"ADDRESSING AFRICA'S CHALLENGES THROUGH MATERIALS DEVELOPMENT"

9th International Conference of the African Materials Research Society

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BOOK OF ABSTRACTS





Welcome Address: AMRS2017 Conference Chairperson

It is with great pleasure that I welcome you to the 9th African Materials Research Society (AMRS) conference that is taking place here in Gaborone, Botswana. I am indeed grateful to all of you for honouring our invitation to attend this conference. Very few people in August 2000 could have imagined that when the National Science Foundation (NSF), USA and the National Research Foundation (NRF), South Africa organized the first meeting to deliberate on how to develop material science in Africa, that the meeting would lead to a vibrant African Materials Society and to this series of conferences. This week we proudly start the 9th edition of this series of conferences and I look forward to successful interactions; networking and strengthening of friendships.

It is what responsible materials research can do for Africa that excites me the most. Yes, we have to be mindful of what we add to our environment, as at best it should enrich the soil's fertility and keep our groundwater prestine. I am delighted that today we have several research groups from laboratories that are driven by scientists based on the African continent, who are engaged in developing materials to solve some of the challenges facing the continent and the world at large. The Botswana Institute for Technology Research and Innovation (BITRI) is a prime example as its research agenda defines the current trends in materials research in Africa. Therefore I would like to invite all our visitors to make time to visit the BITRI stand situated in the exhibition area or better still, get to the BITRI campus to see the range of research as well as the world class facilities available at the Institute. BITRI is keen to collaborate with researchers on the continent and indeed the rest of the world to use materials to develop products that can address challenges facing Botswana and the African continent. So please talk to BITRI!

No conference these days can be run successfully without the support of sponsors, and the AMRS 2017 is no exception. We have received support, both material and otherwise, from various quarters for this conference. We would like to express our sincere appreciation to all our sponsors for their support and will do so in various ways during the course of this conference to let everyone know how grateful we are for the support.

A conference cannot go on without delegates. Our delegates have come from far and near; for some of you this is your first time in Botswana, for others it is your second, third or even forth visit. We feel very lucky that you are able to join us to talk about what materials can do 'to transform lives and provide for equal opportunities'. I am sure you will enjoy your stay here in Botswana and will see it fit to come back with your friends and families in the near future. In the meantime enjoy AMRS 2017; and on behalf of the AMRS family, the Local Organizing Committee and the host of this conference, BITRI, I say Welcome to Botswana and to AMRS 2017.

Let me conclude by saying a special thank you to His Honor, The Vice President of The Republic of Botswana, Mr Mokgweetsi Masisi. Mr Vice President, AMRS2017 is in Gaborone because of you, we are grateful for your leadership.

Nelson Torto PhD FBAS FAAS FRSC Conference Chair

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HO-Health, EO-Energy, NO-Nanotechnology, WO-Water, AO-Agriculture, MO-Mining/Construction, CO-Computational, EDO-Education

PLENARY LECTURES

PL 01 Dynamic Materials Towards Functional Adaptive Materials Jean-Marie Lehn

ISIS, Université de Strasbourg, France

Supramolecular chemistry is intrinsically a *dynamic chemistry* in view of the lability of the non-covalent interactions connecting the molecular components of a supramolecular entity and its resulting ability to exchange components. Similarly, dynamic covalent chemistry concerns molecular entities containing covalent bonds that may form and break reversibility, so as to allow a continuous modification in constitution by reorganization and exchange of building blocks. These features define a *Constitutional Dynamic Chemistry* (CDC) on both the molecular and supramolecular levels. One may define *constitutional dynamic materials*, as materials whose components are linked through reversible covalent or non-covalent connections and which may thus undergo constitutional variation, i.e. change in constitution by assembly/deassembly processes in a given set of conditions. Because of their intrinsic ability to exchange, incorporate and rearrange their components, they may in principle select them in response to external stimuli or environmental factors and therefore behave as *adaptive materials* of either molecular or supramolecular nature.

Applying these considerations to polymer chemistry leads to the definition of *constitutionally dynamic polymers*, DYNAMERS, of both molecular and supramolecular types, possessing the capacity of adaptation by association/growth/dissociation sequences. *Supramolecular materials*, in particular *supramolecular polymers* may be generated by the polyassociation of components/monomers interconnected through complementary recognition groups. *Dynamic covalent polymers* result from polycondensation via reversible chemical reactions. They may undergo modifications of their properties (mechanical, optical, ect.) via incorporation, exchange and recombination of their monomeric components. These features give access to higher levels of behavior such as healing and adaptability in response to external stimuli (heat, light, medium, chemical additives, etc.). CDC introduces a paradigm shift into the chemistry of materials and opens new perspectives in materials science. A rich variety of novel architectures, processes and properties may be expected to result from the blending of supramolecular and molecular dynamic chemistry with materials chemistry, opening perspectives towards *adaptive materials and technologies*.

PL 02

Soft Matter-Hard Matter Synergy for Flexible Electronics and Solar Cells <u>Tobin Jay Marks</u>

Department of Chemistry, Argonne-Northwestern Solar Energy Research Center, and the Materials Research Center Northwestern University, Evanston IL USA

This lecture focuses on the challenging understanding-based design, creation, and realization of new materials combinations for creating unconventional, flexible electronic circuitry and third-generation solar cells. Fabrication methodologies include high-throughput, large-area, high-resolution printing techniques. Materials design issues for electronics include: 1. Rational design of high-mobility p- and n-type organic semiconductors for organic CMOS, 2. High-*k* nanodielectrics enabling ultra-large capacitance, low leakage, high breakdown fields, minimal trapped interfacial charge, and radiation hardness, 3. Polycrystalline and amorphous oxides for transparent and mechanically flexible electronics, 4. Combining these enabling materials sets to fabricate high-performance thin-film transistor circuitries. Materials design issues for photovoltaics build upon the above work and include: 1. Tailored nanolayers to modulate charge transport across hard matter-soft matter interfaces in diverse solar cells, 2. Controlled exciton and carrier generation at active layer donor-acceptor interfaces, 4. Transparent, flexible oxide charge-filtering interfacial layers and electrodes with enhanced properties. In both areas, the symbiosis of green materials synthesis, computational modeling and simulation, and materials characterization over multiple length scales are central.

PL 03 Materials for Sustainable Energy Sossina Haile

Northwestern University (Materials Science and Engineering, Evanston, IL, USA) *Email: sossina.haile@northwestern.edu*

Perhaps the greatest challenge facing our planet is sustainable energy. Sunlight delivers many more times the energy used by modern society, and thus the challenge is in the development of cost-effective means for storing that energy for on-demand utilization. Hydrogen is an attractive candidate for solar energy storage, and fuel cells, with their high efficiencies and zero emissions, are an attractive means for converting the chemical energy of hydrogen into electricity. We describe here recent breakthroughs in the materials for two technologies relevant to sustainable energy. In the area of solar-driven thermochemical hydrogen production, we show that ceria (CeO_{2+2}) and its doped derivatives display exceptional kinetics for hydrogen kinetics. In the realm of fuel cells, we show that the double perovskite $PrBa_{0.5}Sr_{0.5}Co_{1.5}Fe_{0.5}O_{6+2}$ is highly effective for oxygen reduction in the cathodes of fuel cells based on proton conducting oxides. Such breakthroughs are essential for bringing a sustainable energy future to realization.

Keywords: energy, water-splitting, fuel cell, electrocatalysis, hydrogen

PL 04

Global Opportunities in Nanoscience and Nanotechnology Paul Weiss

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Two seemingly conflicting trends in nanoscience and nanotechnology are our increasing ability to reach the limits of atomically precise structures and our growing understanding of the importance of heterogeneity in the structure and function of molecules and nanoscale assemblies. By having developed the "eyes" to see, to record spectra, and to measure function at the nanoscale, we have been able to fabricate structures with precision as well as to understand the important and intrinsic heterogeneity of function found in these assemblies. I will discuss the challenges, opportunities, and consequences of pursuing strategies to address both precision on the one hand and heterogeneity on the other. In our laboratories, we are taking the first steps to exploit precise assembly to optimize properties such as perfect electronic contacts in materials. We are also developing the means to make tens to hundreds of thousands of independent multimodal nanoscale measurements in order to understand the variations in structure and function that have previously been inaccessible in both synthetic and biological systems. Another outcome of the development of our field has been our ability to communicate across fields. This skill that we develop in our students and colleagues has enhanced and accelerated the impact of nanoscience and nanotechnology on other fields, such as neuroscience and the microbiome. I will discuss the opportunities presented by these entanglements and give recent examples of advances enabled by nanoscience and nanotechnology.

Keywords: nanoscience, nanotechnology, heterogeneity, contacts, interfaces

PL 05 A fantastic personal materials story Nelson Torto

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This plenary lecture will relate my life story in material science research that started in 1991 as part of my Hons project at the University of Manchester Institute of Science Technology (UMIST), where I had the opportunity to collaborate with ICI in designing and optimizing a gold based electrochemical detector for saccharides, under the guidance of Peter Fielden. The second phase of my material story evolved at Lund University, Sweden where I worked with the first two commercially available gold based electrochemical detectors (from Dionex and HP). At Lund University, with the talented Tautgirdas Ruzgas, we had fun when we collaborated to fundamentally investigate the use of copper as a possible electrode material in alkaline media. Because of the anticipated application of the electrode material, we also looked into in-situ sampling and sample clean-up for monitoring of enzymic broths with microdialysis and thus found deep interest in polymeric material for hollow fibres. We found the interaction of enzymes with native polysulfone membranes as well as modified polysulfone with PEG-PEI to be fascinating as possible reactors and in-situ devices. The third phase of the work was at the University of Botswana where we tried to maximize hollow fibre membrane performance for inorganic analytes, with some theoretical studies on inner cannula dimensions impact on microdialysis recovery. The fourth phase was at Rhodes University where the desire was to have complete control of the material characteristics and for that reason, electrospinning was chosen as the mode of material production. We wanted to produce the smallest devices for sample clean-up that would benefit from the larger surface area afforded by nanomaterial and tailored molecular imprinted polymers. The large surface area, when functionalized with various ligands, was found to be very efficient in the extraction of various metals. Inspired by filter paper based diagnostic approaches, we started looking at how we could optimize nanoparticle-analyte interactions to ensure that we maximize benefit from phase changes that would produce characteristic and distinct colours. Having realized the potential that electrospun materials presented, the setting-up of BITRI presented another phase where diagnostics and other applications were seen to be the most cost-effective way of producing 21st century products. The talk will conclude by giving a perspective of how I see material, through material science research, would impact Africa in my current pan African role.

KEYNOTE LECTURES

HK 01

Neurotransmitter Sensing via Aptamer-Field-Effect Transistors

Nako Nakatsuka, Kyung-Ae Yang, Kevin Cheung, Chuanzhen Zhao, Leonardo Scarabelli, Liv Heidenreich, Brenda Huang, Peter Sun, Olena Lukoyanova, Yang Yang, Harold Monbouquette, Paul S. Weiss, Milan N. Stojanović, <u>Anne M. Andrews</u>

Measurements of neurochemicals in the extracellular space are limited by combinations of poor chemical, spatial, and temporal resolution. Brain chemistries, therefore, are unable to be investigated dynamically, particularly at the level of neural circuits and across numerous signaling molecules. To understand neural signaling at scales pertinent to encoded information, micro- to nanoscale sensors are needed for multiplexed, highly selective readouts of extracellular neurotransmitter concentrations with sub-second response times. We have designed, developed, and tested sensors that are approaching these critical attributes. Neurotransmitter recognition is by oligonucleotide receptors (aptamers) linked to field-effect transistor (FET) arrays for electronic transduction of reversible binding events *via* conductance changes. For example, using aptamer-FETs, we have selectively detected serotonin and dopamine over five orders of magnitude with fM detection limits in artificial cerebrospinal fluid. Serotonin was measured in brain tissue at physiological concentrations. Currently, we are investigating and tuning temporal resolution of aptamer-functionalized FETs using microfluidics. We are investigating the impact of different surfaces chemistries on sensitivity and biofouling. We are also lithographically fabricating FETs on silicon microprobes for *in vivo* testing. Beyond serotonin and dopamine, we are developing sensors for a broad array of monoamine, amino acid, and peptide neurotransmitters.

HK 02 Biopolymers in 2D, 2.5D and 3D scaffolds for tissue engineering Archana Bhaw-Luximon

Biomaterials, Drug Delivery and Nanotechnology Unit, Center for Biomedical and Biomaterials Research, MSIRI Building, University of Mauritius, Réduit, Mauritius Email: abluximon@gmail.com, <u>a.luximon@uom.ac.mu</u>

Both the healing of diabetic wounds and osteodegenerative diseases associated with the ageing population have impacts on health, social and economic systems. The worldwide trend during the past 30 years has been to look at the use of tissue engineered products which not only provide more efficient healing but also allows the application of personalized medicine and thus improves quality of life. Tissue engineered (TE) scaffolds take into account cell biology, biodegradability, material mechanical properties and biomolecules. The success of TE is highly dependent on the scaffold and hence, much attention has been devoted towards their design and fabrication. The trend nowadays is moving towards the use of naturally derived materials for scaffold fabrication. Indeed, biomaterials have been shown to lead to better cellular attachment, proliferation and differentiation. Moreover, they lead to minimal inflammatory reactions when implanted *in vivo*. Bio-inspired hierarchically structured scaffolds englobing new hybrids 2D (flat), 2.5D (structured surfaces/fibers on thin hydrogel layers) and 3D (composite materials) have the capacity to provide the correct bio-milieu for cells and subsequently tissues to evolve and regenerate. We will here present our work on the efficacy of biopolymers in 2D and 3D scaffolds for tissue regeneration.

Keywords: biopolymers, nanofibers, scaffolds, hydrogels, tissue engineering

HK 03

Engineering Approaches to Combat Infectious Diseases: An Example of Broad-Spectrum Antiviral Peptides

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Viral infections are a leading cause of global morbidity and mortality that urgently need effective therapeutic strategies. While there have been important advances in antiviral drug development over the past few decades, there remain major challenges associated with the large number of emerging and re-emerging viruses as well as with the rise of drug-resistant virus strains. Developing broad-spectrum antiviral strategies that work against multiple viruses is a high priority to counter emerging viral threats. One promising strategy involves utilizing antiviral agents that target the lipid membrane surrounding a wide range of enveloped viruses such as Zika (ZIKV), Dengue (DENV), and Ebola. Unlike other antiviral targets, the lipid envelope is derived from host cell membranes and there is a high barrier to the emergence of drugresistant virus strains. In this talk, I will present ongoing work to develop a membrane-active peptide that exhibits broadspectrum antiviral activity against medically important viruses by selectively destabilizing high-curvature viral membranes. By utilizing biophysical assays, we have characterized the mechanism of action of drug candidates down to the single-virus particle level with real-time measurement readouts. Based on these characterization efforts, we have identified a lead peptide drug candidate that exhibits potent, in vitro antiviral activity against ZIKV and DENV (all four serotypes) at nanomolar concentrations whereas it is nontoxic to mammalian cells at 1000-fold higher concentrations. The therapeutic efficacy of the peptide was also evaluated in a lethal ZIKV mouse model and treatment started three days after infection. Therapeutic administration of the peptide not only significantly reduced mortality, clinical symptoms, viremia, and inflammation, but also prevented neurodegeneration and brain damage. Furthermore, in a humanized mouse model of DENV infection, peptide treatment reduced viremia levels in vivo to nearly undetectable levels. Other arboviruses as well as filoviruses have also proven to be susceptible to this targeting strategy. Looking forward, our findings support that selective targeting of viral membranes holds great potential for combing emerging viral threats, including ZIKV and beyond.

HK 04

Organic bioelectronics for bio-chemical detections at ultra-low detection limits

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Counting the molecules present in a solution instead of assaying its concentration is the ultimate and visionary goal in chemical analysis. Its actuation however, necessarily requires reliable technologies that can "count" the molecules one by one. Such an approach would enable not only fundamental understanding of subtle effects in an affinity interaction likely hidden in ensemble measurements, but also it would pave the way to striking applications. Indeed, proteins and biomolecules detection at the physical limit are foreseen to generate ground-breaking technological fallouts such as for instance, label-free biosensors endowed with high selectivity as well as sub-femtomolar (10⁻¹⁵ M, fM) sensitivity for non-invasive label-free quantitative analysis of pathogens or diseases' markers in bio-fluids such as saliva or tears. The present lecture thus aims at presenting an overview on the challenges and the exciting perspectives that are associated with the quantification of ultra-low concentrations of proteins. An outlook on the extremely high performance level of millimetresize organic bioelectronic sensors integrating a trillion of capturing molecules, will be provided showing that sub-fM detection limits can be reliably reached. As cases of studies, the selective and ultra-sensitive assay of immunoglobulins and C-reactive protein in saliva will be discussed. The organic bioelectronic transistors used are mm-size, low-cost and are operated at physiologically relevant conditions as well as in human saliva setting the ground for a revolution in immunoassay for early bio-markers detection.

