lattice substitution as well as investigate if Sn4+-doped LTP formulations exhibit an improved ionic conductivity compared to LTP. Materials of the general formula Li⊠Ti⊠_(2-x) ⊠Sn⊠_x (⊠PO⊠_4)_3 (for 0, 2, 4, 6, 8, 10, 50 mole % Sn) have been synthesized following the conventional solid-state method. Room-temperature X-ray diffraction was employed as the primary characterization technique, giving insight into the phase compositions and relative phase purities of the products. Room-temperature Raman spectroscopy was used to further establish the structural properties of LTP as a function of dopant percentage. Information about the phase stabilities of the aforementioned materials was obtained by differential thermal analysis, establishing whether or not there was any temperature-dependent polymorphism exhibited by the said products. The room-temperature conductivities were determined using electrochemical impedance spectroscopy.

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Parallel-Chemistry and Materials / 15

Superionic conductors for solid oxide fuel cells: structure-bulk property relationships in Bi2O3 based solid solutions

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Solid oxide fuel cells (SOFCs) are electrochemical devices that convert chemical energy directly to electrical energy with reduced CO2, SO2 and NOx emissions [1]. They are highly efficient and when operated in combined heat and power mode they can reach efficiencies above 80% [2]. These devices have been known since Bauer and Preis reported their first use to produce electricity in 1937 [3]. Over 100 years have passed but no large scale production of such efficient devices have been achieved. The main problem is the high temperature at which they operate (800-1000℃). The operation temperature is mainly determined by the electrolyte; an oxide ion conducting ceramic that rely largely on thermally activated oxide ion hopping mechanism (vacancy mechanism) for ionic transport. The state of the art electrolyte is yttria-stabilized zirconia (YSZ). YSZ has conductivities ranging between 0.01 Scm-1 and 0.1 Scm-1 at 800℃ and 1000℃ respectively [4]. These high temperatures require the use of expensive materials with high melting points such as doped LaCrO3 for interconnects.

Electrolytes that show promise are the solid solutions of Bi2O3. Bi2O3 in its fluorite δ-phase is highly defective, with 25% of the oxygen sites vacant and is reported to have conductivities of about 1 Scm-1 at 730 ℃, the highest for an oxide ion conducting ceramic reported thus far [5]. Unfortunately, the δ-phase is only stable within a narrow temperature range of 730-824℃ [6]. Below this range, a monoclinic α-phase exist which is predominantly an electronic conductor and Bi2O3 melts at 825℃ [7]. To stabilize the highly conductive defect fluorite phase, isovalent and aliovalent cations have been used to substitute for the Bi3+ cation in the structure. In our work, we have fabricated solid solutions of Bi2O3 using the double and triple doping strategies. We have also followed crystal phase changes and measured conductivities with variable temperature XRD and electrochemical impedance spectroscopy respectively. The local environment was probed with variable temperature Raman spectroscopy. This enables us to study the cubic phase and get insight into the structure-property correlations of materials reported to have high conductivities.

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Parallel-Paleo / 16

Whiskers, nipples, venom, and head-butting: how imaging unravels the brain and paleobiology of our pre-mammalian ancestors

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What is probably considered among the most influential paper about pre-mammalian palaeo-neurology states that "early cynodonts possessed low-resolution olfaction, poor vision, insensitive hearing, coarse tactile sensitivity, and unrefined motor coordination" (Rowe et al. 2011). This reflects the fact that the fossilized neuro-anatomy of mammalian ancestors has long been considered extremely conservative. Using X-ray microtomography to access previously out-of-reach internal structures on the extraordinary wealth of South African Karoo fossils - which chronicles the origin and evolution of therapsids in exquisite details - our research team was able to trace back the evolution of several important neurological features through geological times. This work supports that there is more to therapsids palaeo-neurology that has usually been assumed. For instance, it highlights that the therapsid brain and inner ear display an unsuspected variety of shape and size. This hidden diversity relates to the onset of some important biological features, such as hearing, balance, intelligence and warm-bloodedness. Our research furthermore shed some fresh light on the evolution of the pineal eye and trigeminal nerve, which support an early origin of hair, whiskers and lactation some 241 million years ago, well before the origin of crown mammals. The study of the maxillary canal in therapsid also provides a gateway to the evolution of many other palaeobiological traits. It showed that sexual display and head to head fighting likely played a major role in mammalian evolution since the very origin of therapsids and that some mammalian ancestors evolved envenoming capacities millions of years before snakes. Overall, it is safe to state that imaging is currently revolutionizing our understanding of the palaeobiology of mammalian forerunners.

Parallel-Paleo / 17

A Tale of Two Dinosaurs

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The Iron-rich fossil-bearing rocks of South Africa have tempered the success of traditional lab-CT scanning protocols, with results often lacking sufficient resolution and density contrast required for detailed analysis of fossil material. Two dinosaur specimens, from opposite sides of the dinosaurian family tree, were recently scanned on the BM05 and ID-19 beamlines at the ESRF. The results produced were not only of a high-enough calibre to permit allow analysis of already-known material, but simultaneously permitted the recovery of previously unknown and obscured material. The first dinosaur scanned, the basalmost ornithischian - Heterodontosaurus, is currently the largest fossil specimen visualised at the ESRF; and synchrotron-scanning of this specimen (AM4766) revealed a suite of anatomical elements previously unknown from the family that this dinosaur belongs to. The second dinosaur, the coelurosaurian theropod Nqwebasaurus, was scanned and formed the basis for my project at the 2016 ESRF Summer-School program. Nqwebasaurus is known from a single well-preserved specimen (AM4060) that contains most of the postcranial skeleton, but very little of the taxonomically-informative cranial anatomy. Synchrotron scanning of the Nqwebasaurus holotype revealed an abundance of unknown and unsuspected cranial elements – more than tripling the known elements for this species. These results would have been impossible to obtain without the technology and engineering of the ESRF. We will present digital reconstructions of these dinosaurs as well as pertinent new information on aspects of their biology. Our results are a testament to the power of the ESRF facilities to allow maximum utilization of exceedingly rare specimens, produce ground-breaking scientific discoveries, and redefine the status quo.