Keywords: organic electronics, bioelectronics, sensing devices

HK 05 Engineering Materials for Medical Imaging and Therapy Naomi Matsuura

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Medical imaging is a fundamental tool in medicine. The practice of medical imaging is customarily associated with clinical medicine and its essential role in diagnosing disease in sick patients. In reality, at its core, medical imaging is an inherently interdisciplinary field, connecting medicine, the natural sciences, technology and engineering. In parallel with the development of improved imaging systems and techniques, there is increasing interest in designing new classes of materials that can be used for both imaging and therapy once inside a patient. A new opportunity in materials science is the development of new biomaterials that can be activated *in situ* by medical imaging radiation under image guidance to treat specific diseases, such as cancer or heart disease. In this talk, the application of materials research in the design of new and useful contrast materials for medical imaging in the climate of ever-increasing specialization in both radiology and the physical sciences will be discussed. Challenges in designing new materials for *in vivo* imaging will be introduced and a template for how such materials can be more efficiently designed in the future will be proposed. Specific examples of new activated contrast materials will be given, emphasizing the use of perfluorocarbon bubbles, droplets and nanoparticles as multifunctional contrast agents for ultrasound imaging and therapy applications.

Keywords: medical imaging, cancer, contrast materials, colloids

HK 06 Imitating Cartilage with Polymers Nicholas Spencer

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While humans lubricate their machines with oil, the lubricating mechanisms to be found in nature are all water based, and generally involve sugar units in brush-like configurations, supported on soft substrates. Cartilage is an example of such a system. This combination of brushes and gels appears to be an effective one for the establishment of low-friction sliding with low wear. While it is possible to imitate such structures with synthetic polymers, and achieve low coefficients of friction, the tribological and mechanical investigation of these systems, both natural and synthetic, presents a number of technical challenges. In our laboratory, we are synthesizing a range of synthetic brush-gel systems, mostly by atom-transfer radical polymerization, and investigating these by means of colloidal-probe atomic force microscopy.

Keywords: Cartilage, Lubrication, Polymer Brushes, Gels

HK 07 Emerging biomaterials for complex applications in medical surgery Patrick Sharrock

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Bone grafts are the best solution for orthopedic surgeons in need of bone replacement materials for their patients. It has been commonly termed as « the gold standard », enven if many problems still arise due to sterilisation and availability in the operating room. Synthetic bone also termed « bone substitute» is an example of a class of biomaterials with widespread availability in sterilised form. Such biomaterials were described many years ago and current research tends to make more complex and bioactive materials. We present results descibing how to make a bone substitute material with properties analogous to real bone. This calcium-phosphate (hydroxyapatite) is simple to make and much simpler than recently described printed ceramics or other recent advances in manufacturing methods. A composite material made with hydroxyapatite and hydrolysed collagen has mechanical strength and some elasticity analogous to real bone. Production of such artificial materials can be achieved in Africa and made available to all.

Keywords: bone grafts, hydroxyapatite- collagen composite

HK 08 The Importance of HIV and TB Genetic Amplification in the Scaling Up of National AIDS and TB Treatment Programs in Africa Richard Marlink

Crystalline and Vitreous Metal Phosphates Synthesis, Structural Characterizations and Properties Abdelaziz E.L. Jazouli

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Metal phosphates in both crystalline and glassy forms are extensively studied for their applications in renewable energy, biomedical engineering, and environmental remediation. They can be used as cathodes in lithium ion batteries, as lasers and Light Emitting Diodes (LEDs) components, as sunscreens for UV radiation absorption, as pigments, as biomaterials, and last but not less, as hosts for nuclear wastes. Phosphate glasses possess a series of interesting properties such as low glass transition temperature (T_g) and low melting temperature, in comparison with silicate glasses. The diverse properties and applications of phosphates depend on their structure, which is based on [PO₄] tetrahedra. These tetrahedra can be isolated or connected to each other by sharing corners to form condensed phosphates. To illustrate the relationships between structure and properties of phosphates, this presentation will focus on examples of compounds in which [PO₄] tetrahedra are connected with [MO_n] polyhedra (M is a metal and n its coordination number). These materials were obtained as microcrystalline powders, single crystals and glasses. They have been characterized by X-ray and neutron diffraction, thermal analysis (DSC/DTA-TGA), and by EPR, NMR, Raman, infrared and UV-Visible spectroscopies. Electrical, optical and magnetic properties of these materials will be discussed.

Keywords: Phosphates, Glasses, Synthesis, Structure, Properties

EK 02 Porous Structured Wide Bandgap Semiconductors and Light Harvesting Materials for Solar Cell Applications

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Wide bandgap semiconductors have a lot of interesting practical applications in devices such as solar cells, light emitting diodes (LEDs), surface acoustic wave (SAW) etc. In the porous state, wide bandgap semiconductors usually have high specific surface area and pore volumes to accommodate other materials. In the case of dye-sensitized solar cells for example, they are used as the photoelectrode and when coated with a thin layer of dye, can absorb photons from sunlight to start the process of converting sunlight to electricity. In this presentation, preparation and characterization of porous wide bandgap semiconductors such as titanium dioxide, zinc oxide and tin oxide and their role as important components in dye-sensitized solar cells will be discussed. Also, I will give brief description of the working mechanism of the spray pyrolysis deposition system and explain why it is very useful in preparing different porous structured materials. I would also describe certain metal-free organic complex dyes, their properties, advantages over metal-based organic complex dyes, their light harvesting capabilities and finally their combination with different porous wide bandgap semiconductors in the construction of dye-sensitized solar cells.

Keywords: Bandgap, Semiconductors, Spray deposition, dyes, solar cells

EK 03 Advanced Nanofunctional Materials for Li-ion Batteries Boppana V.R. Chowdari

Surface Organometallic Chemistry on MOFs and inorganic oxides for CO₂ and N₂ reduction: *en route* to renewable energies storage

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Partial replacement of fossil-fuel by renewable energy is a central approach toward global carbon footprint reduction. CO_2 , N_2 and biomass can be key vector molecules to enable such renewable energy insertion in the value chain of process industry. A frontier in catalysis connected with this challenge is the development robust and stable solid catalysts which can be integrated in 3D devices capable of harvesting renewable energy (be it a "green electron" or photon) to perform the targeted reductions. Mono-metallic atomically precise systems are emerging which contribute to such approach. Some recent research achievements around N_2 activation, CO_2 catalytic reduction or biomass conversion by single-atom catalytic centers developed by surface organometallic chemistry will be presented here. Among them, two recent examples based on the integration of well-defined rhodium-based catalytic system in MOF and in microporous-based material for CO_2 reduction, with formate as the sole carbon-containing product (Figure 1), which result more stable and selective than their homogenous counterpart while preserving the predictive structure-activity correlation known for the metal complexes in solution. MOF can also be interesting mediators for the electroreduction of gas phase CO_2 at carbon based cathodes (see Figure 2).



Figure 1. MOF-based catalytic system containing Cp*Rh@UiO-67 (MOF structure UiO-67 shown in green) for the photocatalytic-reduction of CO₂ to formate



Figure 2. a) Schematic representation of cathodic compartment for CO₂ electroreduction by Pt-doped Carbon nanotube (CNT) whose faradaic efficiency is increased by the presence of a MOF layer over the gas diffusion layer, GDL. b) and c) TEM images of SIM-1 crystallites grown on the GDL.

Keywords: Single-atom catalysts, MOFs, electro or photo - reduction of CO₂ and N₂, surface organometallic chemistry

Metal-Organic Framework-based Materials for Adsorptive Hydrogen Storage

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One of the key challenges facing the realization of the Hydrogen Economy is the lack of safe, reliable and efficient hydrogen storage systems. Metal-organic frameworks (MOFs) have continued to receive intense interest over the years for a variety of applications due to their remarkable properties. They possess low weight, exceptionally high surface areas, large free volumes, and tunable pore sizes and functionalities, which make them very attractive for hydrogen storage applications. These properties set MOFs apart from other porous materials like zeolites, polymers and carbon nanostructures. At the material-level many studies have revealed the potential of MOFs for adsorptive hydrogen storage. However, for MOF materials to be applicable at a system-level, they need to undergo further processing since most of the known MOF materials are synthesized as fine powder with small crystals. In order to have substantial capacity as well as acquire desirable properties for practical H₂ storage, MOFs must be capable of being shaped into suitable structures. This presentation will focus on our work on the development of Cr- and Zr-based MOFs, and their composites for hydrogen storage. The employment of electrospinning and compaction in the shaping of Cr-MOF and Zr-MOF powders to develop unique MOF/nanofiber composites will be reported, together with an assessment of the composites gas adsorption properties.

Keywords: Metal-organic frameworks; Hydrogen storage; MOF composites

EK 06 Microwave and Fluorination Treatments for Enhanced Electrochemistry of P2-type Na_{0.67}[Mg_{0.28}Mn_{0.72}]O₂ Cathode Material for Sodium-ion Batteries Kenneth I. Ozoemena^{1,*}, Funeka P. Nkosi^{1,2}, Kumar Raju², Nithya Palaniyandy²

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Sodium-ion batteries (SIBs) have begun to attract research attention as one of the next-generation energy storage system and as the most viable alternative to lithium-ion batteries (LIBs) for stationary or grid-scale electricity storage applications. Advantageously, sodium is cheap and abundant as it is the 4th most abundant element in the earth's crust and is uniformly distributed around the world. SIBs also have high voltage, high energy density and long cycle life. The cathode materials for SIBs include layered oxides, notably layered P2-type manganese oxide (MnO2)-based materials. Mn is naturally abundant, and P2-type MnO2-based materials provide large tunnels for sodiation and de-sodiation processes. Sodium magnesium manganese oxide, Na0.67Mg0.28Mn0.72O2, abbreviated herein simply as NaMgMnO, is well known as high-volumetric capacity/energy cathode material for sodium-ion batteries. One of the problems confronting the commercial utilization of NaMgMnO is poor cycling stability or capacity fade. As part of our ongoing research on microwave-assisted synthesis for cathode materials for LIBs and SIBs, we have explored microwave irradiation and fluorination treatments as part of the synthesis strategy to improve the cycling performance of NaMnMgO. In this presentation, we will show for the first time how both treatment processes have been able to tune the physico-chemical properties of the NaMnMgO for improved electrochemistry (such as coulombic efficiency, capacity retention, cycling cyclability and interfacial impedance). The results clearly indicate the synergy offered by the combined microwave irradiation and fluorination processes in suppressing P2-O2 phase transformation process and the Mn³⁺induced Jahn-Teller distortion effect.

1D, 2D, and 3D Electro-fabrication of Nanofiber-based Devices for Flexible Energy Storage Applications <u>Meifang Zhu</u>

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The key pressing world issues that can be solved by science are energy, water, health and environment. In the last decade we have witnessed the growing energy demand which has greatly affected the quality of water, health and environment especially in regions where raw materials are harvested for example in Africa in the pursuit to provide solutions. To curb the related problems, various novel nanotechnologies utilization to fabricate various materials in 1D, 2D and 3D morphologies have been devised. Amongst such techniques, the most commonly used nanofabrication techniques are electrospinning and electrospraying owing to their ease, scalability, affordability and capability to provide materials with unique and boundless properties especially for energy storage applications. This current presentation will provide an insight in ways to electro-fabricate materials with 1D, 2D, and 3D morphologies as the next generation and alternative solutions to flexible energy storage. Nanofiber-based electroactive nanostructures produced via proven techniques of electrospinning/electrospraying possess great porosity, better ion conductivity, high chemical reactivity, high surface area, low density, as well as favorable light weight compared to their bulk counterparts. So, when research is focused to this synthetic method, better properties and performance are guaranteed with wide industrial applications.

Keywords: Nanofiber, Energy storage, Electro-fabrication

EK 08 Development of Advanced Semiconductor Materials and Devices for Next Generation Photovoltaics: Opportunities and Challenges

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Renewable energy production is a key component in the drive towards a safe, secure energy supply for future low-carbon economies. Using energy from the sun to generate electricity provides a sustainable source of free, abundant, safe, clean energy, without use of any fossil fuels and without waste or pollution. Solar cells (photovoltaic cells) are made of semiconductor materials that convert energy from the sun directly into electrical energy. Sunlight consists of a spectrum of different wavelengths (colours) of light, each corresponding to a different energy level. Semiconductor materials can only convert sunlight of specific wavelengths and energy into electrical energy. Remaining energy from the sun is lost. Existing semiconductors cannot utilise the entire spectrum distribution of sunlight. The strategy to increase the efficiency of solar cells is to use semiconductors optimised for different wavelength ranges of the spectrum. Existing 'three junction' solar cells, which utilise three different semiconductors, are capable of converting sunlight from three regions of the spectrum into electrical energy. The drawback is that state of the art solar cells currently only convert 33% of solar energy into electricity. There is a great interest worldwide into developing innovative semiconductor materials capable of converting sunlight from a fourth specific portion of the solar spectrum into electrical energy. Retrofitting this fourth generation material onto current solar cells should significantly improve solar cell efficiency to >60%. Currently a wide range of semiconductors is explored for their potential use in photovoltaic applications. However, solar cells are already an important part of our lives. The simplest systems power many of the small calculators and wristwatches. The complicated systems provide electricity for pumping water, powering communications equipment, and even lighting our homes and running our appliances. With the growth of the satellite industry and the increase of power requirements, larger solar arrays are needed to produce the required power. The familiar wings of most modern satellites are made of solar arrays. In this talk, I will give an overview of the principles of solar cells, the properties of semiconductors suitable for solar cells, and some selected recent achievements in III-V solar cells.

EK 09 Energy Storage for the Electric Grid – MegaWatts from picoWatts Sean Hearne

Center for Integrated Nanotechnologies, Sandia National Laboratories, Albuquerque, NM

The rapid expansion of non-dispatchable renewable generation onto the US electric grid is driving the need for new grid energy storage options. The impetus for this need is largely based on the variable nature of renewable energy, which can cause instabilities in power delivery and directly impact our daily lives (e.g. our ability to watch Netflix). However, the deployment of energy storage technologies is hampered by high initial cost, often inadequate service lifetimes, and the low monetary value of the services provided. In this presentation, we will discuss the current state of drivers for the utilization of grid energy storage and dive into a few specific examples of how nano-science is being used to understand and control degradation in Li-ion batteries. This work was performed, in part, at the Center for Integrated Nanotechnologies, an Office of Science User Facility operated for the U.S. Department of Energy (DOE) Office of Science. Sandia National Laboratories is a multi-mission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA-0003525.

EK 10 The Role of Structural Water in Electrochemical Energy Storage of Tungsten Oxides <u>Veronica Augustyn</u>

Dept. of Materials Science & Engineering, North Carolina State University

Nanoconfined fluids in materials, such as interlayer structural water, could lead to new mechanisms of electrochemical energy storage with significantly enhanced kinetics. Hydrated tungsten oxides are model materials for the systematic investigation of the effect of structural water in electrochemical energy storage because of their stability in acidic and non-aqueous electrolytes, reversible redox, and multiple hydrated phases. Our results show that hydrated tungsten oxide exhibits surface-limited (pseudocapacitive) kinetics for proton intercalation even with high mass loadings and large particle sizes, which leads to high power capability. On the other hand, the anhydrous tungsten oxide exhibits primarily semi-infinite diffusion-controlled kinetics, typical of battery materials. With *in operando* atomic force microscopy, it is possible to track electrode height changes on timescales of a few seconds and with sub-Ångstrom resolution. Our results on hydrated and anhydrous tungsten oxides show a difference in the structural response of both materials as a function of potential and sweep rate. These results ultimately demonstrate fundamental differences in the structural response of pseudocapacitive, hydrated layered oxides and battery-type oxides that both store charge via intercalation reactions and exhibit the same surface area and morphology.

Keywords: transition metal oxides, layered oxides, energy storage, electrochemistry

Laser-Produced Sm_{1-x}Nd_xNiO₃ Plasma Dynamic Through Langmuir Probe and ICCD Imaging Combined Analysis and Their Correlations to Films Properties <u>Balla D. Ngom</u>

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We report on the presence of an interesting cross-correlation among the pulsed laser deposition (PLD) thin films parameters, which are usually overlooked in the usual empirical approach used by PLD growers. The fast intensifiedcharge-coupled-device (ICCD) photography imaging and Langmuir probe studies of the plasma generated by the KrF excimer laser ablation of Sm₁- xNd_xNiO₃ at x=0.45 in the presence of oxygen background gases at different pressures are reported. The analysis of the oxygen pressure dependence of the ion yield points out to four different regimes. More accurately, the specific ionic current shows a first drop at about 2.10^{-2} mbar corresponding to the appearance of two peaks in the profile of the ionic signal. Likewise, this pressure marks the early stage of the plume splitting into two prominent components as observed by the ICCD imaging. Below 2.10⁻² mbar, the dynamic of the plume is directive (1D), while a quasistable behavior on the ionic signal is observed. In the 0.2- to 0.5-mbar region, a quasi-stationary regime is obtained. More accurately, both the ionic yield and the plume stopping distance vary very slowly in such pressures range. Above 0.5 mbar, the ionic yield is altered again corresponding to the appearance of the diffusion regime. At a pressure of 1.5 mbar we observe a second appearance of an ionic signal peak. A correlation between the results obtained by Langmuir probe and ICCD imaging is made, presented, and discussed within this contribution. The experimentally determined behaviors are compared with the predictions of an analytical model, which gives a complete description of the expansion of the plume and with some recent results reported in the literature. Evidence of the strong influence of the expansion plasma regime on the final thin films properties, was found, which showed that it is not simply related to the overall reactive gas content. Our findings demonstrate that the optimization of the pulsed laser deposition parameters, such as gas pressure and target substrate distance, should be performed also taking into account the chemical pressure induced by the substrate nature. The analysis of the experimental results allowed us to estimate the average deposition oxygen pressure for Sm_{0.55}Nd_{0.45}NiO₃ in the typical range used for Pulsed Laser Deposition (PLD) of complex oxides.

NK 02

Mulling over Emulsions: Molecular Assembly at Nano emulsion Surfaces Geraldine Richmond

NK 03

Nonspherical Colloidal Nanoparticles for Broadband Plasmonics

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Near field techniques, such as surface enhanced Raman spectroscopy (SERS), rely on the ability of plasmonic nanoparticles to induce localized electromagnetic field enhancements in close proximity to the metallic surface. The possibility of achieving SERS signal enhancements high enough to enable sensitive identification of analytes down to the single molecule level depends on the presence of the so-called "hot spots", which can be located at the vertices, edges, or crevices in isolated nanoparticles or at narrow junctions between assembled nanoparticles. In turn, the presence of finely tunable hot spots correlates to the possibility of applying SERS as a reliable spectroscopic technique in the analytical and biomedical fields. Our group has worked for several years on the implementation of SERS sensing substrates and imaging tags, in which gold nanostars have demonstrated to be excellent substrates. However, bottom-up synthetic protocols for gold nanostars are hampered by lack of monodispersity and batch-to-batch reproducibility, and by the difficulty of quantitatively determining relevant physical and optical properties due to the complex nanoparticle morphology. For these reasons, we have initiated a combined experimental and computational effort that has enabled us not only to determine surface area, volume, and extinction coefficients of gold nanostars, but has also yielded a new synthetic protocol for the synthesis of nanostars with high monodispersity and reproducibility and localized surface

plasmon resonances tunable between 600 and 2000 nm. Based on our computational work, these particles promise to become interesting testbeds for the study of the plasmonic properties of highly anisotropic colloidal nanomaterials. In the final part of my talk, I will also present some interesting applications of these nanoparticles for SERS and beyond.

Keywords: gold nanostars, plasmonics, colloidal synthesis, SERS, finite element modeling

NK 04

Metal and Semiconductor Nanoparticles and their Polymer Fibres

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Quantum dots (QDs) are semiconductor nano-particles, which have many unique properties and show interesting phenomena, such as size dependent emission wavelength, narrow emission peak and broad excitation range. QDs have been studied for almost three decades and are nano-crystals in which excitons are confined in all three spatial dimensions. The confinement can be realized by fabricating the semiconductor in very small size, typically several hundred to thousands of atoms per particle. Due to quantum confinement effects, QDs act like artificial atoms, showing controllable discrete energy levels. QDs were first fabricated in the 80's by Louis E. Brus and the unique properties of these special nano-structures attracted interest from many fields. CdSe is a binary semiconducting material of cadmium and selenium. CdSe is being developed in research for use in opto-electronic devices, nanosensing, and biomedical imaging. This presentation will be focused on CdSe and other metal based chalcogenides such as AgSe, CuSe and Ag. Various methods have been explored in making metal chalcogenide nanoparticles and for example, CdSe nanoparticles are prepared using a solution of cadmium and selenide under controlled conditions. The incorporation of nanoparticles prepared into the polymer PMMA using electrospinning technique in order to make polymer fibre. Variation of percentages of CdSe nanoparticles into the polymer cause coiling of fibres and decreased luminescence intensity. CdSe nanoparticles were also used as core in the synthesis of CdSe/ZnO and CdSe/PbS nanomaterials using thioglycerol, hexadecylamine and trioctylphosphine oxide. The semiconducting, metal nanoparticles and polymer fibres will be discussed for their synthesis and characterization; their properties will be explored from their synthetic conditions.

NK 05

Green bio-synthesis of multifunctional nanoscaled oxides using natural extracts as effective biochelating agents M. Maaza¹⁻²

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Nano-scaled oxides have numerous applications in areas ranging from catalysis, photonics, molecular, energy storage, fuel cells, tunable resonant devices, sensing & antibacterial applications. This is due to an increase in reactivity when compared to their micro-sized counterparts since nanoscaled materials exhibit larger surface-to-volume ratio which provides unsaturated and, thus, more reactive surface atoms. To consider nanoparticles for biological applications, such as drug delivery. The standard physical and chemical methodologies used for the synthesis are either non cost effective or use harsch chemicals and hence generate non green waste byproducts. Green chemistry is the utilisation of a set of principles that reduces or eliminates the use or generation of hazardous substances in the design, manufacture and application of chemical products. *Green Chemistry* is an emerging field, at the frontiers of an interdisciplinary science that attempts to reduce the environmental impact of the chemical enterprise by developing a technology base that is inherently non-toxic to living things and the environment. This contribution reports on the possibility of biosynthesis of several nano-scaled ighly crystalline oxides and their physical properties using natural extracts as effective chelating agents. This includes TCOs, rare earth and PGMs family based oxides.

The importance of nanoarchitecture in advanced high performance heterogeneous catalyst

Mike Scurrell

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Our current lifestyle in the developed countries would not be possible if we did not have access to high performance heterogeneous catalysts. These materials lie at the heart of our industrial processes for oil, petrochemicals, polymers, pharmaceuticals, energy conversion and environmental protection and ever increasing demands are being placed on catalysts for the future. Very high performance heterogenous catalysts will almost always demand that considerable attention is paid to the detailed nanoarchitecture of the solids. This point will be illustrated by several examples, including thermostable gold catalysts for environmental protection, based on the use of nanoflower-structured support decorated with nano-sized metal particles. These materials have greatly improved thermal stabilities against conventional materials and this could see new applications in several areas, especially environmental protection. Catalysts for the decomposition of methane in low carbon footprint conversion of natural gas to electricity can also be improved by incorporation of suitable nanomaterials such as medium and wide-pore zeolites. A further example is provided by photocatalysts for biomass conversion to syngas and hydrogen, where at the nano level the inhibition of charge pair recombination is required for high reaction rates. The devices and procedures available for manipulation of nanoarchitecture include microwave radiation treatment and the use of non-thermal plasmas. The extent to which these approaches can be used in improving solid catalysts will also be discussed.



TEM image of a thermostable Au-rutile nanorod catalyst system active in CO and hydrocarbon oxidation and hydrocarbon-NO reactions.

Keywords: catalysis, nanoarchitecture, energy, environment

NK 07

Delivering Interesting Functional Materials at the Nanoscale using Simple Chemistry

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Metal chalcogenide semiconductor nanocrystals have been identified as an important class of materials due to their applications in emerging technologies. A key objective of many research groups is the fabrication of nanostructures with controlled diameters, aspect ratios and morphologies, which are essential for their applications in electronic devices. The use of metal complexes to prepare metal chalcogenide materials at the nanoscale is a well-established route. The talk will focus on recent work done in my laboratory on the synthesis of semiconductor nanomaterials. I will discuss the recent synthesis of new complexes which have been used to prepare iron, bismuth, antimony and tin chalcogenide nanomaterials. The talk will highlight three major routes, ie. hot injection, aerosol assisted chemical vapour deposition (AACVD) and melt method. Examples of novel ternary materials and 2-D materials will also be highlighted. The lecture will also focus on the use of green materials as capping groups for nanoparticles. An application in drug delivery will also be presented.

Measuring spillover effects using nanoreactors

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Hydrogen spillover is thought to be one of the mechanisms by which a noble metal promoter can enhance the reducibility of a metal oxide. The effect of these noble metals is attributed to their ability to easily dissociate H₂ molecules at low temperatures to hydrogen atoms that are transferred to the metal oxide nanoparticles via a spillover mechanism. In this study Co and Ru nanoparticles were separated by encapsulating the Co nanoparticles inside a mesoporous hollow carbon sphere support (MHCS) while the Ru was exclusively loaded on the outer surface (i.e., Co@MHCS@Ru). Other catalysts, Co/MHCS, and Co@MHCS and promoted CoRu/MHCS and CoRu@MHCS were also prepared. TEM analysis of the materials showed Co₃O₄ particles with an average size between 7.1-7.4 nm and Ru nanoparticle sizes of 2.6 nm with the shell thickness of the MHCS defective carbon between 20-30 nm. By using pulse chemisorption (after reduction at 350 °C), primary hydrogen spillover was invoked to explain the high Co dispersion of CoRu@MHCS in relation to the Co@MHCS@Ru and Co@MHCS dispersion. Using in situ PXRD a secondary hydrogen spillover process over the porous carbon was invoked to explain the complete reduction of the Co₃O₄ on Co@MHCS@Ru when compared to unpromoted Co@MHCS. Finally, the primary spillover effect was revealed to be more favourable than the secondary hydrogen spillover effect. Fischer-Tropsch testing of the catalysts showed that the Fischer-Tropsch activity was proportional to the degree of reduction that increased with the Co-Ru intimate contact. The Ru promoter also enhanced the production of paraffinic products and methane. The study indicates that the use of hollow carbon spheres are readily suited to investigate reactions in which metals can be separated by a carbon layer of varying thickness and with varying functional groups.

Keywords: Spillover effect; Hollow carbon sphere; catalysis; nanoreactor; synthesis

NK 09

Syntheses and characterization of 2D-layered metal chalcogenide nanocrystals for application in chemo-resistive sensors

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Electronic and optical properties of bulk semiconductor surfaces exploited in the design of chemical sensors have been reported to be as a result of the electronic structure of the surface and carrier dynamics associated with the semiconductors [1]. In the nanoscale size regime, the opto-electronic properties can be tuned during synthesis by manipulating the size and the shape of the semiconductor nanocrystals thus making the nanocrystals potential candidates for sensor application. This happens as a consequence of the change in the density of states as a result of spatial confinement [2]. In addition, the nano-size provides the semiconductor nanocrystals with a high surface area which is important for adsorption of the analyte vapour [3]. The process of the analyte detection on the semiconductor surface is usually due to the changes in the band bending or surface recombination velocity caused by the bound species from the analyte-substrate surface states interactions. Therefore, these changes can be used to derive relevant information about the distribution of the density of state in the semiconductor, thus an understanding about the substrate's electronic and optical properties. For instance, a semiconductor might possess a high density of surface states that pins its Fermi level near mid-gap, making it resistant to analyte induced perturbation of electronic properties, and therefore, prohibiting analyte detection. In contrast to such a pinned system, a distribution of surface states that is substantially perturbed by interaction with adsorbate orbitals can lead to reversible or irreversible changes in opto-electronic properties and allow real-time or integrated sensing to occur [1]. Herein we focus on 2D layered metal (In, Mo, W and Nb) chalcogenides. We look at how different synthetic parameters affect their properties and eventually use them as active layers in chemoresistive sensors.

Keywords: 2D layered materials; nanostructures; metal chalcogenides; chemical sensors

Industrial development of nano-enabled products and technologies: Challenges and Opportunities

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South Africa seeks to advance local value addition of various strategic minerals in order to transform our resource-based comparative advantage into a national competitive advantage. For the past ten years, metallic nanomaterials research in SA received substantial funding and support from the government and small industry. While excellent nanoscience research is ongoing at various universities and science councils, the pace of industrial development for nano-enabled technologies and products require an accelerated effort/strategy in order to make a significant impact. This presentation will highlight the opportunities and challenges associated with the development, industrialisation and commercialisation of metal-based nano-enabled technologies and products for socio-economic benefits.

NK 11 Recent scientific & technological advances: Potential implications for the African continent Solomon Assefa

WK 01

Advances in Photocatalysis: The Ethiopian Experience

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This review briefly describes the developments in photocatalysis research in our laboratory focusing on synthesis, characterization and photocatalytic applications of nanomaterials (doped metal oxides/sulfides, binary/ternary oxide/sulfides heterojunctions, Supported nanocomposite sand Metal Organic Frameworks). Various synthetic approaches and state-of-the art characterization techniques have been employed to fabricate and characterize the as obtained nanoparticles. Photocatalytic application of these materials have been investigated for degradation of model organic/inorganic pollutants making use of a variety of approaches to make the as synthesized materials visible active. We also made domestic research progress on the fabrication of supported ternary systems. Zeolites, polymers, ion exchangers and biomaterials have been used as supports with demonstrated efficiency. Recently, our research group is working on nano-exchangers and metal-organic frameworks for potential application in photocatalysis.

WK 02 To Purify Water with Nanocellulose Benjamin Hsiao

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The fabrication of nanocellulose can be accomplished by chemical and mechanical treatments of any natural biomass, including agricultural waste, weeds and shrubs, where some sources can provide "effortless extractability" with very low energy consumption. Nanofibrous scaffolds have very unique properties including interconnected pores, a very large surface-to-volume ratio and a high capacity for surface modifications, making them ideal candidates for fabrication of high throughput separation membranes (e.g. microfiltration and ultrafiltration) and/or highly efficient sorptive media. Directed water channels in the barrier layer of reverse osmosis and nanofiltration membranes can also be formed through the formation of interface between the nanofibers and barrier layer polymer matrix, while the gap thickness can be regulated by physical interactions or chemical bonding. In the present context, advances in fundamental studies on cellulose microfibrils, the building blocks from the cell wall of any plant, and their interactions with metal ions by means of synchrotron x-ray and neutron techniques have provided us with new insight into the design and fabrication of highly permeable nanofibrous membranes, having a hierarchically tiered structure, that can enable higher flux, higher retention and lower energy consumption water purification. Nanocellulose may serve as a revolutionary platform technology for the design and fabrication of low cost, sustainable and highly efficient filtration and sorptive media.

WK 03 Anti-Bacterial Activity of TiO₂ Nanostructured Materials Darren Sun

Darren Delai Sun, LiLin Zhang, Hong Wei Bai and Zheng Tao Li, School of Civil and Environmentl Engineering, Nangang Technological University, Singapore 639798

TiO₂ is one of the wonder materials that possess extraordinary engineering versatility in terms of nanostructures, shapes and morphology. TiO₂ nanomaterials have shown superior antibacterial capability, it is however still unclear about the dimensional effects on antibacterial mechanisms. It is therefore highly important to carry out studies and investigations on the fundamentals of antibacterial mechanisms and capability of the engineered nanostructured TiO₂ materials (ENMs) – from three aspects 1) the structures of such nanoparticles, rods, tubes, fibres and spheres; 2) sizes/dimeters/length of the ENMs; 3) combined effect due to dimensions and structures. By knowing these, *E. Coli* cells were used as the targeted bacteria of study in this work for its inactivation responses towards the exposure to the as mentioned TiO₂ ENMs. The studies revealed that, the 1D nanotubular TiO₂, being the smallest individual ENMs possessed the highest toxicity towards E. Coli; further studies showed that 3D dendritic nanostructure incorporated with 1D ultrathin TiO₂ nanorods had the highest antibacterial efficiency. Comparative studies have suggested that, the well-engineered 3D TiO₂ nanomaterials (microspheres) with enhanced surface properties such as evenly grown 1D sub-structures were more aggressive than the clustered aggregated 1D nanomaterials. In-depth research concluded that with well controlled nanorods density and length, the integrated 3D ENMs exhibited most efficient antibacterial activities. Such results were crucial information which could benefit the future antibacterial applications and the agent fabrications.

WK 04

Biopolymer Metal Oxide Nanocomposite for Fluoride and Arsenic removal from water: An Invention

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Heavy metal and fluoride contamination in groundwater affects about 150 million people worldwide. In this study we focused on synthesizing biopolymer metal oxide nanocomposite for arsenic (V) and fluoride removal from and antimicrobial activity against *E.coli*. Nanocomposite material was done using SEM, HRTEM, XPS, XRD, BET and FTIR. As(V), AI, Ti, Zr and Fe water samples were analyzed by ICP-MS (Inductively coupled plasma-mass spectrometry). Fluoride level were determined using standard method-Ion-Selective Electrode method. Preliminary results indicate arsenic (V) removal was below the 10 ppb and fluoride less than 1.5 ppm as prescribed by WHO. The removal efficiency was after 60 -70 minutes with a recyclability of 11 cycles. The nanocomposite worked well in all pH ranges 6.5 –8.5. A filter cartridge biopolymer metal oxide nanocomposite constituting of template aluminium homogenized in the aggregated network of chitosan was developed as an adsorbent for fluoride, arsenic, lead and Chromium removal from water with better adsorption limit

Keywords: biopolymer metal oxide nanocomposite; antimicrobial activity

WK 05 The challenge of sustainable potable water supply: Consideration of novel and appropriate technologies

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Lack of safe water, presents a challenge to sustainable living. The United Nations reports that although worldwide "2.6 billion people have gained access to improved drinking water sources since 1990, 663 million people are still without". It is estimated that as many as 40% of the 783 million people of sub-Saharan Africa are under-served with safe water. The consequences are disturbing; "**115 people in Africa die every hour** from diseases linked to poor sanitation, poor hygiene and contaminated water". The need for simple but effective water treatment and sanitation infrastructure cannot be overstated. The impetus of our work is to increase the effectiveness of affordable point-of-use household units in providing health improvements in under-served areas. In this presentation, we will discuss current research in the development of novel materials for application in these household units as well as proven technologies recently introduced commercially. In a novel material under development, we seek to combine TiO₂ semiconductor photocatalysis and anti-microbial nanomaterials to enhance the technological design of Solar Disinfection (SODIS) units, and improve their effectiveness in water treatment and disinfection.