Parallel-Chemistry and Materials / 19

Relevance of Synchrotron Radiation in Inorganic Medicinal Chemistry

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Abstract

Relevance of Synchrotron Radiation in Inorganic Medicinal Chemistry

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This study entails how three synchrotron radiation spectroscopic techniques (infrared microspectroscopy, microphobe X-ray fluorescence imaging, and X-ray absorption spectroscopy) are useful instrumentations to medicinal inorganic chemists in order to solve inorganic medicinal chemistry challenges. The study focuses on cellular uptake circulation, conventional bio transformed conventional agents, and future therapeutic agents.

Keywords: Challenges in inorganic medicinal chemistry; synchrotron radiation spectroscopic techniques; therapeutic agents

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Poster Session 1 / 20

Structure-property correlation of cerium doped bismuth vanadate for energy application.

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The demand for electricity is rapidly growing in developing countries and electrochemical devices such as solid oxide fuel cells (SOFCs) have shown promising developments to mitigate the demand. SOFCs are devices that convert chemical fuels (such as CO, H2 and ethanol) directly into electrical energy and this process is more efficient than any combustion process. They reduce the dependence on coal and oil to produce electricity and are largely composed of pollutant-free materials. Bismuth vanadate (Bi2VO5.5) is commonly doped or co-doped with transitional metals to enhance its ionic conductivity and function as a SOFCs electrolyte. The study of Bi2VO5.5 doped with rare-earth metals is under-reported and this study addresses the current literature gap. We report the impact of doping Bi2VO5.5 with cerium at different concentrations levels using a soft chemistry method (the citrate method). The study focuses on understanding how cerium substitution affects Bi2VO5.5

properties, (such as thermal stability, phase transition behaviour and ionic conductivity). It was determined that lower dopant concertation of Ce (<13% mol) form multi-phased material composed of monoclinic and orthorhombic phases, while higher dopant concentrations (>23% mol), form orthorhombic phase. At room temperature, Raman spectroscopy for 13% mol Ce doped, the predominate phase was orthorhombic which also showed weak signals nassociated with a monoclinic phase which was not detected by PXRD measurements. Selected results will be presented.

Poster Session 1 / 21

Synchrotron light source to aid where traditional SCD experiments fall short

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The discovery of actuating materials, or materials that respond to external stimuli (light, heat, pressure etc.) has shed light on an entirely new area for exploration in the fields of crystal engineering and the chemistry of the solid state. Many of these actuating responses coincide with some sort of phase transformation or solid state reaction. Although the mechanisms of the transformations that result in the photosalient effect are fairly well understood, very little is known about the thermosalient effect and its causes.

Work done on 4-(dimethylamino)-benzonitrile (DMABN) showed a thermosalient event by hot stage microscopy (HSM) upon cooling at 240 K and the reverse upon heating at 290 K. DSC traces and VT-PXRD confirm this phase change. Additionally, cooling below 182 K showed crystals rolling under HSM, and a small change in the PXRD pattern appeared. However neither single crystal diffraction (SCD) nor DSC showed any indication of an event or change. A recent study by Klaser et al. suggested that, potentially, the thermosalient event may not have to correspond to a phase change but may simply be due to thermal expansion.1 However, when comparing the changes in the PXRD patterns collected from DMABN to the PXRD patterns corresponding to thermal expansion in the study by Klaser, it appears to be more than just thermal expansion. Due to methods employed to prevent a thermosalient crystal from jumping off the mount for a SCD experiment, solving the structure from VT-PXRD data may be more useful to elucidate the structural change causing the thermosalience.

Another area where conventional SCD instruments present limitations, however powerful modern ones have become, is the size of the incident X-ray beam. On an Incoatec microfocus IµS 3.0 source, a beam size of about 110 µm (Mo) can be expected. When trying to focus the analysis on a small area of a crystal, for example the bent area of a plastic/elastic molecular crystal, the beam is still too large to isolate studies on that area alone. In light of the above, we hope that the capabilities provided by a synchrotron light source may aid where traditional SCD falls short.

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Poster Session 1 / 22

Doped bismuth oxide materials for low-temperature solid oxide fuel cell electrolyte

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Bismuth-oxide based electrolytes are well known for their high oxide ion conductivity at intermediate temperatures (300-700℃). Indeed, the defect fluorite structured δ-phase of Bi_2O_3 shows the highest known oxide ion conductivity of any material. Unfortunately, this phase is only stable above 730℃ and much research has been carried out on stabilizing this phase to lower temperatures through solid solution formation with other oxides. The aim is to work towards a better understanding of these materials in terms of structure and ion conductivity so that better SOFC electrolytes can be designed to run at lower temperatures (between 300 – 600℃). These materials will thus be studied at elevated temperature ranges. The longer-term stability of promising materials will also be investigated to determine how thermal cycling degrades the material and affects the conductivity.
The effects of Y^{3+} and Pb^{2+} double substitutions in Bi_2O_3 has been examined in the Bi_2O_3-PbO-Y_2O_3 system using X-ray powder diffraction (XRD), differential thermal analysis/thermal gravimetry (DTA/TG), and VT-Raman spectroscopy. All these characterization techniques show that samples having Y^{3+} as a major substituent have a single (δ-phase) phase structure. Pb^{2+} is isoelectronic with Bi^{3+}, thus the aim of including Pb^{2+} is to eventually try and gain insight into the effects of the lone pair of electrons in the mobility of the oxide ions through the lattice.

Poster Session 1 / 23

The effect of Cs content on the structural and photo physical properties in mixed cation hybrid-perovskites.