Keywords: Safe-water; Sustainable; Nanomaterials; Solar Disinfection
From curiosity-driven basic research to new insights and improved applications of moringa in water treatment and materials research

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Moringa is a tropical tree known for its wide range of uses. Nearly every part of the tree has socio-economic benefits and hence it is often referred to as the "miracle tree". The presentation will review some of the advances our research has made in the recent years in the cultivation and use of Moringa tree, a natural resource that can easily be grown in Namibia, for its water treatment, medicinal and nutritional properties. For instance, curiosity research about the water treatment properties of seeds has led to the development of a new technology that eliminates the use of chemicals, fully sustainable, cheap and easy-to-use for rural community use. The use of chemicals is normally expensive and has health and environmental effects associated with them. Two prototypes of the water treatment system using Moringa seed powder have been developed. The next prototype to be developed in conjunction with NUST Innovation Design Lab will not use power but solely depend on gravity. The ultimate objective of this research is to create a point-of-use continuousflow water purification device that couples the filtration capabilities of sand and charcoal (both readily available) with the antimicrobial and flocculating properties in a Moringa seed. The Moringa research has recently been extended with the aim of empowering communities in rural areas towards sustainable and environmentally-sound development by facilitating access to improved nutrition, eradicating poverty, hunger and malnutrition, income generation and mitigating effects of climate change through growth, use and advocacy of the Moringa. The effects of climate change include perpetual droughts, famine, crop failure, desertification, food shortages, to mention but a few. The planting of the Moringa tree, can play one important role in mitigating the effects of climate change because it grows fast and well in dry areas. The presentation will also review what is known about this important resource and will further discuss results of some of the studies we have done about this peculiar tree which have been aimed at addressing antimicrobial activity of different parts and the global issue of antibacterial resistance. Combining Moringa extracts and silver nanoparticles (AgNPs) with antibiotics has been found to be a potential method to overcome bacterial drug resistance. The presentation will also show how Moringa seed proteins can be used as a gue to stick particles to solid surfaces.

Coagulation and flocculation are important processes in water treatment system and their primary purpose is to removal of turbidity, caused by suspended particles, from the water. The suspended particles vary considerably in source, composition charge, particle size, shape, and density. Correct application of coagulation and flocculation processes and selection of the coagulants depend upon understanding the interaction between these factors. The structure of flocs has direct relevance to applications. For example, the fractal dimensions of the aggregates of impurities obtained in water treatment has been related to the ease with which sludge can be dewatered. Obviously, the choice of flocculating agent and conditions is of crucial importance when designing a range of processes that are required to produce aggregates. The presentation will show measurements using neutron scattering made on samples of aggregates of polystyrene latex made by addition of salts sodium chloride (NaCl), ferric chloride (FeCl₃) aluminium sulfate (Al₂(SO₄)₃) and protein of Moringa seeds. Flocs resulting from addition of Moringa seed proteins gave high fractal dimension values (tightly packed flocs) as the concentration of particles increased.

Keywords: Antibacterial resistance, Antimicrobial activity, Critical coagulation concentration, flocs, Moringa, Nanoparticles, Polystyrene latex, Water treatment

Lignocellulose-based nanocomposites: synthesis, characterization and possible application as adsorbents in water treatment

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Composite materials based on lignocellulose were prepared, characterised and evaluated as adsorbents for the removal of pollutants (dyes and heavy metals) from aqueous solution. The need to reduce the cost of adsorption technology has led to such investigations seeking the development of low cost adsorbents from renewable resources and adsorbents that can simultaneously remove pollutant mixtures. In this work lignocellulose-montmorillonite nanocomposites were prepared by in situ intercalative polymerisation using silanes. Clinoptilolite was also chemically modified with silanes after removal of impurities by treatment with hydrochloric acid. Dibutyltin dilaurate catalyst was used in subsequent reactions. Both modified lignocellulose and clinoptilolite were reacted at 140°C in DMF to form the Lignocellulose-clinoptilolite composites. Montmorillonite clay was also organic-modified while lignocellulose-montmorillonite was functionalised through esterification to increase hydrophobicity before being evaluated as adsorbents. Characterisation methods used included FT-IR, XRD, BET, TGA, SEM and NMR. The main pollutants removed from solution included Methyl Orange, Cd²⁺, Pb²⁺, 1,10-phenathroline. For the study of competitive adsorption analysis of binary mixtures of methyl orange with Cd²⁺ and methyl orange with Pb²⁺ in aqueous solution were carried out to see the effect of combining organic and inorganic pollutant mixtures. Some kinetic studies were also undertaken and various models suggested for the different processes.

Keywords: adsorbent, siloxane, pollutant, lignocellulose, nanoclay

WK 08

Development of a Laterite Composite for Removal of Fluoride from Borehole Water: Collaboration Research and Educational Experience

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In certain areas of the world, water obtained from boreholes have high fluoride levels due to contamination from geological rock formations. For example in the Bongo District, located in the upper east region of Ghana, some boreholes contain an excess of 3 ppm or more above the World Health Organization (WHO) recommended intake for Fluoride in drinking water, that is 1.5 ppm. Dental and skeletal fluorosis are some of the immediate obvious manifestations of ingestion of excessive fluoride. A survey of scientific literature shows several approaches such as use of hydroxyapatite, bone ash etc. as tested treatment remedies, however this study seeks to find a locally sustainable and cost effect way to eliminate the excessive fluoride from water. In this study, a composite of local laterite activated with alumina was found to increase fluoride uptake and thereby improving the defluoridation to a level at or below the WHO 1.5 ppm. Additionally, studies on two 10-kg configurations of the composite laterite and bio-sand filtration system were tested in columns with: 1) laterite composite column with a bio-sand filter that contained 10:2 laterite to alumina ratio, and 2) 10:0.183 laterite to alumina (or 10:1 laterite to alum) ratio. Column adsorption tests were conducted by passing fluoridespiked water samples at fluoride concentration of 5.02mg/L and 6.4mg/L. SEM micrographs of physically coated lateritealumina composite and chemically coated laterite-alumina composite show an intimate association of elements including Fe, Si, Ti and Al. The EDX spectrum of the composites confirmed higher aluminum content in the composite than that of raw laterite. Overall, the performance of the column with chemically coated alumina was much better than that of the physically coated. In this NSF International Research Experience for Students project, SU students traveled to Kumasi, Ghana and worked with faculty and students at KNUST supported by funding from US National Science Foundation.

Keywords: Fluoride, laterite, alum, alumina, water purification

Photodegradation of Organic Dyes using Cobalt-based metal Organic framework (Zif-67) Catalysts supported on graphene oxide under simulated solar irradiation

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The photocatalytic degradation of methylene blue and methyl orange was achieved under solar light simulated conditions using Zeolitic imidazolate framework-67 (ZIF-67) anchored on graphene oxide (GO) sheets. -The composition, structure and morphology of both the self-standing ZIF-67 and the graphene oxide supported analogue, GO@ZIF-67 composites, were analysed and confirmed using a variety of techniques such as FTIR, BET, SEM, TEM and Zeta potential. The ZIF-67 frameworks structures retained their crystallinity (octahedrals of 300 - 500 nm size) even when supported on GO sheets. ZIF-67 crystals had a high specific surface area *ca*. 1185.1 m² g⁻¹ with a pore volume of 0.0069 m³ g⁻¹ and the pore diameter of 2.6 nm. The GO@ZIF-67 composites exhibited high adsorption for methylene blue (MB) compared to that of methyl orange (MO). The maximum adsorption capacity reached up to 220.00 mg g⁻¹ within 2 h for MO. Further catalytic degradation of the same dyes (MB and MO) showed that degradation efficiency was quantitative for MB and reached a maximum for MO. The GO@ZIF-67_(0.1) composites proved to be the best photocatalyst for MB as compared to the rest of the combinations. The kinetics of the adsorption and photocatalytic processes will be presented and related to the nature of the dyes, i.e. cationic versus anionic.

Keywords: ZIF-67, GO@ZIF-67, adsorption, photocatalytic, methylene blue, methyl orange

WK 10 Synthesis of hybrid nanostructured membranes for use in water purification Sabelo Mhlanga

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Contamination of drinking water sources by pollutants originating from agricultural, industrial and/or anthropogenic activities has been observed in many areas due to escalating industrialization and urbanization, poor sanitation, ineffective water treatment processes, and lack of access to purified water. Pollutants can be predominantly of microbial, organic or inorganic nature, depending on the environment. Studies have been conducted to monitor the quality of water in selected rural communities in Mpumalanga, South Africa and novel hybrid nanostructured membranes and nanofibers have been fabricated and used to remove target pollutants from contaminated water sources. Membrane properties were controlled by adding various nanomaterials such as multi-walled carbon nanotubes, silver, iron and silica nanoparticles, and nanoparticles from leaf extracts in order to obtain high pollutant rejection and water permeation properties as well as low fouling propensities. Unique membranes for use as membrane distillation (MD) membranes and have been fabricated and tested or saline groundwater. The presentation will focus on the sustainable processes used to prepare these nanostructured materials, their characteristic properties and their performance in purifying real water samples.

Keywords: nanofiltration, membranes, nanomaterials, water purification

Zeolites for the purification of water (removal of hardness and heavy metal specifically Cr and Pb)

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Zeolite is inorganic ion exchange used as a suitable low coast and locally available solution for water treatment in many regions of the world. Dissolved calcium and magnesium are the two most common minerals that make water "hard". Cr and Pb are also the common poison metals present in water especially from industrial waste. In this study the hardness of water decreased by 68.6620% by modified natural zeolite. The zeolite A and X synthesized from Ethiopian Kaoline removed Cr and Pb in high percentage. According to the experimental data the optimum condition for lead adsorption with synthesized zeolite Na-X were obtained pH (5, 97.1%), contact time (60 min, 96.2%), adsorbent dosage (0.1 g, 97.0%) and initial concentration (10 mg/L, 96.0%). The % removal of Cr(III) or its adsorption from the synthesized zeolite Na-A at pH 6, adsorbent dose of 0.4 g and time of 10 h removal efficiency were found to be 99.56%.

Keywords: zeolite, natural, water, purification, heavy metal

AK 01 Biowaste as a source for nutriments, micro-elements and sustainable fertilizers (biofertilizers) <u>Ange Nzihou</u>

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Fertilizers need to be produced in a more sustainable and resource-efficient manner to raise crop yields to meet the food demand of a growing population. These products are manufactured using processes based on feedstock such as phosphate rocks using energy intensive processes. The use of biobased fertilizing products from biomass and biowaste increases the sustainability of fertilizing practices and the productivity of the agriculture. Mineral fertilizers represent most of the market value of fertilizers used worldwide. The development of biofertilizers from biowaste and biomass could lead to replace up to 30% of mineral fertilizers in coming years. The use of biofertilizer should be developed because this increases the stable fraction of organic matter in the soil. These fractions are more resistant to decomposition and therefore are crucial for increasing soil carbon sequestration. These fertilizers are expected to show beneficial environmental footprint due to mobilizing side streams and residues within the value chain. Return of biowastes to soil is a step towards more closed to nutrients cycles, greater sustainability, and reduced environmental loads. For their growth, plants need macro elements as N, P, K, carbon (C), Ca, S and Mg, micro elements such as B, Cl, Mn, Fe usually in trace amount. The concentration of species such as heavy metals in the biowaste is the main quality criterion on their utilization as biofertilizers. There is a need to determine the amount, nature and speciation of these elements on the feedstocks and biofertilizers produced to prevent health and agronomical risks. This presentation will cover various biomass and biowaste by-products namely char from thermochemical conversions, compost and digestate and highlights the main issues linked to their use as biofertilizers In a long-term perspective, effects on soil fertility, included storage, turnover od added carbon and nutrients and impacts on soil organisms should be considered.

Keywords: biofertilizers, biowaste, biomass

AK 02

High Throughput Electrospinning/Electrospraying Applications of Interest in Food, Pharma, Biomedicine and Packaging

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Looking genuinely at nature, nanofibers often serve as a basic platform where either organic or inorganic components are built upon. For instance, cellulose nanofibers would represent the building block in plants while collagen nanofibers in the animal body. To follow this extraordinary nature's design, a process that is able to fabricate fiber nanostructures from a variety of materials and mixtures is an indispensable pre-requisite. Control of the nanofibers arrangement is also necessary to optimize such structural requirements. Electrospinning is a physical process used for the formation of ultrathin fibers by subjecting a polymer solution to high electric fields. At a critical high voltage (5-25 kV), the polymer solution droplet at the tip of the needle distorts and forms a Taylor cone to be ejected as a charged polymer jet. This stretches and is accelerated by the electrical field towards a grounded and oppositely-charged collector. As the electrospun jet travels through the electrical field, the solvent completely evaporates while the entanglements of the polymer chains prevent it from breaking up. When the breaking up of the jet is purposely sought, then the process is termed electrospraying and nanoparticles or nanocapsules are formed instead. Thanks to recent innovations in the scaling up of these technologies (see www.bioinicia.com), industrial applications are making their way forward and have become affordable for specialty applications in the biospace. The current paper will highlight some recent advances carried out within our research group in which various applications of the above electro-hydrodynamic processing techniques making use of nanoparticles, biopolymers and biopolymeric blends will be reviewed. These include examples in which new antimicrobial nanostructured fiber mats with strong biocide efficiency were successfully developed, as well as nanostructured systems for bone implant interfaces with significant bioactivity, antiinflamatory and antibiotic properties, novel nanoencapsulation of bioactive food ingredients and also biopackaging nanostructures with high gas barrier and oxygen scavenging capacity.

AK 03

Conversion of Agricultural Waste Streams into Value Added Product

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The unique structural architecture of carbon-based nanoporous structures such as activated carbon (AC) has made activated carbon one of the most viable materials to address current environmental challenges. The highly developed porosity, large surface area, tunable surface chemistry, and high degree of surface reactivity make AC the most widely used adsorbent for the removal of wide variety of organic and inorganic pollutants dissolved in aqueous media or from gaseous environments, as well as the use as electrodes in energy related applications. Traditional feedstocks for AC production include, primarily, mineral carbons, and lignocellulosics from biomass and wood. However, any cheap material, with a high carbon content and low mineral content, can be used as a precursor for the production of AC. Agricultural wastes are proving to be promising precursors for the production of ACs mainly due to their availability, low cost and zero carbon foot print. We present preliminary investigation on utilized mechanical ball milling followed by chemical activation technique to convert agricultural waste (cocoa and coconut husks, palm midribs and calabash) into ultra-high surface area activated carbon suitable for myriads of environmental and energy related applications. Our preliminary investigation indicates about 70% increase in BET surface area with ball milling to as high as ~ 3000 m²/g.

Keywords: agricultural waste streams, activated carbon, chemical activation, specific surface area

MK 01 Translating Africa's comparative advantages in minerals into competitive advantages in materials Francis P. Gudyanga

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Materials derived from minerals are intrinsically linked to all industries across all supply chain stages, and consequently are essential for our way of life. For example, the healthcare sector uses equipment containing high performance magnets made from rare earth elements, electricity distribution relies on pylons and cables constructed of aluminum and copper respectively. The rapid development of hi-tech goods and environmental applications over recent decades has led to shifts in demand patterns for mineral-based materials. The growth in use of flat panel televisions and touch screens is reliant on the supply of indium used in transparent conducting layers. The complexity and sophistication of these products is growing, leading to a corresponding increase in the number of materials used in their production. This is coupled with increasing product complexity, for example a modern mobile phone may contain 500 to 1,000 different components. Exhaust emissions from internal combustion engines are managed through catalytic converters containing platinum group metals. Many wind turbines designs use magnets containing rare earth elements, and solar panels rely on metals such as silicon, tellurium and indium amongst others. Similar cases are seen for electric vehicles and energy efficient lighting. If the quality and way of life is to be maintained and improved, continued access to mineral-based materials is essential. The African continent is richly endowed with these minerals required for modern industry and society. Africa's export-oriented mining and quarrying is driven primarily by the commodity hunger of the world's largest economies. Many African countries are highly and dangerously dependent of such exports. This paper attempts to illustrate how the African countries can leverage on their mineral endowments for their socio-economic developments. The African countries can do this through value addition to, and market influence on, their minerals/metals that are strategic to global economies.