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Hybrid-perovskite solar cells have shown rapid development over the last decade reaching 25.2% efficiency in 2019 [1]. Their commercialization is precluded by device stability. The use of mixed cations to substitute the A-site cation site in the prototypical $MAPbX_3$ has shown to greatly improve stability, tune the bandgap and modify the microstructure of the photoactive layer towards a more optimal device. [2][3][4]. A better understanding of the substitution effects on structure and the associated changes in device stability is fundamental in the development and commercialization of these devices.

In the context of phase stabilization, our work investigates the structural, photo-physical and electronic properties of these hybrid-perovskites using both variable-temperature in-situ XRD and time resolved in-situ photoluminescence measurements. Various methods of analysis of the diffraction data are used focusing on sequential and parametric Rietveld refinements along with Pawley fits to extract unit cell parameters, bond lengths, structural distortions and polyhedral orientations for the metal halide framework of the hybrid-perovskites. The inclusion of MA suppresses the formation of the perovskite gamma phase while the inclusion of both MA and Cs changes features of the alpha/beta phase transition.

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Parallel-Bio / **24**

MicroCT provides novel insights into plant form and function

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MicroCT has tremendous potential to provide novel insights into plant form and function My research uses this and other, novel, non-invasive optical techniques to view the process of leaf and stem xylem embolism formation within intact plants to resolve long-standing questions in plant physiology. Here, I will highlight two recent experiments performed at the Australian Synchrotron in Melbourne Australia and the Lawrence Berkeley Laborartory in Berkeley, California in the USA. We used multiple visual techniques, including X-ray micro- computed tomography and the optical vulnerability method, to investigate the spread of embolism within intact stems, leaves and roots of Solanum lycopersicum (common tomato) and North American oak species. We found that roots, stems and leaves of tomato plants all exhibited similar vulnerability to embolism, suggesting that embolism rapidly propagates among tissues. Although we found scarce evidence for differentiation of xylem vulnerability among tissues at the scale of the whole plant, within a leaf the midrib embolized at higher water potentials than lower order veins. In oaks, air-entry water potential varied 2-fold in leaves, ranging from −1.7 ± 0.25 MPa to −3.74 ± 0.23 MPa, and 4-fold in stems, ranging from −1.17 ± 0.04 MPa to −4.91 ± 0.3 MPa. Embolism occurred earlier in leaves than in stems in only one out of eight sample species, and plants always lost turgor before experiencing stem embolism. Our results show that herbaceous species (tomato) and long-vesseled oak species are more resistant to embolism than previously thought and support the hypothesis that avoiding stem embolism is a critical component of drought tolerance in plants.

Parallel-Bio / **25**

Heterologous expression, crystallization and structural determination of Schistosoma mansoni Universal stress G4LZI3 protein by X-ray crystallography.

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The formation of high quality and perfect crystals forms the bottleneck and rate-limiting step for structure determination by X-ray crystallography. Protein crystallography has formed an intricate part of the chemical, biotechnology and pharmaceutical industry as an important tool towards drug design, protein engineering and in understanding various biological systems. In this study, a Universal stress G4LZI3 protein, identified as a 'lead' molecule for the design of alternative treatment against schistosomiasis, was subjected to protein crystallization trials. Schistosoma mansoni, a parasitic helminth, is responsible for the neglected tropical disease schistosomiasis that ranks second to malaria in public health significance. It accounts for over 280 000 deaths per year and is equally to blame for the physical life-long disability and disfigurements associated with the infection with

an estimated global prevalence of 200 million. Praziquantel, which has been the gold standard for treatment for over 3 decades, has now exhibited drug resistance. Over-expression of the G4LZI3 protein throughout the schistosome's lifecycle caused by conditions of stress, has warranted the need to determine its structure in a bid to design new schistosomides. The gene sequence coding for the G4LZI3 protein was first cloned into a pQE-30 vector using BamH1 and HindIII restriction enzymes. The resultant pQE30-G4LZI3 construct was transformed into M15 bacteria cells. Expression screening was done to determine the best expressing clone, and was used for heterologous expression of sufficient amounts of recombinant G4LZI3 protein, followed by purification on a Ni-NTA column. Thereafter, the G4LZI3 protein was purified to homogeneity using size exclusion chromatography; purified fractions under the chromatogram was pooled together and concentrated down to 10mg/ml, 15mg/ml, 17mg/ml, 20mg/ml and 24mg/ml. These various concentrations were subjected to various crystallization trials and various conditions yielded considerably sized and 3-dimensional shaped crystals. Complete datasets of 3.5 – 3.99A were collected and molecular replacement was achieved using the MR Rosetta software. Coot was used to visualize and perform model building on the generated solution. Future studies will aim to perform structure-based virtual screening of identifying small molecule inhibitors that can serve as anti-schistosomals.
Keywords: Crystallization, G4LZI3, Praziquantel, gel filtration, Schistosomiasis

Parallel-Chemistry and Materials / **26**

Synchrotron light and ore geology research

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The world's future supply of crucial metals hinges on sound scientific research and geological discovery. To this end, researchers and industry experts apply a range of traditional techniques such as microscopy, whole-rock geochemistry, and field mapping (among others). However, the world's easily-discovered resources have been exhausted and new mineral discoveries are becoming more difficult to uncover. Geoscientists must thus apply increasingly specialised and novel study techniques towards locating and optimally exploiting future resources.

Synchrotron techniques represent one approach that can advance this ultimate goal. Already, several research groups have applied synchrotron techniques towards understanding the micrometer and submicrometer scale mineral associations between ore minerals and the host rock (i.e., using synchrotron XRF). Similarly, the complexation and solubility of crucial metals within geological fluids are now better understood through insight obtained using synchrotron XANES and EXAFS analyses. These techniques further advance our understanding of trace metal coordination within mineral structures (e.g., gold in pyrite, silver in galena, germanium in zinc).

For southern African researchers to remain at the forefront of the global trends in geological research, it is crucial that they become familiarised and indeed, start to employ these high level synchrotron techniques towards their research questions. The current contribution critically reviews the global trends in synchrotron use for ore geology research. Key findings, and anticipated future directions will be highlighted during the seminar.

Parallel-Chemistry and Materials / **27**

Magnetic-electronic studies at a megabar: the new frontier

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The main consideration in this presentation is the interplay amongst magnetic-electronic, structural and charge-gap responses in strongly correlated 3d electron systems (transition metal oxides) evolved to very high static densities. Tuning through the large, ˜eV, energy scales necessitate employing diamond anvil cells for requisite static pressures to the vicinity of ˜100 GPa.
Consequently pertinent onsite-repulsion to bandwidth U/W and crystal-field splitting to spin-pairing energy CF/J ratios can be varied over large ranges. Profound effects on physical properties may ensue, including the breakdown of Hund's rule resulting in a high-spin (HS) to low-spin (LS) transition (CF/J > 1) and a Mott insulator-metal transition (U/W <1).
Variable temperature 57-Fe nuclear resonance (Mössbauer) spectroscopy extended to cryogenic temperatures, is one of the few and most powerful means of revealing the magnetic-electronic groundstate stabilized at high densities. Synchrotron XRD monitoring of the pressure evolution of the unit-cell volume provides evidence of crystallographic phase transitions or corroborating evidence of HS to LS transitions, from signature shrinkage effects in the cation radius due to spin pairing in lower lying 3d orbitals.
Complementary resistance pressure measurements help to ascertain whether magnetic collapse is associated with HS to LS crossover or correlation gap closure (insulator to metal transition) or the concurrence of the two phenomena.
Highlights from a selection of studies, which include synchrotron XRD and nuclear resonance probes, on various ferrous spinels pressurized to the vicinity of ˜100 GPa will be presented [1-3]. These include, as a result of compression: (i) orbital moment quenching effects, (ii) site-inversion at room temperature and subsequent spin crossover occurring, (iii) transitions to post-spinel structures and subsequent triggering of partial/site-specific spin crossover, (iv) charge-gap resilience in spite of anticipated appreciable bandwidth broadening and an attempt to rationalize this.
We will further indicate why probing magnetic-electronic and structural aspects of these transition metal oxides beyond ˜100 GPa would be useful, is beyond home laboratory based capabilities and that synchrotron probing with appropriately tightly focused probes of micron or sub-micron dimensions is imperative.

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Poster Session 1 / 28

Structural characterization of Ti6Al4V/TiC thin films produced by RF Magnetron Sputtering.

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TiC thin film has many industrial and scientific applications due to its favourable properties. In this study, TiC thin film was deposited on Ti6Al4V alloy substrate to improve the surface properties. Structural characterization of the evolving properties was carried out. Grazing incidence X-ray

diffractometer GIXRD was used to determine the crystallographic structure of the film. Structural defects and the stoichiometric ratio of the film was studied using Raman Spectroscopy. Field emission scanning electron microscope FESEM was used to understand the distribution of the TiC thin film morphology and the surface topography analysis was done on an optical profilometer. The results show that the TiC thin-film properties evolved with change in the process parameters of the RF magnetron sputtering. Crystalline TiC thin film was noticed on the XRD spectra and the Raman results confirm the presence of both stoichiometric and non-stoichiometric TiC thin film. Homogenous distribution of the TiC thin film was also observed.

Parallel-Chemistry and Materials / **29**

Materials preparation for the future hydrogen economy: PEC water splitting

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Semiconductors have been used in solar water splitting since the initial report on hydrogen production using TiO2. Thus far, materials explored to achieve theoretical solar to hydrogen efficiency (STH), included cadmium selenide (CdSe), zinc oxide (ZnO), copper(I)oxide (Cu2O), tungsten trioxide (WO3) and hematite (α-Fe2O3). All these failed due to their band edge alignments that do not straddle water oxidation and reduction potentials. Of these materials, hematite has received much attention for photoelectrochemical water splitting attributed to its stability in aqueous solution, a small band gap of 1.90 eV-2.20 eV, non-toxicity and abundance. However, it has associated limitations such as high electron-hole recombination rate, short hole diffusion length (2-4 nm) accompanied by short excited lifetime of 10 ps, and poor minority charge carrier mobility of 0.1 cm2 V-1s-1, leading to low photocurrent during water splitting. Furthermore, hematite promises a maximum theoretical STH efficiency of ˜16.8 %, with photocurrent densities above 12 mAcm-2, but the reported findings are far below 10 mAcm-2. The future is in the hydrogen economy which requires clean energy production to reduce the carbon foot print and consequently combat climate change.

Plenary / **30**

Residual Stress Characterization using Synchrotron XRD for the Development Laser Shock Peening Applied to Steam Turbine Blades

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The lifespan and integrity of critical metal components such as steam turbine blades for the power generation industry can be limited and compromised by mechanisms such as fatigue and stress corrosion cracking. Conventional surface treatments such as shot peening and roller burnishing are commonly used to introduce beneficial compressive residual stresses to mitigate crack related phenomena. Laser Shock Peening (LSP) is an advanced surface enhancement process that potentially achieves superior performance compared to conventional treatments due to deeper levels of compressive residual stresses. Although LSP has successfully been adopted in the aerospace sector for titanium blade performance enhancement, the technology is not yet typically applied for power generation applications. Systematic development of the LSP process parameters applied to 12Cr steels for low pressure stream turbine blades has been performed using a number of complimentary residual stress characterization techniques such as synchrotron XRD, laboratory XRD, incremental hole-drilling, neutron diffraction, and the contour method. High energy synchrotron X-Ray Diffraction performed at the ESRF (beamline ID15A experiment ME1440) has allowed for qualitative evaluation of a number of LSP parameter combinations leading toward the selection of an optimized parameter combination to be applied to full scale components.