Keywords: Africa's minerals and global economies

MK 02

Mining contribution to the Botswana economy through local content Joseph Ramotshabi

MK 03

Performance of Cement Mortar with waste ground clay brick

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Cement industry consumes a lot of energy and is responsible for more than 5% of total global emissions from industrial sources. An effective way to reduce the impact of cement production on the environment is to use supplementary cementitious materials (SCM) as a partial substitution to cement. The use of SCM in cement for the manufacture of mortar and concrete also reduces the cost and enhance the performance at both fresh and hardened state. In this paper, cement was partially substituted by fines obtained from crushed recycled waste bricks recovered from a brick plant. The level of substitution was either 0%, 5%, 10% or 15% by weight of cement. The results show that cement substitution by brick fines results in a slight loss of workability with the increase of the substitution rate. Substitutions rates of 5% and 10% produced at long-term comparable strength as control mortars. The differential thermal analysis (DTA) and thermos-gravimetric analysis (TGA) results show that the mass loss is more important for mortar with brick powder at 28 and 180 days of age and hence cement hydration improved significantly with different rates of substitutions.

Keywords: cement, waste brick, strength, workability, hydration

MK 04

Minimising the risk of thermally induced cracking in mass concrete structures through suitable materials selection <u>Yunus Ballim</u>

CK 01 Application of Molecular Structure Methods to Materials Problems David S. Perry

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Thin-film solar photovoltaics pose a formidable challenge to computational simulation. The donor and acceptor materials responsible for charge separation are often combined in a bulk heterojunction containing nanoscale domains of the two materials. These interfaces, together with electrode interfaces, will have a major impact on device performance. This talk will address the application of molecular structure methods to the characterization of key interactions within organic polymers used in solar photovoltaics. These results may then be included in the force fields used for molecular dynamics simulations of pure materials, interfaces, and

eventually model devices. After reviewing the computational technologies, opportunities and limitations of molecule-based density functional calculations, the talk will focus on the torsional conformational properties of the conjugated polymers, P3HT and PTB7, which are used as electron-donor materials.

The extended conjugation in these polymers tends to stabilize a coplanar configuration of adjacent ring systems in the polymer chain, whereas steric hindrance tends to stabilize non-coplanar geometries. Multi-dimensional torsional potentials for P3HT and PTB7 will be presented, along with results on the band gaps, the long-chain limit and conjugation length. The evidence points to substantial torsional conformational disorder for these conjugated polymers at the interfaces in practical devices. The implications for materials optimization and device efficiency will be discussed.



Computed torsional potential energy map for a PTB7 oligomer. The angles α and β are the two kinds of dihedral angles between adjacent ring systems. (R. Bhatta, D.S. Perry and M. Tsige, J. Phys. Chem. A **117**, 12628 (2013).) http://dx.doi.org/10.1021/jp409069d

Keywords: solar photovoltaics, poly-(3 hexylthiophene), PTB7, torsional potential, conjugation length

CK 02

Polymer topology in surface absorption of binary blends

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Physical techniques for surface modification of plastics use surface-active agents, which are allowed to selfassemble at the surface. Many techniques, which are important in modern technologies, use polymer blends, and there is considerable interest to understand the extent the composition of the surface layer differs from that in the bulk for molten polymer mixtures. Dynamical and structural properties of polymers in the melt state are strongly influenced by molecular architecture [1-4] and blending polymers with different molecular topologies could be potentially exploited to control interfacial segregation of the polymer film, and to achieve optimal mechanical properties of the plastic material. However, a deep understanding of the role of chain architecture and molecular mass in determining which species preferentially adsorb at a given interface is lacking. Experiments to resolve the matter are typically conducted by mixing polymers possessing the same repeat chemistry, but different molecular architecture. Here we show the results obtained in large-scale molecular dynamics simulations of linear-cyclic polymer films, and we find clear evidence of enhancement of linear polymers at the interface [7], in agreement with recent experimental results [8]. The behavior predicted by the self-consistent field theory (SCF), i.e., enhancement of cyclic polymers at the interface [9], emerges for relatively long chains. In our presentation, we provide a picture of the microscopic mechanisms through which the chain length arbitrates the competition between the different packing constraints imposed by the loop and linear geometry of the two polymers. We also discuss the role of enthalpic and entropic factors of the interface linear geometry of the system in determining which species in the blend preferentially adsorbs at the interface.

CK 03

Large-scale simulations of solid-liquid interfaces under realistic electrochemical conditions for energy conversion and storage

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Pennsylvania State University (Materials Science and Engineering/Materials Research Institute, University Park, United States)

Solid-liquid interfaces are at the heart of a wide array of electrochemical technologies such as batteries, supercapacitors, fuel cells, electroactuators, and dye-sensitized solar cells. To optimize these technologies, the interactions of the charged electrodes and the ions from the surrounding electrolyte need to be understood at the molecular level. While existing quantum-mechanical models are applicable to either the electrolyte or the electrode in isolation, their combination is challenging using available computational approaches. This presentation will highlight progress in the quantum-continuum modeling of solid-liquid interfaces. The focus will be on the storage of energy in electrochemical capacitors and the production of chemical fuels in photoelectrochemical reactors. We will describe the use of newly developed, embedded quantum-mechanical techniques and large-scale finite-temperature sampling methods to elucidate pseudocapacitive storage at ruthenia electrodes and to predict the electrification of silicon photoelectrodes in realistic aqueous media.

Keywords: Energy Storage and Conversion, Computational Electrochemistry

CK 04

Simulated synthesis and characterisation of metal oxide nano-architectures

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Electronic structure and atomistic simulations are capable of elucidating structural, transport and predicting performance of lithium ion battery electrodes. A major challenge associated with generating atomistic models is to capture the wealth of microstructural features observed experimentally and to follow evolvement of lithiated phases obtained after intercalation, associated with charging and discharging of batteries. One technique that is capable of spontaneously generating various nanostructures and introducing complex microstructures is the simulated amorphisation and crystallization method. We have used the method to synthesis metal oxide composites with complex nano-architectures of binary MnO₂, TiO₂. Recently, we laid a framework for modelling ternary composites of layered and spinel structures, reported amongst high capacity lithium-metal-oxide cathodes for lithium-ion batteries by Thackeray, but with potential for performance enhancement. Our simulated microstructures were characterised and validated with high resolution transmission electron microscope images and X-ray diffractions results. The performance of such composites was predicted from mechanical properties which demonstrated, at a nanoscale, that electrochemical activity of batteries is sustained by maintaining open pathways for lithium ion transport during charging and discharging processes. This is mainly achievable in certain nano-architectures which confer long battery life, whilst enabling fast charge by providing access for electrolytes into voids and pores of battery electrodes.

Keywords: Atomistic simulations, Li-ion batteries, nanostructures, mechanical properties

CK 05 Dusk of Moore's Law: opportunities for HPC and materials science?

Thomas C. Schulthess

Whether and for how much longer CMOS based microelectronic fabrication will continue to scale is a matter of some debate. Several changes, however, have already had profound effects on high-performance Computing (HPC). With the end of Dennard scaling, on-chip parallelism has increased exponentially over the past decade. It is also clear that new, more performant processor generations cost more. Furthermore, the increased commoditization of HPC hardware has led to a diversification of architectures used in scientific computing. While some see this negatively, I will argue to the contrary. Several of the most performant supercomputing systems today consist of hybrid, accelerated nodes that required adoption of new programming models. The need to refactor software for divers architectures encourages HPC practitioners to rethink algorithms and invest in software development. Scientific application software has to be portable across all these architectures and at the same time perform optimally on each individually. We will discuss software strategies that allow us to tackle this challenge while maintaining high productivity of scientists who have to use and further develop application software. Specific examples will be given for codes used to study electronic structure in condensed matter physics and materials science.

EDK 01

Facilitating Industry Driven Research and Innovation: a fully integrated systems approach

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The development of an inclusive Science Technology and Innovation sector of the economy relies to a larger extent on existence of a fully integrated National System of Innovation (NSI). To achieve the latter, there is need to synergise conflicting policies that negatively impact on the development of the NSI and establishment of new policy instruments that support Research and Innovation in the wider economy. To address these deficiencies, the Botswana Innovation Hub (BIH), a company registered under the Companies Act, has been setup to develop and operate a Science and Technology Park in Gaborone, Botswana. BIH has identified a number of initiatives aimed at developing working relationships with similar research institutes within the Botswana Science, Engineering and Technology (SET) landscape as well as externally. A case in point is the relationship that has been developed between BIH and the Botswana International University of Science Technology (BIUST), a world class research oriented and future entrepreneurial University that has been setup to drive national efforts towards creating a more synergised industry based education that is part of the wider Research and Innovation agenda. In this paper, the focus and emphasis is placed on key policy initiatives and configurations that allow for significant investment in Research and Development by government and to ensure that research outputs contribute to economic diversification and national competitiveness. Under these frameworks, innovative processes, services and products are envisaged through the development of a strong University and industry collaboration that is feasible and sustainable and is a real engine of economic growth and prosperity.

Keywords: Innovation systems, Policy, Research, Science, Technology, Engineering, Competitiveness

EDK 02

The Early Days of Cold Sintering: Where We Are, Where We Are Going, and Our Dreams <u>Clive Randall</u>

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In the form of a tutorial, we will review the basic concepts of sintering and then consider generally low temperature precipitation processes in ceramics. We will then consider how these concepts can be combined to enable ceramics to be sintered at low temperatures. I will give some background information that exists in the hydrothermal literature, in the geochemistry literature, and possible non-equilibrium processes that can all synergistically accelerate the kinetics that allow a low temperature densification. I will review the basic processes that we are applying to enable the densification. I will particularly concentrate on the opportunities that we have realized within the electroceramic materials, including the development of cold sintered multilayers and thick films.

Keywords: sintering, microstructure, processing, composites, energy materials

EDK 03

Mentorship for Young Scientists: Developing Scientific Survival Skills

Federico Rosei

In this lecture, I will try to convey a feeling for our course on "Survival Skills for Scientists" [1]. This is a graduate course designed and developed in my department, in which we give basic advice and offer mentorship to our graduate students and post-docs. The central theme of this presentation is that succeeding in Science requires skills (often referred to as 'soft professional skills') beyond those needed for Science. The lecture aims at giving basic guidance and mentoring to young scientists (typically science and engineering undergraduate and first year graduate students). The main topics are:

- The job market for graduates in science and engineering (industry, national labs and academia; advantages and disadvantages)
- Funding in modern science
- Publish or perish; publishing quality papers, having an impact
- Presenting your work to your peers
- The fundamental laws of 'scientific survival' (know yourself, plan ahead, and play chess)
- Ethics in modern science
- Alternative careers

EDK 04

Building the SciBridge: Bringing together African and U.S. Scientists John Paul Eneku

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Scibridge is a science based collaboration project based at North Carolina State University (U.S.) and Makerere University in Kampala, Uganda (Africa). Scibridge Project-Uganda Chapter has six member public universities spread evenly across the country, Uganda. The coordination center is Makerere University and superintended by Mr. Eneku John Paul (MSc), Lecturer at the department of physics. The department of physics in each member university is the primary participating unit and undergraduate students of Bachelor of Science (Bsc) in physics plus graduate (MSc) students in some cases. The academic dialogue between Ugandan universities with their counterparts in the United States began in October 2014, with a novel science experiment kit (dye sensitized solar cell). Once a class of students performed the experiments under the supervision of their lecturer, a webseminar is arranged involving a U.S. researcher (live online), the students and their lecturer. Activity photos are posted on the project websites: www.scibridge.org; www.facebook.com/scibridge; taken and www.twitter.com/scibridge. In May 2015, a second experiment developed by Texas Materials Institute, University of Texas was delivered to Uganda. In this experiment, students build an aluminum/air (Al/air) battery and then use this battery to light different color LED lights and power any other devices. More experiments continue to be designed and assembled by the U.S based collaborators led by Scibridge group of North Carolina State University (U.S home of Scibridge). This activity is headed by Dr. Veronica Augustyn, Assistant Professor of the Department of Materials Science and Engineering in the same university. The first project review workshop for the Ugandan network was held on July 1st, 2017 and participants were coordinators from all the six member universities.

Keywords: Scibridge project, Uganda chapter, Physics, Experiment kits, web-seminar

EDK 05 Educating Engineers for Africa in the 21st Century <u>Michael Adewumi</u>

EDK 06

Learning Chemistry on Computers in African Contexts

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The public education system in East Africa is seeing a huge influx of computers for digital learning. Kenya in particular has made incredible strides in equipping its public schools at all levels with computers in an effort to increase the technological literacy of its students. This is actively contributing to students becoming fluent on computers at early ages, and national curricula for computer labs at the high school level are shifting from general computer skills to specific science content lessons. This project is a small effort to help ease that transition. The authors have explored advanced materials science computational software, and they have repurposed and retailored the software for easy-to-implement chemistry lessons appropriate for classrooms in East Africa - including rural labs which may not have readily available or high-speed internet access. The lessons feature global chemistry learning standards coupled with locally inspired examples - from minerals to natural products. Pilot lessons are being carried out with coordination from staff at the University of Dodoma and learning advantages to the newly developed lessons will be examined.

Keywords: Education, Visualization, Pedagogy, Computation, Chemistry

EDK 07

Recent scientific & technological advances: Potential implications for the African continent Solomon Assefa

EDK 08

Educational networks to face new challenges in global teaching: Project Based Learning and Service Learning in Materials Science courses

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In an increasingly globalized world, the challenges in education turn out to be global as well. The arrival of the TIC to the education field during the last years has resulted in a global revolution by closing the gaps among different countries and cultures. The use of TIC enables to connect teachers and students from all around the world, decreasing the technological gap among countries while granting access to more people to all levels of education (e.g. MOOC, remote supervision of master and doctorate projects, etc). Moreover, TIC opens the way for real-time collaboration between people from different cultures and backgrounds, allowing students and teachers from different countries to work in common problems under the maxima "think global act local". This collaborative work could be a mighty tool to improve people skills for better understanding of "the other", thus reducing xenophobic and racist feelings, while enhancing other professional skills such as working in multicultural, multiracial and multilingual teams. In this regard, teachers from Materials Science and Engineering from two Spanish universities have developed together some Service Learning projects in collaboration with local institutions and NGOs working in third countries. The pedagogy selected was Project Based Learning as it has proven to work perform properly in achieving both specific and professional competences. Examples of some of these experiences will be presented and discussed. Nevertheless, whenever a real and long-term change in education is intended, integration within the curricula, institutional support and proper systematization is required. In this direction, we are currently working in a proposal to the Erasmus + K2 program from the European Community we would like to present here. The project is SEEDs: "Service learning in engineering and architectural studies: an instrument for social transformation in Europe".

Keywords: Materials Engineering, Teaching Networking, Project Based Learning, Service Learning

Oral Presentations

HO 01

Electrochemical sensor for determination of pyridine-2-aldoxime methochloride and dopamine at poly(3,4-ethylenedioxythiophene) modified glassy carbon electrode Abera Demeke

Electrochemical sensor for determination of pyridine-2-aldoxime methochloride and dopamine at poly(3,4-ethylenedioxythiophene) modified glassy carbon electrode Abstract A simple and sensitive elecrochemical method was developed for simultaneous determination of pyridine-2-aldoxime methochloride (PAM-2) and the neurotransmitter dopamine (DA) at poly(3,4-ethylenedioxythiophene) (PEDOT) modified glassy carbon electrode. The electrochemical behavior of PAM-2 and DA were investigated using cyclic voltammetry. PAM-2 was irreversibly oxidized at 650 mV while DA was reversibly oxidized and reduced at about 185 mV and 147 mV, respectively. The observed significant oxidation peak potential difference between PAM-2 and DA allowed the simultaneous determination of both species using square wave adsorptive stripping voltammetry. Under optimized conditions, the voltammetric the responses gave linear ranges of $3.0 \times 10^{-6} - 1.5 \times 10^{-4}$ M and $1.0 \times 10^{-7} - 1.0 \times 10^{-4}$ M with detection limits of 1.9×10^{-7} M and 3.1×10^{-8} M for PAM-2 and DA, respectively. The determination of PAM-2 and DA in human blood serum samples was successfully carried out with a very good recovery result 95.17 % and 101.6 %, respectively.

Keywords: Pyridne-2-alidoximemethochiloride, Dopamine, Adsorption stripping voltammetry, poly(3,4-ethylenedioxythiophene)

HO 02

Effect of Sintering Time on Mechanical Properties of Porous Ti-6Al-4V Implant

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Titanium alloy is popular in biomedical application owing to its low density, good biocompatibility (i.e. biological and chemical inertness) and excellent mechanical properties but due to high disparity between the implant and bone Young's moduli, it causes stress shielding in the body. Porous Ti alloy implant has proven to be effective in addressing this issue, so in this work, we created porous Ti-6Al-4V implant by sieving the as-received Ti-6Al-4V powder into different particle sizes and sintering it without pressure at 980°C for 0.5hrs, 1 hr, 2hrs up to 5 hrs. The wettability and the mechanical properties of the sintered samples are elucidated using a contact angle measurement setup, nanoindentation and universal testing machine. The results show that there is a direct relationship between the Young's modulus of the samples and the sintering time.

Keywords: Ti-6Al-4V implant, Biomaterials, Young's Modulus, Sintering time and temperature

HO 03

Numerical modeling of laser heating of hydrogel/gold nanoparticles composites for localized hyperthermia

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This paper presents the results of a combined experimental and computational study of the effects of particle size on near-infrared laser heating of gold nanospheres. The temperature changes in the gold nanosphere solutions with different sizes are studied experimentally. Finite element model of P(NIPA) gel-gold nanoparticles composite/tissue illuminated with different levels of laser power intensity are simulated. The measured temperature changes at different levels of laser power intensity are shown to be in the range required for the control of programmed cell death via hyperthermia. The implications of the work are discussed for the killing of tumors, with minimal damage to normal cells. The implications of the results are also discussed for potential applications of gold nanoparticles in laser hyperthermia.