Plenary / 31

Chemical characterization at the ESRF

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The highly brilliant X-ray beam at the ESRF allows application of sophisticated techniques for identification of the chemical state. High-resolution powder diffraction pushes the limits of solving and refining of crystal structures and investigating the structure of crystalline, defective and non-crystalline materials via atomic pair distribution function (PDF) analysis. X-ray spectroscopy provides an element-selective tool to study the chemical state of an analyte. Here, the ESRF has been pioneering the development of photon-in/photon-out spectroscopy that allows for higher spectral resolution and probes unoccupied as well as occupied electronic levels (Figure 1). This technique will enter a new dimension with the upgrade programme ESRF-EBS where it will be combined with a micron-sized beam. This unique technical development provides access to the study of "invisible" elements, i.e. analytes in low concentration in a matrix of elements with similar atomic number.
The presentation will provide brief explanations of the techniques, present the most important technical developments and give examples to illustrate the new possibilities.

Strategy 1 / 32

Towards an African Crystallographic Association

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In recent years, there has been significant effort devoted to the formation of regional crystallographic associations in the developing world. During the International Year of Crystallography in 2014, an IUCr-UNESCO summit was held in South Africa. One of the outcomes of the summit was a declaration that envisaged the formation of an African Crystallographic Association, AfCA. This presentation will discuss progress in the constitution of AfCA, as well as the connections between AfCA, the IUCr and synchrotron users.

Parallel-Chemistry and Materials / 33

Dithiadiazolyl radicals as building blocks for functional materials

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The 1,2,3,5-dithiadiazolyl radicals (DTDAs), R-CNSSN•, are of considerable interest due to their potential as magnetic or conducting materials. However, DTDAs tend to dimerise in the solid state via an interaction known as pancake bonding.[1] Pancake bonding between DTDAs results in spin pairing, rendering the resulting materials diamagnetic. Overcoming this dimerization interaction has been the focus of much effort, and several DTDAs that remain paramagnetic in the solid state have been characterised, with some exhibiting magnetic ordering at low temperatures.[2] This presentation will present our efforts in characterising solid-state materials containing DTDAs using a combination of X-ray diffraction experiments, computational methods and spectroscopy.
In order to better understand (and thus overcome) the pancake bonding interaction, we have turned to experimental charge density investigations.[3] An analysis of the topology of the charge density of a series of DTDAs reveals how pancake bonding differs from both covalent bonding and conventional intermolecular interactions.
We have also explored the incorporation of DTDAs into multi-component crystals, including co-crystals[4] and porous materials,[5] in order to overcome dimerisation. Co-crystal formation with DTDAs has been shown to be highly dependent on experimental conditions. Inclusion of DTDAs in porous hosts shows great potential for the development of functional materials.
Finally, we have investigated the coordination of DTDAs to metalloporphyrins, yielding at least one new material with intriguing properties. [6] It is clear that DTDAs show great potential as building blocks in the construction of molecular materials.

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Structural Biology at the ESRF: present and future

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The ESRF's facilities for Structural Biology comprise 6 end-stations for macromolecular crystallography (MX) 1, one end-station for BioSAXS experiments 2 and one end-station based around a Titan Krios cryo-electron microscope 3. These are supplemented by a number of support laboratories including the iCOS facility for in crystallo optical spectroscopy 4 and a facility for the high pressure cryo-cooling and/or derivatisation of crystals of biological macromolecules 5. This talk will describe the instrumentation and experimental possibilities available on these end-stations, with a particular emphasis on automation, remote access and mail-in services.

The ESRF Extremely Brilliant Source (EBS) project (see http://www.esrf.fr/about/upgrade for details) will provide benefits for many areas of synchrotron-based science. This presentation will thus also look ahead to the evolution of the ESRF's facilities for Structural Biology post-2020, focusing on the possibilities for serial crystallography and time-resolved MX, which ESRF-EBS X-ray beams will facilitate.

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X-ray diffraction using the ESRF-EBS

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Atomic structures can be determined using X-ray diffraction and this technique has already had a huge impact on a wide range of scientific disciplines. The upgrade of the ESRF source will bring another order of magnitude increase in the X-ray flux available for diffraction experiments in many beamlines. Detector upgrades are also planned in order to get the full benefit of these source improvements.

In many cases, these upgrades will increase the range of samples for which we can obtain atomic information, to ever smaller crystals and also with higher resolution in time and space. There are a range of new techniques available where we can obtain images of samples by scanning small beams while recording X-ray diffraction data. The EBS upgrade will enable these very demanding methods to be used for in-situ studies, so that we will be able to see what the atoms are doing inside of complex materials and evolving micro-structures. Examples of recent highlights from ESRF will be presented with a view towards the new possibilities planned for 2020.

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Overview of SA synchrotron activities and its ESRF associate membership status

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Synchrotron radiation has revolutionized basic and applied research in many fields of science and technology. South African, like many countries, has seen an ever increasing number of scientists accessing such facilities around the world. Despite spiralling cost and long distance travel, South African synchrotron usage has therefore increased steadily over the last decade.

This talk aims to give an overview of synchrotron-based activities currently undertaken by South Africans, provide some examples of successes achieved thus far including government support and commitment for accessing international synchrotron facilities, highlight some challenges experienced by the community and outline the long-term goals for the country for the use of synchrotron radiation. An overview of SA's association with the European Synchrotron Radiation Facility, its usage by SA scientists as well as successes and challenges will also be presented. The possibility of political support from the DST and the NRF to create multi-African country partnerships that could jointly participate at the ESRF along with South Africa will be explored.

Parallel-Paleo / **37**

The use of Micro Computer Tomography in the establishment of a new basal sauropodomorph taxon

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Understanding the palaeobiodiversity of the Early Jurassic of South Africa relies on researchers' ability to correctly identify the various fossil taxa from that time. Complicating factors such as ontogeny, sexual dimorphism, and taphonomic deformation often hinder these taxonomic identifications. Micro Computed Tomography (CT) allows for an unprecedented level of detail when studying fossils and therefore more insight into the factors explaining observed morphological disparities. Here, a basal sauropodomorph specimen (BP/1/4779) previously referred to Massospondylus carinatus was CT-scanned and compared to a small ontogenetic series of M. carinatus specimens in order to rule out developmental effects as a reason for the morphological differences observed. Using digital retrodeformation of the reconstructed scans, we assessed if the shapes of the overall skull of BP/1/4779 and of the individual cranial bones can be deformed to resemble that of M. carinatus, therefore excluding taphonomic deformation as an explanation. On the basis of this CT-based investigation, we can confidently reassign BP/1/4779 to a new genus.

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Opening DST/NRF/SRRIC

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ESRF and EBS Overview

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SRRIC Chair: Tshepo Ntsoane - SA and ESRF

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ESRF DG : Francesco Sette - ESRF as the CERN of LSs

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SA Feeder Infrastructure overview and issues

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The role of Large Scale Infrastructure

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International Collaboration

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START - Trevor Sewell

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ASNAEM -Marcus Newton

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ANSDAC - Esna du Plessis

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LAAAMP - Simon Connell

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IUCr/ACr - Delia Haynes

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Round Table - Floor and Panel

Author: Simon Connell[1]

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The Floor puts Questions and Comments to the Panel of seekers who gave talks in the session

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Conclusion and Actions

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The Floor and Panel come to Resolutions and Conclusions.

Conclusions

This SA-ESRF meeting builds on more than a decade long deep commitment to develop the User Base in Africa reflecting the Global nature of Science and the ESRF as a leading international facility.
ESRF-EBS represents a very dramatic increase in figure of merit (FOM) of performance of both source and detector (100x100) or about 10000 time more powerful. In addition completely novel with also novel techniques and opportunities emerge. The novelty means there is not really experience yet and so the exploitation of the new capacity requires partnerships with beamline scientists.
This meeting extends the possibility for all to grow their contacts within the ESRF or launch new ones. This should lead to the development of proposals ready for March 2020

The meeting noted the increased number of projects and organisations involved and shares the vision of working together in a common coherent vision, not only for South Africa, but also for Africa (training, impactful science, science for development….)
For example, there were also talks from the AFCA (IUCr AND PCCR), the START program, ANSDAC, ASNEAM, LAAAMP and also the neutron related complimentary techniques at Necsa.
All programmes and projects were stakeholders and could work together coherently avoiding silos, and build the common vision of growing the User Base in South Africa, with training, mobility and shared local infrastructure.

The ESRF were committed to the concept of coherence and inclusivity of stakeholders.

The coherence of the South African Community had suffered because of the failure of the NRF to provide regular support for the Science@Synchrotrons biennial conference since 2011 and also to not respond to the SAILS Proposal which would replace the SRRIC. The DSI and NRF meanwhile supported other similar programmes, such as the SA-CERN programme.

The SAILS (or SA Light Source user community) would grow even more than this programme, as it was more interdisciplinary, with more members, with at least the same or better opportunities for training, technology transfer and innovation. Meanwhile we are only a volunteer management and are under-resourced to grow coherently, develop joint proposals, provide training and audit and comment our performance.

The meeting agreed to revive SAILS with or without the support of the DST and NRF.

We could go elsewhere to seek funding, but we recognise it made more sense for the NRF and DSI to understand their role to support this group.

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Introduction to workshop: Science with the EBS

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ESRF Materials via Imaging - Julia Villanova

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X-ray diffraction using the ESRF-EBS - Jon Wright

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Structure Property correlation in SOFC & SOEC materials, and the importance of Synchrotron Techniques - Dave Billings

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Chemical Characterization at ESRF- Pieter Glatzel

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Synchrotron microtomography in palaeontology, a bright future for the South African exceptionnal fossil heritage at the ESRF - Paul Tafforeau

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Overview of CT in South Africa

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Structural Biology at the ESRF: present and future - Gordon Leonard

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AfLS, SA and Pan Africa

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Inspired by the rallying call of Science for Development, Science for Peace, and Science itself, a large cohort of Scientists and Policy Makers and others, from Africa and beyond, have identified the African Light Source as a priority. This large scale science research infrastructure is the leading example of a resource hosting multi/inter/trans- disciplinary research activities. These include the medical sciences, cultural heritage sciences, geosciences, environmental sciences, energy sciences, nano-sciences, materials sciences and mineral sciences, industrial R&D, amongst others. It is expected to have an enormous impact on socioeconomic development. As an example, already, we know the HIV drug development was guided by the idea from structural biology that structural information helps to elucidate protein function and, in particular, the mechanisms of enzymes. This understanding inspires the design of new drugs. The same idea of course applies to many other diseases. Similar dramatic and relevant growth can be found in African heritage and also materials research. The call was first sounded in 2002, and it is now rather mature, with a Roadmap, driven by a fully mandated international Steering Committee. Massive gains are now made, particularly in the expansion of the User Base, the profile at the African Government and Pan African Level, and the momentum of the progress on the Roadmap. This talk will review the past, present and future prospects, as we drive the roadmap forward, with some highlights from Africa.