Keywords: Gold nanoparticles; cancer treatment; hyperthermia and laser therapy.

HO 04

The interaction of 200 MeV Protons with green and chemically synthesized AuNPs in malignant and non-malignant cells

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Radiation therapy aims to deliver a lethal and curative dose of radiation to diseased cells whilst sparing surrounding healthy tissue. However, even with the advent of intensity modulated radiation therapy, this remains the limiting factor associated with radiotherapy. The clinical application of proton radiation, previously maligned as a therapeutic option that is too costly, has gained renewed attention. This is due to the lower integral body dose of protons compared to traditional x-ray therapy which stems from the ability to confine the radiation dose to the malignant tissue and the lack of an exit dose. The incorporation of proton radiation with nanobiotechnology presents an even greater opportunity to improve the efficacy of radiotherapy in cancer. Nanotechnology presents a unique option to treat carcinomas individually whilst preserving the integrity of adjacent healthy tissue and potentially reducing the side effects associated with cancer therapeutics. Gold nanoparticles (AuNPs) have been proven to exhibit a plethora of characteristics that can be exploited for medicinal use. AuNPs have the potential to sensitize or improve the sensitivity of cancerous cells to radiation therapy. The combination of gold nanoparticles and proton radiation therefore presents an ideal mixture to ameliorate the effects of radiotherapy. This study explored the potential radioenhancement effect of AuNPs of varying sizes in vitro at increasing depths along a modulated proton beam. Based on preliminary results, it is clear that all the AuNPs on their own induced a G_0/G_1 block. However, in combination with proton radiation, a G_2/M block was revealed. A significant G₂/M block is expressed at the most distal depths of irradiation in the Spread Out Bragg Peak (SOBP). Quantification of micronuclei, indicative of radiation damage, showed a significant (p<0.05) dose enhancement effect by the AuNPs. In both cases, the effects seen were dependent on the size of the AuNPs and depth of radiation.

Keywords: Radiation therapy, protons, gold nanoparticles, radiosensitization, cytotoxicity

HO 05

Preparation and Characterization of Chitosan-Ascorbic Acid Complex Microspheres with Encapsulated Prodigiosin for Localized Drug Release in Breast Cancer Treatment

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Chitosan (CS) has been shown to be an effective anticancer drug carrier. However, it requires internalization by cells to potentiate the effect of the drug upon drug release inside the cell. Ascorbic acid (AA) is transported into many cells through the sodium-dependent vitamin c transporters (SVCTs) on the surface of the cells. Thus, functionalizing CS with AA may facilitate the entry of drug-loaded microspheres of CS-AA complexes into cancer cells and subsequent drug release inside the cells. We have prepared CS-AA complexes with the aim of functionalizing CS with AA facilitating the cellular internalization of CS-AA microspheres encapsulated with prodigiosin (PG), an anticancer drug. CS is first synthesized from prawn shells, and its moisture content at varying concentrations in 1% acetic acid solution is investigated. It is also characterized using SEM to study its morphology, FTIR to investigate its chemical bonding structure and tensile testing to assess its mechanical properties. Thereafter, CS-AA complexes are produced and a single emulsion (water/oil) technique is used to synthesize CS-AA microspheres with encapsulated PG at varying concentrations. The PG loaded microspheres are designed to act as scavengers for metastatic cells and deployed in a systemic blood circulation to erase the reticula-endothelial system and functionalized to target circulating tumors. We prepared gels of CS-AA to act as resolvable drug eluting entities. These resolvable gels are designed to be inserted after tumor resection. The microspheres and gels are characterized using FTIR, SEM and XRD. UV-Vis spectrophotometry is used to determine the drug encapsulation efficiency, the swelling kinetics of the microspheres and gels as well as the drug release kinetics in vitro, which is modelled according to the zeroth order, first order, Higuchi and Korsmeyer-Peppas kinetic models. This study demonstrates that microspheres of CS-AA complexes with encapsulated PG can be synthesized for potential targeting of breast tumours.

Keywords: chitosan, ascorbic acid, microspheres, prodigiosin, cancer, drug release.

HO 06

Water Solubilization of CuInS₂/ZnS QDs and their Bioconjugation to Fibroblast Growth Factor for In-vitro Imaging

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Fibroblast Growth Factors (FGFs) play a major role in angiogenesis, which is important in cell development/proliferation and wound healing, but has been implicated in a wide range of cancers. Finding new methods to image and understand angiogenesis under physiological conditions may eventually lead to developing better cancer treatments. Fluorescence imaging is particularly attractive due to its high sensitivity and spatial resolution and quantum dots (QDs) are currently one of the most attractive fluorescent probes due to their high brightness and photo stability and long fluorescence lifetime. However, most current biomedical imaging with QDs use Cd-based QDs. Developing fluorescent QDs that utilize non-toxic materials will allow for a safer use of fluorescent probes in more biological environments. CuInS₂/ZnS is an excellent candidate for this, but their synthesis and application is much less well-developed than Cd-based QDs. In order to be able to use such QDs they need to be made soluble in water and to maintain stability in physiological environments, after which they can be bioconjugated to proteins such as FGF. Here we report on the water solubilization procedures for CIS/ZnS, and how this affects their fluorescence properties. Then, we study the bioconjugation of these water-soluble CuInS₂/ZnS to FGF. We accomplish this by first labeling the FGF with an acceptor dye and then

determined the QD:protein conjugation ratio under various conditions by FRET. Once an optimal QD:protein ratio was determined, we began performing *in-vitro* fluorescent imaging studies to determine FGFs function and specificity is not affected, which will be followed by *in-vivo* studies to determine how FGF affects angiogenesis.

Keywords: Quantum Dots (QDs), Bioconjugation, Fluorescence Resonance Energy Transfer (FRET), Imaging, Fibroblast Growth Factor (FGF)

HO 07

Green synthesized silver nanoparticles for optical detection of Escherichia coli

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Optical detection is usually determined based on the measurement obtained through fluorescent, colorimetric signals generated by the interaction of microorganisms with the specific analytes. More so, several strains Escherichia coli (E. coli) has been reported as a leading cause of diarrhea in the populace, especially in sub-Saharan Africa. The aim of this study is to biosynthesize silver nanoparticles using culture supernatant and wet biomass of Bacillus subtilis and assess a rapid method for detection of pathogenic strains of E. coli using the synthesized nanoparticles. Culture supernatant as well as wet biomass (cell pellets) of Bacillus subtilis (NCIB 3610) were exploited for the synthesis of Silver nanoparticles (AgNPs). Synthesis was confirmed using UV-Vis Spectrophotometer. They were further characterized by Scanning Electron Microscope(SEM), Energy Dispersive X-ray(EDX), Fourier Transmission Infrared(FT-IR) and X-ray Diffractometer (XRD). The optical detection study was investigated by the use of several strains of E. coli (EPEC, ETEC, EIEC, STEC, EAEC and EHEC) which were cultured and standardized to 0.5 McFarland (1 x 10^{^8}). Silver nanoparticle was coated with Poly-L-lysine (PLL) and mixed with each of the E. coli standardized strains, optical density was monitored at 540nm wavelength. The result showed Surface Plasmon Resonance (SPR) peaks at 410-450 nm for culture supernatant (Room and elevated temperature) and wet biomass (Room temperature). The biosynthesized AgNPs were also found to have the size range of 45-95 nm with a cuboid shape. Standardized inoculum of E. coli in the presence of coated AgNPs changed from pink to colourless for the strains. This shows promising pathway to inhibit and detect E. coli.

Keywords: Escherichia coli; Silver nanoparticle; Bacillus subtilis; Detection.

HO 08

Electrochemical field effect transistor for glucose detection

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Among the many biological compounds found in nature, glucose is arguably one of the most critical for life. The level of blood glucose may be related to the diabetes disease which is a world-wide public health problem. In this work, we report on ElecFET (Electrochemical Field Effect Transistor) devices potentially of interest for the detection of different molecules in solution such as glucose. ElecFET are electrochemical microsensors in liquid phase, based on two elements : (i) a pH-sensitive chemical field effect transistor (pH-ChemFET) and (ii) a metallic microelectrode deposited around the sensitive gate. The coexistence of these two elements combines potentiometric and amperometric detection effects at the microscale. Design, fabrication and experimental validation of ElecFETs based on silicon and polymer micro-technologies, are reported. We first demonstrate the detection of hydrogen peroxide (H_2O_2) in solution, showing a sensitivity of 5mV/mM in the [10–100mM] concentration range. The sensor response depends on the main influential parameters such as: (i) polarization

parameters on the microelectrode, *i.e.*, voltage (Vp) and time (tp). The ElecFET concept is then extended to the detection of glucose in the [1-30mM] concentration range. The sensitivity are between 2-6mV/mM. This new ElecFET device paves new ways for sensor applications, opening several new opportunities for pH-ElecFET devices for H₂O₂-related enzymatic detection of biomolecules.

Keywords: Glucose, biosensors, Hydrogen peroxide, Transistor

HO 09

Graphene Oxide/ZnO for Antibacterial Cytotoxic Impact Against MCF-7, A549 and Hep2 Cells Comparative Studies: Bio-Medical Application

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7 Graphene oxide (GO) is a two-dimensional (2D) materials with fascinating properties such as large surface-tovolume ratio, strong optical transparency, tough mechanical and electronic transport capabilities. Respectively, non-toxic zinc oxide proves the bio-activity and the nanosized ZnO particles with diameters of 10 nm quantum dots were prepared with a solution based co-precipitation method at low cost and high yield. The synthesis of the particles was functionalized by the organic solvent dimethylformamide, and the particles were covalently bonded to the surface of GO. The morphology of the graphene oxide sheets and ZnO particles was confirmed with field emission scanning electron microscopy (FESEM) and HRTEM. Fourier transform infrared spectroscopy (FTIR), photoluminescence (PL), micor-Raman scattering spectroscopic methods and X-ray diffraction were used to analyse the physical and chemical properties of the ZnO/GO nanocomposites (NCs) that differed from those of the specific components. Excellent enhanced antibacterial activity of nano ZnO/GO composites were observed with a well-diffussion method in which minimum inhibitory concentrations of 5.94 µg/mL for Escherichia coli (E. Coli) and Salmonella typhimurium (S. typhimurium), 10.87 µg/mL for Bacillus subtilis (B. subtilis), and 25 µg/mL for Enterococcus faecalis (E. faecalis). The NCs showed good cytotoxic impact against MCF-7, A549 and Hep2 cells compared to normal cell lines. Compared to control plates, the percentage of cell growth inhibition was found to be high with as concentrations of ZnO/GO- NCs becomes more as determined by MTT assay. The AO / EtBr staining observations demonstrated that the mechanism of cell death induced by Ag-NPs was due to apoptosis in cancer cells. Therefore, the synthesised nanocomposites (ZnO/GO) were exhibit extraordinary antimicrobial and anti-cancer activity. The reactive oxygen species formed on the surface of composites, improving antibacterial properties and enhance to anti-cancer activity.

Keywords: Graphene oxide, ZnO, FESEM, TEM, Antibacterial, Anticancer properties.

HO 10

The effect of cassava cellulose microfibre reinforcement on the mechanical, morphological and microstructural characteristics of three-dimensional gelatin composite scaffolds

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Gelatin is mostly used as polymer matrix in the development of tissue engineering three-dimensional composite scaffolds to serve as a substrate for seeded cells to promote cellular activity and tissue production in vitro and in vivo, however, gelatin polymer has low mechanical stability which undermines the characteristics needed for tissue engineering scaffolds. This study examined the effect of incorporating cassava cellulose microfibres as reinforcement on the mechanical, morphological and microstructure characteristics of gelatin scaffolds. Threedimensional cassava cellulose microfibre/gelatin scaffolds with different fibre weight fractions were fabricated using phase separation and freeze-drying methods. The cassava cellulose microfibre/gelatin scaffolds fabricated showed rough surfaces compared to pure gelatin scaffolds and were highly porous with surface porosity ranging between (84 – 90 %) and interconnected pores of average size of 36 \pm 12 μ m. The effect of the fibres on the scaffold surface roughness and porosity could improve cell-matrix adhesion and also facilitates efficient cell seeding and diffusion of nutrients and oxygen during cell culture. Cassava cellulose microfiber/gelatin composites containing up to 7% cellulose fibres can withstand higher mechanical loads than pure gelatin scaffolds. The 7% fibre load composite scaffold recorded a maximum compressive strength of 0.29±0.02 MPa, about eight (8) times higher than the pure gelatin scaffolds, and also increased the Young's modulus of pure gelatin scaffolds from (0.31 ±0.03 MPa) to (1.31 ±0.03MPa), about four times higher. The strength and stiffness of the cassava fibregelatin composite scaffolds were improved with increasing cassava cellulose microfibre load, demonstrating the potential use of these scaffolds in the tissue engineering field.

Keywords: Gelatin, Tissue engineering, Scaffold, Cassava, Cellulose microfibre

HO 11

Complementary strategies to target the tumor microenvironment with gold nanorods

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Gold nanorods have received attention as contrast agents for key applications in biomedical optics, such as the photothermal ablation and photoacoustic imaging of cancer. These particles feature a unique combination of optical absorbance, non-cytotoxicity and potential to home into tumors upon systemic injection, thanks to their capacity to pervade hyper-permeable lesions and ease of conjugation with molecular recognition probes. However, targeting malignant cells is hampered by their molecular variability and poor accessibility through the blood, due to a variety of biological barriers. Instead, shifting the focus from the malignant cells to the tumor microenvironment (TME) opens new perspectives. For instance, the hyperproliferative profile of malignant cells entails a combination of poor oxygenation and high oxygen consumption, which makes the TME hypoxic. As hypoxic cells need to switch from aerobic respiration to fermentation, there occurs a variety of processes that include the expression of transmembrane isoforms of carbonic anhydrases. Conjugates of gold nanorods and inhibitors of carbonic anhydrases act as a multimodal tool to hit hypoxic cells by hampering their pH homeostasis and imparting an optical sensitization. In addition, the abnormal conditions of the TME trigger the recruitment of various types of immune and stem cells that track gradients of chemokines. These cells may be harvested from a patient, loaded with plasmonic particles ex vivo and then re-injected into their host, in order to exploit their innate tropism to the TME. For instance, polycationic particles undergo massive uptake from macrophages that retain their chemotactic profiles and gain optical contrast. We exploit the unique asset of this strategy to manage the nano/bio interface ex vivo, rather than in vivo, in order to optimize a hybrid coating of gold nanorods. We are confident that our work shall provide new inspiration for the development of innovative strategies to deliver plasmonic particles to tumors.

Keywords: Plasmonics, Photoacoustic imaging, Photothermal therapy, Drug delivery

Converging blockchain and next-generation artificial intelligence technologies to decentralize and accelerate biomedical research and healthcare

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The increased availability of digital healthcare data introduces new challenges both in data analysis and management. To speed up the biomedical research, new technologies are needed. To identify the outlook of next-generation artificial intelligence technologies and blockchain for integration on healthcare systems, we highlight recent advances in machine learning (deep learning in particular) for healthcare data analysis and drug discovery and also describe blockchain technology as a tool for data management. We discuss discriminative and generative approaches in deep learning and present considerations in the transfer learning techniques, including one and zero-shot learning. Our goal is to introduce emerging strategies that have a potential to integrate and decentralize biomedical data and advance health sciences.

Keywords: artificial intelligence, deep learning, data management, blockchain, digital health.

HO 13 Polysucrose-based scaffolds for tissue engineering applications Itisha Chummun, Archana Bhaw-Luximon*

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The development of scaffolds that mimic the structure, bio-functions and dynamic nature of the extracellular matrix (ECM) has been a major challenge, which requires materials science, a crucial tool for modern tissue engineering. Hydrogels and electrospun nanofibers have been widely explored as attractive macro- and microporous 3D scaffolds, with similar aqueous and hierarchical fibrous architecture to the ECM. However, the limited number of 3D hydrogel scaffolds progressing to clinical implementation and concerns with commercially available hydrogel scaffolds such as immunogenic response and production inconsistency of Matrigel® have led to renewed interest in hydrogels based on novel materials that can offer potential alternatives. Polysucrose (PSuc) has excellent biocompatibility with cells, virus, and microorganisms. It is commercially used for density gradient filtration of cells and is also not readily degraded in the bloodstream. However, its capacity to support cell growth and proliferation has been scarcely investigated. 3D culture systems provide a more pertinent platform inducing *in vivo*-like cellular behaviour such as adhesion, morphology, proliferation and differentiation. Parameters such as mechanical properties, interconnective porosity, and surface properties of 3D scaffolds play key roles in cellular functions and cell fate determination. We report here on the fabrication of nanofibers from amorphous, hydrophilic polyether polysucrose (PSuc, Ficoll-type) blended with poly (L-lactide) (PLLA) and polydioxanone (PDX) respectively and on the synthesis of chemically and physically crosslinked hydrogels from derivatives of polysucrose, tailored to meet specific requirements for tissue engineering applications. The physicochemical properties of the scaffolds were determined using a range of characterization techniques such as Scanning Electron Microscopy (SEM), Instron tensile tester, thermogravimetry analysis (TGA), differential scanning calorimetry (DSC) and drop shape analyser (DSA). The biological performance of the scaffolds was evaluated using L929 mouse fibroblasts and MTT assays on the cell seeded scaffolds.