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Whiskers, nipples, venom, and head-butting: how imaging unravels the brain and paleobiology of our pre-mammalian ancestors - Julien Benoit

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Image quality in X-ray tomography: the case study of a fossil embedded in rock - Muofhe Tshibalanganda

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A Tale of Two Dinosaurs - Viktor Radermacher

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The use of Micro Computer Tomography in the establishment of a new basal sauropodomorph taxon - Kimberly Chapelle

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Structure-property correlation of cerium doped bismuth vanadate as potential SOFC electrolyte - Dennis Malhase

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Magnetic-electronic studies at a megabar: the new frontier - Giovanni Hearne

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Synchrotron light and ore geology research - Bjorn von Heyden

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Synchrotron light source to aid where traditional SCD experiments fall short - Thalia Carstens

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Research Activities: Advanced Manufacturing Technologies - Fred Mada

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MicroCT provides novel insights into plant form and function - Robert Skelton

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Heterologous expression, crystallization and structural determination of Schistosoma mansoni Universal stress G4LZI3 protein by X-ray crystallography - Abidemi Paul Kappo

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The structure and function of HIV neutralizing antibodies and their targets

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Biophysical characterization of Plasmodium falciparum Hsp70-Hsp90 organizing protein (PfHop) reveals a monomer that is characterised by folded segments connected by flexible linkers - Stanley Makumre

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Thin films of VC/SiC - Kuda. Jakata

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The Search for an Improved SOFC Electrolyte Material: Stabilizing the $Fm\bar{3}m$ Phase of Bismuth Oxide to Lower Temperatures - Kiefer Mattias

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Dithiadiazolyl radicals as building blocks for functional materials - Delia Haynes

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Micro-Raman and X-ray Diffraction stress analysis of residual stresses in fatigue loaded leached Polycrystalline Diamond - Maxwell Vhareta

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Innovations in Energy Materials - Marcus Newton

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X-ray and Neutron Radiography/Tomography at Necsa: A success story - Frikkie De beer

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HARPIA: High Resolution Powder X-ray Diffraction beamline at Sirius - Dean Barret

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Complimentary diffraction techniques at Necsa- Deon Marais

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ESRF and EBS Overview

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TBA

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ESRF as the CERN of LSs

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SA Feeder Infrastructure overview and issues

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Effective use of Large Scale Research Infrastructures (LSRI) requires considerable local infrastructure to first be in place. In the case of a LSRI for analysis of samples or materials, a strong local capacity in acquisition and preparation of research material is required as well as an established excellence in the understanding of that material in the general research context. The proposers of experiments at analytical LSRIs need to demonstrate the research material has the capacity to yield new information and insight into a specific research programme. This material or class of materials therefore needs to be first studied locally. Both the acquisition / production and pre-charaterisation / preliminary studies of the research material require local infrastructure. In the context of the structural biosciences, a local or regional laboratory for bio-crystal growth and characterisation is necessary. The production of the samples requires a well equipped biological and chemical laboratory with advanced equipment, such as robotic apparatus for high throughout production of the crystals, and

ancillary and major equipment for the characterisation of these crystals. In addition, advanced local equipment (lab scale x-ray diffraction equipment and electron microscopy equipment) whereby the general research programme is established and advanced is crucial. Suitcase science alone is not sufficient. Indeed, this phase of the research is still highly competitive and impactful. It establishes the base from which successful proposals to the LSRI can be made, and provides the main part of the training for the research team, especially the students. The situation is very similar for all the other sciences and industry programmes which plan to access the LSRI. This talk reviews the situation for such feeder equipment in local laboratories, which then enable effective access of the LSRI.

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Lightsources for Africa, the Americas, Asia and Middle East Project (LAAAMP): An IUPAP and IUCr ISC-Funded Project

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We describe an initiative funded by a 3-year, 300K-Euro grant from the International Science Council (ISC) to the International Union of Pure and Applied Physics (IUPAP) and International Union of Crystallography (IUCr) in collaboration with over 30 partner organizations that include 16 advanced light sources to enhance the utilization of advanced light sources and crystallography in five targeted regions of the world, namely Africa, the Caribbean, Mexico, Southeast Asia, and Middle East. LAAAMP's programs include the development of a Strategic Plan for each region; a Colloquium program that sends experienced light source and crystallography users to those regions; establishment of new IUCr-UNESCO Crystallography OpenLabs; design and distribution of a Brochure that describes advanced light sources and crystallography for government officials and the public; 2-month Faculty-Student (FAST) Team training visits to advanced light sources, with approximately 30 new users participating in 2019; and culminating in a December 2019 thematic session at the World Science Forum 2019 in Budapest, Hungary to chart a path forward beyond the ISC grant.

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The African Neutron and Synchrotron Data Analysis Competency (ANSDAC)

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The African Neutron and Synchrotron Data Analysis Competency (ANSDAC) project aims to develop expertise amongst emerging Africa-based faculty researchers to engage with and make use of large scale international institutions such as neutron and synchrotron light sources. It is funded by the Newton Fund administered by the Royal Academy of Engineering, and the DST-NRF Centre of Excellence in Catalysis c*change, in kind contributions by the Universities of Glasgow, the Western Cape and SASOL and partnering with the Global Challenges Research Fund project START (Synchrotron Techniques for African Research and Technology). Three workshops on synchrotron and neutron data analysis were / will be offered in 2018 to 2020. Lectures are held by experts from the Diamond Light Source and the ISIS Neutron and Muon Source in the UK as well as South African specialists. The most recent workshop took place from the 16th to the 24th of October 2019 in Cape

Town. In 2020, ten of all workshop attendees will travel to the Diamond Light Source and the ISIS Neutron and Muon Source in the UK to experience beamtime first hand. This is possible through a collaboration with the UK Catalysis Hub. This presentation will provide further details on ANS-DAC.

Poster Session 1 / 94

Same as Monday

Plenary / 95

What is new in X-ray imaging at ESRF?

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X-ray characterization provides opportunities for scientists in the exploration of materials and living matter in many fields: chemistry, material sciences, archaeology and cultural heritage, structural biology and medical applications, environmental sciences, information science and nanotechnologies. A wide range of techniques are available one of which is X-ray imaging. This term is usually associated with absorption radiography but, in fact, it is related to any X-ray technique that provides spatially resolved information. In this overview, common 3D X-ray imaging i.e. computed tomography that reveals 3D microstructure of materials from the micro to the nano-scale will be presented. The ultimate state-of-the-art instrumentation offered by the ESRF, especially in terms of spatial and temporal resolution, will be addressed based on examples from the field of materials science studies. Furthermore, we will explore the field of micro and nano-chemical mapping. Materials and environmental sciences examples will detail and illustrate the benefits and limitations of this technique with ESRF-EBS.

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Proposal Clinic

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There is a strong competition for beam time at the ESRF. Access is based on submission of a Research Proposal. The proposal success rate averages 45%, but certain facilities are more in demand than others. Proposal are judged primarily on scientific merit. Technical feasibility, safety and ethics must also be assured. Although the EBS project has led to a service interruption, the proposal submission deadlines for the next round of beam times are in January and March next year - depending on the type of access required. The purpose of this session is to provide information on the proposal writing and submission process, so that South African researchers can be ready for the Proposal Submission deadline early next year. There is also opportunity at this conference for new users to identify parters who are experienced users. This can greatly increase the success rate of applications for new users. It is particularly useful to partner with beamline scientists from the ESRF, or other

collaborators, who are familiar not only with the proposal process, but also the samples preparation, the measurements and the analysis of synchrotron data.

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Sponsors (Flash Talks)

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ESRF Data Policy

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The effect of Cs content on the structural and photo physical properties in mixed cation hybrid-perovskites

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Synchrotron light source to aid where traditional SCD experiments fall short

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Research Activities: Advanced Manufacturing Technologies

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The Search for an Improved SOFC Electrolyte Material: Stabilizing the $Fm\bar{3}m$ Phase of Bismuth Oxide to Lower Temperatures

Parallel-Bio / 104

Structural characterization of neutralizing antibody lineages from an HIV-infected donor

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HIV broadly neutralizing antibody (bNAb) responses develop in chronic infection in only approximately 25% of HIV-1-infected individuals. Understanding how bNAbs develop has been a major focus in HIV vaccine research in recent years. The aim of this study is to solve the structures of co-evolving strain-specific and bNAbs from an HIV-infected donor, CAP314. We have recently isolated three antibody lineages from this donor. The first lineage is an N332/glycan-dependent lineage which matured from being strain-specific to broadly neutralizing through the course of infection. Comparison of early and late antibodies by X-ray crystallography techniques may thus provide insight into the differences between the binding of broadly neutralizing and strain-specific antibodies within a single lineage. Preliminary data suggest the second lineage of interest can be classified as a "helper" lineage which aided in the development of the broad N332/glycan-dependent lineage. Therefore, using X-ray crystallography to obtain the structures of these antibodies will aid in understanding how this lineage shaped viral populations and drove the development of neutralization breadth. The third lineage identified from this participant recognizes an undefined epitope consisting of elements of both the N332/glycan and the CD4 binding site. Therefore, solving the structure of this antibody by X-ray crystallography will provide insight into the binding of a neutralizing antibody lineage targeting a novel epitope. Collectively, structural data for three antibody lineages from a single HIV-infected individual represents a unique opportunity to investigate the underlying mechanisms used by the humoral immune response in responding to swarms of HIV variants.

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Characterisation of Materials using X-rays and Deep Training

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Africa does not have a synchrotron, and while the establishment of a synchrotron light source on the African continent continues to be discussed, these initiatives get stalled by the lack of expertise on the African continent in successfully designing an experiment and analysing the large amount of data. In this contribution, I will highlight some collaborative projects between African researchers and the technology and expertise around the world. I will also highlight the South African "Indaba", a series of interdisciplinary workshops, organised by the South African Crystallography (SACrS), which assembles scientists from around the world particularly in chemistry. Lastly, I will also present the "deep learning" experience at ID22 - High resolution powder diffraction beamline – ESRF. Included will be my scientific work at the institution which can be summarised as participation in in-house research programmes, the operation of the beamline, providing support to external users as local contact and development of a personal research program.

Plenary / 108

SA Bioscience Overview

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The discipline of structural biology has had a rocky start and chequered history in South Africa. Despite structural biology having transformed the life sciences over the last half century and the continued relevance being documented almost daily through novel revelations in the premier scientific journals such as Nature, Science, Proceedings of the National Academy of Sciences (USA), New Scientist, and novel drugs being developed continuously based on its insights, the field has been systematically underdeveloped in South Africa. In the 1970's to the 2000's, structural biology was seen as too expensive for universities and funding agencies in South Africa. Hence the first rotating anode generators were installed only in the early 2000's in Cape Town and Johannesburg under the respective leadership of Profs Trevor Sewell and Heini Dirr. From these late beginnings, the discipline has expanded slowly but steadily to secondary centres throughout the country including Bloemfontein, Stellenbosch, Pietermaritzburg, Pretoria, Richards Bay, Potchefstroom, Makhandla/Grahamstown and others. As centres are not all equally well equipped in hardware, expertise and manpower, a complex network of extensive collaborations have developed between the groups helping researchers and students in different parts of the country to push their projects forward.

Despite the hardships encountered over many years and enduring into the present, the community of structural biologists is currently fairly cohesive and still growing. However, many dangers lurk that could rapidly derail the gains made over the last years. These include the weak financial support in the South African funding landscape, the (imminent) retirement of the trailblazers in the field, limited employment prospects for graduates and a resulting associated brain-drain out of the country, the poorly developed drug industry in South Africa, to name just a few.

Thus while structural biology appears passably well established in South Africa at present with fairly good links to international infrastructure such as the ESRF and Diamond, the continued development of the discipline will require significant will power, hard work, the identification of alternate funding sources, the further development of international ties, and the engagement with and support from appropriate representatives in the South African funding agencies and ministries.