Keywords: polysucrose, nanofibers, scaffolds, hydrogels, tissue engineering

HO 14

Development and Nano-optimisation of actinic damage retarding treatments for Albinistic persons incorporating various nanotechnologies

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Oculocutaneous albinism (OCA) is a congenital amelanistic pigmentation disorder that affects all known vertebrates and has no known cure. It affects one in every 20 000 people worldwide but is geographically biased towards Sub-Saharan Africa where it affects one in every 1000 people. Melanin and melanogenesis are the body's primary protection from actinic damage, medically this damage summarizes all the acute and chronic solar induced adverse dermatological conditions from sunburn to various skin cancers. This impairment therefore makes Albinistic persons highly susceptible to all forms of this damage. No treatment has ever been developed specifically to retard actinic damage in PLWA. Chemical sunscreens used by PLWA a e ineffective and do not treat other symptoms of actinic damage. The aim of this research was to develop a treatment based on nanometric TiO₂ and ZnO incorporating nano structured lipid carriers and other novel nanoscale drug delivery systems. The nanomaterials dermato-pharmacokinetics, stability, efficacy, toxicity and aesthetics of the resultant formulation on albinistic skin types were also investigated in this study. Nanometric emulsion formulation was done according to FDA-CFSAN, COLIPA, and OECD mandated technical guidelines and testing methods. Nano optimised formulation skin sensitivity tests were evaluated through Draize ocular and skin sensitivity tests as well as in-vivo patch tests guided by OECD 428/404 technical guidelines and opinion SCCNFP 0750/03. Percutaneous absorption and albinistic skin dermato-pharmacokinetics were evaluated ex-vivo using Franz diffusion tests and sequential adhesive tape stripping respectively according to OECD guidelines 428 and SCCNFP opinions. Analysis for nanometric Ti and Zn were done by ICP-AES and Flame AAS respectively. Efficacy and SPF testing was done as per FDA-CFSAN, Colipa and OECD M389/EN mandated test methods. SPF 16, aesthetic and stable nanostructured emulsions incorporating nanometric metallic oxides were formulated. Negligible irritation indices for the treatment were recorded for Draize and human patch testing. No percutaneous absorption was observed for ex-vivo diffusion tests and sequential tape stripping tests. Different skin reservoir properties were observed at different skin sites. The studies demonstrate for the first time, direct evidence that neither nanometric Zn nor Ti can penetrate actinic damaged skin regardless of anatomical site and that albinistic dermato-pharmacokinetics are depended on anatomical region and extent of UVR exposure. All sensitivity tests showed negligible irritation potential for nanostructured emulsions and materials on compromised albinistic skin types. Based on the foregoing, it was concluded that, nano structuring using various nanotechnologies and incorporation of nanometric TiO₂, ZnO and herbs in treatments to retard actinic damage in albinistic persons is feasible, aesthetic, efficacious, and commercializable and does not pose any health risk.

Keywords: Albinism, Titanium dioxide, Zinc Oxide, sunscreens, actinic damage

HO 15

Antiproliferative effects on human lung cell lines A549 activity of cadmium selenide nanoparticles extracted from cytotoxic effects: Investigation of bio-electronic application

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Cadmium selenide (CdSe) nanoparticles make necessary to acquire more information against the cytotoxic effects on human lung epithelial cells A549 potential adverse to health effects. More biological studies highlighted their cytotoxic potential like pulmonary or respiratory diseases were focused on toxicity nanoparticles mechanisms are involved. The aim of our research, is the comparison of cytotoxicity effect between cells-particle interactions, viability test, membrane integrity and oxidative stress were investigated. XRD showed a strong peak associated with (111) plane of hexagonal CdSe suggesting formation of highly orientated nanoparticles. The longitudinal optical phonon shifted slightly due to strain whereas strong low-energy shoulder shift can be explained within a model for surface optical phonons. Photocatalytic activity of CdSe nanoparticles were investigated by exploiting photocatalytic degradation of Rhodamine B (RhB). The typical UV-vis absorption spectra of RhB solution at different time intervals it can be clearly seen that the relative intensity of the absorption peak corresponding to RhB, with the catalyst for different concentration time intervals (0 mM, 2 mM, 5 mM & 10 mM) of the prepared CdSe nanoparticles. After completion of 5 mM % the dye was completely degraded and the absorption spectra act as a photocatalyst. CdSe nanoparticles exhibits antibacterial activity over a broad range of bacterial species and in particular against P. vulgaris where it out competes four other commonly used S. aureus, E.coli, P. vulgaris and E. hermannii, well as testing four different appropriate concentration from the results showed a significant gain in viable cell numbers of all four bacteria species, with 5 mM and 10 mM being the most effective and 2 mM being the worst, where it provided only a slight improvement from the control in detail.

Keywords: CdSe nanoparticles; Cytotoxic effects; Rhodamine B; Photocatalytic; Electron microscopy; Antibacterial activity.

HO 16

Characterizing the Motions of Hedgehog-Signaling Proteins on the Surfaces of Live Cells by Single-Molecule Tracking

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Single-molecule techniques are well suited for investigating the heterogeneity of populations, which is of particular interest in biophysics where the properties on the nanoscale are often defined by their complexity. Single-molecule fluorescence microscopy incorporates the three main advantages of fluorescence imaging: biocompatibility, target specificity, and extreme sensitivity, and improves upon the spatial precision by an order of magnitude relative to traditional, diffraction-limited imaging (down to tens of nanometers). Here we describe the application of single-molecule tracking to the Hedgehog signaling pathway, a critical player in the development of organs and tissues during embryogenesis. Aberrant pathway signaling can lead to birth defects and cancer. Despite its importance, many of the key mechanisms underlying pathway transduction remain unknown, although it has been shown previously that these steps take place in a small, rod-like cellular protrusion called the primary cilium, which is 2-10 microns long and 400 nm in diameter. Using single-molecule

fluorescent imaging, we have tracked the motions of the individual pathway proteins, Patched1 and Smoothened, in cilia of live, cultured, mouse embryonic fibroblast cells with high temporal and spatial resolution (10 ms, 30 nm). These proteins exhibit specific behaviors in activated/deactivated conditions, i.e., a change in affinity for binding sites that interrupt the normally diffusive movement. These changes are consistent across a broad range of treatments, whether it be the natural pathway agonist (Sonic Hedgehog), small-molecule ligands, or genetic manipulation, indicating that the observed behaviors reflect the pathway activation state. This work has deepened our knowledge of the Hedgehog pathway, and also provides a possibly new roadmap for measuring the efficacy of potential treatments on tumor-derived cells by characterizing the nanoscale movements of pathway proteins.

Keywords: Microscopy, single-molecule tracking, nanoscience, Hedgehog signaling

HO 17

Selective induction of cell death (apoptosis) using multifunctional gold nanoparticles

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Angiogenesis, which is the formation and growth of new blood vessels, is indispensable for growth, development and progression of chronic diseases such as obesity and cancer. This tissue remodelling is required for nutrients and oxygen supply to diseased cells. Inhibiting angiogenesis by targeting specific cells represents a promising strategy for treatment of these diseases. The aim of this study was to develop targeted anti-angiogenic gold nanoparticles (AuNPs) that can be delivered selectively to the target cells and trigger apoptotic cell death. The AuNPs were bi-functionalized with a targeting peptide and a pro-apoptotic peptide. The targeting peptide (AHP) binds to a protein that is overexpressed by endothelial cells in the white adipose tissue (WAT) vasculature of obese subjects. The bio-distribution of nanomaterials functionalised with the AHP demonstrated that these nanoparticles accumulated in the WAT of animal models of obesity. In the current study, the bi-functionalized AuNPs were synthesized then characterised by UV-Vis, Zeta potential and TEM. The selective targeting and toxicity of the AuNPs were investigated on three human cancer cell lines (Caco-2, MCF7 and HT29), of which Caco-2 cells express the cell surface receptor for AHP. The AuNP toxicity was evaluated using the WST-1 and the APO-Percentage apoptosis assays, while the AuNP uptake was confirmed by ICP-OES analysis. The bifunctionalized AuNP cytotoxicity and uptake were more pronounced in Caco-2 cells, cells that express the receptor for AHP. The bifunctionalized AuNPs showed receptor mediated targeting and targeted destruction of Caco-2 cells following the apoptosis pathway, which demonstrates the potential for the development of targeted therapy for colon cancer. The therapeutic efficacy and specificity studies for the bi-functionalized AuNPs in animal models of obesity and cancer are currently underway.

Keywords: Gold nanoparticles, angiogenesis, apoptosis, targeted drug delivery

HO 18

Developing FRET assays to study the binding of Fibroblast growth factor to its receptor

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Fibroblast growth factors binding to their receptor (FGFR) govern signaling pathways that trigger physiological responses which can be wound healing and cellular proliferation. However, skeletal dysplasia disorder and a significant number of cancers such as breast cancer have been closely associated with the unregulation of FGFR signaling. As a result, regulation of FGFR is highly required to maintain homeostasis so as to lessen the profuse proliferation of cells, which could then lead to cancer. Therefore, there is a need to develop assays that seek to understand the binding of FGF-FGFR and regulation of FGFR to better develop effective therapies for cancer. The

use of Fluorescence resonance energy transfer (FRET) has shown to be a suitable technique for such binding studies since the structural and kinetic information of FGF-FGFR interactions can be effectively elucidated. For FRET, respective binding proteins are site specifically labelled with donor and acceptor dyes using highly fluorescent maleimide dyes that form thiol bonds only with cysteine residues of the proteins. Our results using UV/Vis spectroscopy, fluorescence correlation spectroscopy (FCS) and SDS-PAGE showed that FGF was successfully labelled with maleimide Alexa series dyes (488, 594, 546 and 647). In the future, FGFR will be labelled with suitable dye pairs to the already labelled FGF followed by investigation of ensemble and single molecule FRET between the two proteins.

Keywords: Fibroblast Growth Factor (FGF), Fibroblast Growth Factor Receptor, Single Molecule Fluorescence Resonance Energy Transfer (FRET), Fluorescence Correlation Spectroscopy (FCS).

HO 19

Functional Materials through Surface and Interface Engineering

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Challenges in materials (supply and utility) and energy pose a significant challenge to our existence, especially with our dependence on technology. This calls for new thinking in energy efficiency and manufacturing. Thermodynamics offers a route to sustainable engineering and resource use. Classical thermodynamics relies on the notion of equilibrium, but, not all equilibria states are equally stable – some are 'more equal than others'. A droplet on a poorly wetting surface exemplifies these inequalities in that; evaporation, imbibition, and flux renders an apparent sessile state chaotic. Metastable equilibria states are prevalent in nature especially across surfaces and interfaces, existing in forms of functional concentration gradients (e.g. the synaptic cleft), as self-organized surface-adsorbed adventitious contaminants (e.g. water), among many others. Metastability is a challenge in engineering; however, can we exploit these states as pathways to new materials, technologies, or energy-efficient process? In this talk, I will present our efforts to design new technologies and processes based on understand of metastability on surfaces and interfaces. I will discuss how we adopted emulsification to process metals and how that simple process led to various technologies and capabilities in our laboratory. Highlighted technologies will include heat-free solders, flexible electronics, smart composites, and low-cost diagnostics.

Keywords: Functional Materials, frugal science, surfaces, interfaces.

HO 20

Metal Oxide-Carbonaceous-Polymer nanocomposite based sensors for the detection of lung cancer volatile organic compounds Biomarkers

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Exhaled breath biomarkers are a promising solution for early detection of lung cancer on its early developmental stages. The analysis of specific Volatile Organic Compounds (VOCs) in exhaled breath give an insight of metabolic and physiological activities of an individual. Application of nanoscience using metals oxides and polymer nanocomposites through gas sensing is an interesting research path that brings cost-effectiveness and fast results using the non-invasive route for the detection of biomarkers. This mode of detection will be employed for the detection of Lung cancer exhaled breath biomarkers. This study is aimed at developing metal-oxide-carbonacious polymer nanocomposites based sensors of high sensitivity and tuneable selectivity towards specifically targeted lung cancer VOC biomarkers to improve the detection methods for lung cancer VOCs. Materials such as Manganese dioxide, Titanium dioxide and Tin dioxide, carbon nanoparticles and polymer nanocomposite based Volatile organic compounds sensors were utilized. Synthesized materials were characterized using TEM, SEM, XRD and Raman spectroscopy. The sensors are fabricated by solution mixing method of metal-oxide, carbon

nanoparticles and a biopolymer to produce a nanocomposite. The prepared nanocomposites are drop-casted onto electrodes and dried under room temperature. After fabrication, gas sensors are conditioned under vacuum overnight. To detect lung cancer volatile organic compounds biomarkers, aldehydes such as pentanal, hexanal, octanal and nonanal investigated as biomarkers under simulated environment. The major goal of this project is to establish the known how in the development of gas technologies. The study adds contribution on technologies showing the capacity and capability of South Africa and technology development.

Keywords: cancer, biomarkers, nanocomposites, gas-sensing, volatile organic compounds (VOCs)

HO 21

Extraction and Characterization of Chitosan from Black Soldier fly (Hermentia illucens)

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Black soldier fly (Hermetia. illucens) is an insect of the Stratiomyidae family. They are important in sustainability by their ability to voraciously degrade organic waste without constituting nuisance to the environment. Chitin was extracted from both the pupae shells and adult black soldier fly through demineralization, deproteinization and decolouration processes. The obtained chitins were converted to chitosan by deacetylation process using NaOH (aq). The chitin yield from dry weight of the pupae shells and adult BSF were approximately 13% and 5%, while chitosan was 11 and 2% respectively. Both the chitin and chitosan were characterized by different analytical techniques including Fourier Transform infrared spectroscopy (FTIR), Scanning electron microscopy (SEM), X-ray diffraction (XRD), elemental Analysis (EA), Thermogravimetric analysis (TGA) and cross polarisation-magic angle spinning nuclear magnetic resonance (CP/MAS-NMR). XRD analysis showed the crystallinity of both products, FTIR spectra indicated the peaks corresponding the stretching and vibration of various functional groups, while TGA indicated the behaviour of the materials under intense heating. The degree of acetylation of the chitins from elemental analysis were 91% for adult and 115% for pupal. Both materials were stable up to 270°C, with the adult having a maximum degradation temperature (T_{max}) of 391°C and the pupae 384°C. The results obtained shows that the extracted materials conformed to an α -chitin structure. On the other hand, chitosan had reduced thermal properties compared to the chitins, with both stable up to 220°C and having T_{max} values of 308°C and 306°C for adult and pupae respectively. The chitosans were found to be of medium molecular weight from viscometry method with a value of 203 KDa. The characterisations were done to determine the effectiveness of the extraction processes, and the purity of the extracted materials. These results have shown that the pupae and adult chitins and chitosans were of high quality when compared with the standards.

Keywords: Black soldier fly, Biopolymer, Chitin, Chitosan, Characterization

HO 22

Development of a nystatin-loaded micellar system for oral mucoadhesion

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Oropharyngeal Candidiasis, also known as oral thrush, is a fungal infection that commonly affects infants and immune compromised patients. Although treatment is available, in the form of a nystatin suspension, the mechanism of application of the suspension does not allow prolonged contact with the affected area. This results in reoccurrence of the infection and a longer treatment period. This research aims to increase contact time of nystatin in the affected area, by incorporating nystatin loaded micelles into a mucoadhesive patch. The polymeric micelle solutions were formed by dissolving nystatin and poly(ethylene glycol) methyl ether-block-poly(lactide-co-glycolide) in dimethyl formamide (DMF), water was then added to the solution and rotoevaporated to create nystatin loaded polymeric micelles. The micelles were then dialysed to remove the DMF from the micellar solution. All the solutions were characterised for size and stability using a zetasizer and the optimal formulation

was determined statistically through the use of Research Surface Methodologies. The optimal solution was incorporated into a mucoadhesive film which was tested for rate of drug release as well as antimicrobial activity. The findings of the research will provide insight into the rate of drug release of nystatin from the mucoadhesive patch as well as the antimicrobial effectiveness of the patch for treatment of oral thrush. **Keywords:** oropharyngeal candidiasis, polymeric micelles, block copolymers, mucoadhesion

HO 23

Electrochemical determination of serotonin in urine samples based on metal oxide nanoparticles / MWCNT on modified Glassy Carbon Electrode

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The electrochemical response of serotonin on the modified electrode based on multiwalled-carbon-nanotube (MWCNT) doped respectively with nickel, zinc and iron oxide nanoparticles coating on glassy carbon electrode (GCE) at physiological pH 7 was determined using cyclic voltammetry (CV) and square wave voltammetry (SWV). The modified GCE/MWCNT-metal oxide electrodes exhibited excellent electrocatalytic activity towards the detection of serotonin at large peak current and lower oxidation potentials compared to other electrodes investigated. The dynamic range for the serotonin determination was between 5.98 x 10^{-3} µM to 62.8 µM with detection limits 118, 129 and 166 nM for GCE/MWCNT-NiO, GCE/MWCNT-ZnO and GCE/MWCNT-Fe₃O₄ sensors respectively. GCE-MWCNT-NiO was the best electrode in terms of serotonin current response, electrode stability, resistance to fouling and limit of detection towards the analyte. The developed sensors were found to be electrochemically stable, reusable, economically effective due to their extremely low operational cost, and have demonstrated good limit of detection, sensitivity and selectivity towards serotonin determination in urine samples.

Keywords: Metal oxides nanoparticles, Multi-walled carbon nanotubes, Serotonin, Cyclic voltammetry, Square wave voltammetry.

HO 24

Quantitative analysis of Foot-and-mouth disease virus-host interactions using a stable isotope labelling proteomics workflow

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Most African countries are endemic with foot-and-mouth disease (FMD). FMD causes severe economic losses due to vaccination costs, production losses, loss of trade due to export restrictions and limited development of the livestock sector. Laboratory characterisation of foot-and-mouth disease virus (FMDV) field isolates and immunological matching to the relevant vaccine is a prerequisite for a successful vaccination campaign. This process requires time-consuming virus culture in primary host cells/host cell lines for growth and subsequent diagnostics. The lead time for prescribing the correct vaccine directly impacts the severity of an outbreak. A greater understanding of the dynamics of virus culture in host cells is needed to design improved systems for FMDV diagnostics. Discovering novel insights into host-virus interactions via quantitative proteomic analysis is the aim of the current investigation. There have been only a few proteomics studies, limited to basic analysis, that have investigated FMDV-host interactions. Liquid chromatography coupled to mass spectrometry (LC-MS) analysis was performed on cell lysates of BHK-21 and IBRS-2 host cell lines to pilot the protein extraction and MS-analysis methods. These methods will be combined with stable isotope labelling using amino acids in culture (SILAC) for the complete workflow which enables accurate quantitation of proteins (rather than identification only) that are differentially expressed in the host cells after infection. LC-MS analysis of the BHK-21 and IBRS-2

cell lines identified 1662 and 1674 proteins, respectively. No evidence of expression of certain integrin receptors ($\alpha V\beta 3$, $\alpha V\beta 6$, $\alpha V\beta 8$) on the cell surface was found which contradicts previous reports that these receptors are crucial for FMDV replication. These findings prompt further investigation into the proteins crucial for viral replication in the host cells (those differentially expressed after infection). Use of stable isotope labelling material allow for accurate quantitative proteomic analysis which are being implemented currently to reveal insights into host-virus interactions. Such insights may allow for the design of adapted host cell lines with enhanced attributes and reveal novel cellular targets for the design of improved antivirals and new vaccine strategies.

HO 25

The Importance of HIV and TB Genetic Amplification in the Scaling Up of National AIDS and TB Treatment Programs in Africa

Richard Marlink

HO 26

Designing affordable biomaterials for the developing world Shathani Nkhwa

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Currently most biomaterials are developed, manufactured, and used in high income countries and not widely available and affordable to approximately 80% of the world population living in the developing world. This means that these biomaterials are generally not designed, tailored and priced to address current health issues and burdens for the developing countries. The precise extent of biomaterial availability in developing countries and their usage is, however, unclear. There is therefore an opportunity to refocus the attention on the development of novel affordable biomaterials for developing countries, such as Botswana, as these countries currently face numerous and complex health issues that need to be solved. This is a necessary piece of the healthcare delivery puzzle, just as drugs, vaccines and diagnostics. There is growing burden of non-communicable diseases, such as diabetes, cancer, heart disease and HIV, with costly and a significant strain to already struggling health systems. Developing countries, such as Botswana, also have high rates of road traffic accidents, as well as high incidence of burn injuries due to poverty and poor housing conditions, and this results in patients needing implants as well as high quality biomaterials for tissue repair. When developing biomaterials that are suitable for low and middle income countries, researchers should consider the cost-effectiveness of introducing the technology in the developing world in relation to the expected outcomes. Herein we present biomaterials for bone tissue regeneration, synthesized and fabricated via freeze drying technique using FDA approved polymers and ceramic materials. These biomaterials had properties that can be tailored to desired specific needs, such as increased mechanical strength, fluid uptake and retaining of those fluids, as well as the ability to incorporate drugs of interest to have the biomaterial function as a drug delivery matrix. The developed biomaterials were found to be suitable not only for hard tissue applications, but also for soft tissue applications.

Keywords: Biomaterials, hydrogel, composites

HO 27

Development and Nano-optimization of *Burkea* africana (Mukarati) and *Zanthoxylum chalybeum* (Mukundanyoka) for the management of actinic keratosis

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Actinic keratosis is a common premalignant lesion that might develop into an invasive squamous cell carcinoma. The lesions develop on skin damaged by Ultra Violet Radiation (UVR). It is mostly prevalent in elderly Caucasians and individuals with albinism. The skin condition is characterized by scaly, hyperpigmented skin that may itch or ulcerate. Treatment methods include freezing with liquid nitrogen, photodynamic therapy and the use of topical creams such as 5-flouroacil and imiquimod cream. These treatment options are expensive and as a result most people in Zimbabwe that develop actinic keratosis opt for herbal remedies. These herbal remedies are usually polyherbal combinations that differ from region to region. Two plants that appeared frequently among traditional herbalists though were Burkea africana and Zanthoxylum chalybeum. Research carried out on Phytoformulations has indicated that the development of Nano dosage forms has several advantages that include improvement of stability, protection from toxicity and enhancement of bioavailability and solubility. As a result, the formulations were optimized by incorporating nanotechnology. The research project sought to obtain crude extracts from the plants and evaluate efficacy of the extracts. To investigate the antibacterial activity of Burkea africana and antioxidant potential of Zanthoxylum chalybeum. Leading to the formulation of a topical Nanooptimised cream that can be used to manage actinic keratosis. All formulation was guided by Cosmetics Toiletries and Fragrances Association (CTFA), COLIPA, CANSA, South African National Standards (SANS), Standard Association of Zimbabwe (SAZ), Medicines Control Authority of Zimbabwe (MCAZ) guidelines and recommendations.

Keywords: Actinic Keratosis, Burkea africana. Zanthoxylum chalybeum, premalignant, Nano-optimization

HO 28

Development of Bio-phytomedicine from the local natural resources of Chad: case of Boscia senegalensis, spirulina platensis and Hyphaene thebaica Soudy Imar Djibrine

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The herbal medicine is practiced in all the countries of the world as alternative or complementary medicine. Used during centuries as the only shape of medicine, it became the main source of the active ingredients used in allopathic. Actually, pharmacologists and professionals of the industry of the medicine agree on the fact that the alone chemistry is not anymore enough for developing medicine of the future and fighting effectively against the serious illnesses and emergent diseases as the cancers, the diabetes, the high blood pressure, the rheumatism and the genetic diseases. Furthermore, medicine against these diseases is more and more expensive. So, thus the proposal of the alternative solution becomes a priority. Biophytomedicine answers this wait and can supply a comparable therapeutic comfort level and at a lower cost while minimizing the undesirable effects often attributed to the chemistry medicine. In the approach of development of Biophytomedicine, the extraction of the plant or a part of the plant (barks, seeds, leaves or roots) is made in the water, in the oil, in the ethanol or in the CO2. According to the desired biological effect, the extract or the mixture of extracts of plants are used in Permeations USSING Chambers with variable concentrations. The USSING equipment uses the fragments of organs of mice, rats or rabbits beforehand were put on an empty stomach during 14 at 4 hours. The active ingredient consists of products which are absorbed in UV between 200 nm and 450 nm. The control of the raw material is made in three stages. At first, seeds, leaves, barks or roots are sorted out in the hand by the collectors to eliminate those who are not in compliance with the recommendations of the Laboratory. The second control is made at the time of the grinding of the dry samples in the form of flour. The third control is chemical and is made from the flour obtained according to the following described methodology: 1 g of flour of Boscia senegalensis is diluted in 10 ml with ultra-pure water heated in 60 °C during 20 min. The mixture is then shaken in the whirlpool and filtered. The mixture is then diluted in 1/100 before being read to the spectrophotometer

to have the total spectrum between 200 nm and 450 nm.lt is as such that we had led research works and developed an antidiabetic Biophytomedicine from a traditional recipe from this plant called Boscia senegalensis used in Chad to fight against the type II diabetes. We had not only to estimate the harmlessness and the efficiency of the traditional recipe, but also its capacity to block the intestinal absorption of sugars and in vitro fatty acids in Permeation USSING Chambers and in vivo on rats. The obtained results show that the phytomedicine repeated with a modern galenic preparation inhibits the intestinal absorption of the glucose and the fatty acids with short in vivo chains as ex-vivo. The peak of boscia extraction is situated in 256 nm. These results confirm the traditional use of this recipe as antidiabetic formulation by the population from the east of Chad and show that the development of the clinical phytopharmacology can contribute to fight against the modern diseases in Sub-Saharan Africa. On the basis of this new concept of development of Biophytomedicine, we plan to use this opportunity which offers itself for developing countries as ours to go out of the economic underdevelopment in the field of the health and of sciences of alive based on the natural substances. Produce according to the modern methods of medicine with plants and food complements for the health of our populations. In fine, the characterization tools commonly used by material scientists such as raman and infra-red spectroscopy, highresolution X-ray diffraction, Magnetic resonance , and so will potential tools to complete the present study and will certainly open the way for increased knowledge and appropriate use of our bioverse substances and materials.

HO 29

Formulation and characterization of a paediatric nanoemulsion dosage form with modified oral drug delivery system for improved dissolution rate of nevirapine

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The development of antiretroviral drugs (ARVs) continues to play a pivotal role in combating the global health effects of HIV/AIDS. The aim of this study was to formulate a nanoemulsion to improve the solubility, dissolution and absorption of nevirapine for paediatric use. A nanoemulsion was prepared using emulsion inversion point and evaluated for particle size, poly dispersity index, zeta potential. The nanoemulsion consisted of ethyl oleate (15.6% w/v), tween 80 (28.1% w/v), PEG 400 (18.7% w/v), water (37.5% v/v) and nevirapine (3% w/w). In vitro drug release studies were performed at pH 2 and 6.4. Permeability studies using the Caco-2 cell model were performed for the nevirapine nanoemulsion. The optimized nevirapine nanoemulsion had a mean droplet size of 36.09±12.27nm, low pdl of 0.598 and zeta potential of -7.87±4.35mV. At pH 2, the nanoemulsion released 76 \pm 2 % of nevirapine within 2 h, while at pH 6.4 value representing the small intestine, amount of nevirapine released was 41.6 \pm 4 % . The permeability rate of the nevirapine nanoemulsion was 30.02 x 10⁻⁶ cm/s and higher than that of propranolol. Efflux ratio was 0.02 indicating low drug efflux. The results showed that modified drug release formulations of nevirapine could be formulated. The permeability of nevirapine remained high while drug efflux was low, potentially improving bioavailability of nevirapine in vivo.

Keywords: Nevirapine, nanoemulsion, dissolution rate, permeability.

HO 30

Kinetics of Paclitaxel[™] Release from Multi-Coated Metallic Stents: Solution to Coronary Cardiovascular Disease

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Atherosclerosis is a common cause of cardiovascular disease. Atherosclerosis is often characterized by the deposits of fatty substances in the inner lining of an artery. Biomedical devices such as stents are therefore used to restore the normal flow of blood in blockage arteries. In this present work, balloon-expandable stents were coated with biopolymers (sodium alginate (SA), poly-lactic-glycolic acid (PLGA) and poly-ethylene-glycol (PEG)) loaded with paclitaxel[™] (PT) via dip-spin-coating. PT is a reliable agent used to destroy build up plaques such as blockage arteries. Release kinetics of multi-layered PT-coated stents in phosphate buffer saline solution, pH 7.4, was studied in the presence of an enzyme. Drug delivery was carried out in an orbital incubator shaker set at 37°C and at 60 revolutions per minutes (rpm)) to simulate physiological conditions for an extended time. Scanning electron microscope was used to study the biodegradability of the coated stents, while UV-Vis spectrophotometer was used to determine the amount of drug release. Release rate of paclitaxel was higher for sodium alginate matrix. Cumulatively, 70% of drugs were released from SA coated stents within 200 h, and 67% was released from PEG, while 58% was the case for PLGA at this time. There are no clear significant differences due to polymer types in drug release. However, the hydrophilicity of SA plays a key role in drug diffusion. Macroroughness' were observed on PEG coated stents, while macro-pores were profound on the SA coated surfaces. Similarly, macro-cracks were observed on PLGA coated surfaces. Diffusion and hydrolysis were the main control mechanisms of drug release. Huguchi model dominated after 24 h time of drug release. The results suggested that coated stents with PT-loaded biopolymers loaded with PT can provide solution to coronary cardiovascular disease.

Keywords: multi-layer coated stents, cardiovascular disease, biopolymers, drug release kinetics, and dip-spin-coating.

EO 01

Fabrication of Electro-Porcelain Insulators from Local Raw Materials in Ghana

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Electro-porcelain insulators are vitrified and fine grained ceramic whitewares which are used either glazed or unglazed as electric insulation materials for both low and high tension insulation. These complex multicomponent ceramic materials are made from clays, fluxes and fillers. These three ingredients react together under thermal conditions to produce the final product. Despite significant research already conducted in this field, challenges still remain in understanding the properties relating to selection and investigation of raw materials, their processing, microstructure and phase evolution which are critical determinants for their use as electric insulation materials. Although the raw materials for electroporcelain fabrications are readily available in Ghana, there is no research conducted for their application as insulation materials. Therefore, this research, reports for the first time, the potential application of locally sourced Ghanaian minerals for electrical insulation. Furthermore, their workability, fabrications processes and characterization methods are also highlighted.

Keywords: Clays, Electro-porcelains, Insulators, Characterization

EO 02 Adsorptive Desulfurization and Denitrogenation of Fuel over Imprinted Polymer **Microspheres and Nanofibers**

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The deleterious effects of refractory polyaromatic hydrocarbons found in fuels such as organosulfur and organonitrogen compounds (dibenzothiophene, quinoline and its alkylated derivatives) are such that they emit SO_x and NO_x to the environment when combusted, thereby reducing air quality. These compounds also deactivate the catalyst used during fuel refinement and in catalytic converters on cars. Hydro-desulfurization (HDS) and -denitrogenation (HDN) processes that are currently being employed in petroleum refineries to eliminate organosulfur and organonitrogen compounds in fuels are limited in treating these refractory compounds. Herein, desulfurization by means of oxidative desulfurization and adsorptive denitrogenation are reported as complementary steps to the HDS and HDN processes, respectively, to meet the mandated environmental protection agency limit of 10 ppm S and 1 ppm N. Refractory organosulfur compounds were oxidized to polar organosulfones followed by the adsorption of the organosulfones over molecularly imprinted polybenzimidazole nanofibers. While synthesized molecularly imprinted 2-(1H-imidazol-2-yl)-4-phenol (PIMH) microspheres and electrospun 6-vinyl-1,1'-binaphthyl-2,2'-diol co-polymerized with styrene [DBN-co-STY] were employed for the selective adsorption of organonitrogen compounds in fuel. All sorbent shows high selectivity for organosulfur and organonitrogen compounds fuel. The sorbent material produces ultra-pure fuel that will meet all international environmental standards and can be applied in petroleum refining processes.



Adsorptive Desulfurization and Denitrogenation

Keywords: organonitrogen; molecularly imprinted nanofibers and microspheres; density functional theory; Solid Phase extraction

EO 03

Hydrogenation of Ti-based Quasicrystalline Powders Produced by Mechanical Alloying <u>A. Takasaki¹</u>, G. Łukasz², D. K. Patrick³, J. Czub² K. Śwerczek⁴

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Icosahedral (i) quasicrystals, which have a new type of translational long-range order and display noncrystallographic rotational symmetry, were firstly observed in an Al-Mn alloy in 1984 by Schechtman et. al. Since the discovery of the presence of Ti-Zr-Ni i quasicrystal phases (i-phases), studies on their hydrogen storages have been extensively performed for not only their industrial applications as hydrogen storage media but also scientific interest in their local structures which are forbidden to normal crystals. In the chemical compositions of Ti-Zr-Ni system, Ti and Zr have strong chemical affinities with hydrogen, while Ni has less but enhances decomposition of hydrogen molecules into protons as catalysis similar to one in LaNi5. Furthermore, the Ti-Zr-Ni i-phases are believed to possess a large number of tetrahedral interstitial sites in the cluster, which makes the i-phase alloys attractive candidate materials for hydrogen storage. The i-phases were directly produced by rapidquenching or melt spinning, but can also be synthesized by annealing amorphous powders obtained after mechanical alloying. We have systematically and widely studied for hydrogenation of Ti-Zr-Ni amorphous and iphase powders synthesized by mechanical alloying and subsequent annealing respectively. At the conference, we review recent progress in studies on hydrogenation of Ti-Zr-Ni alloys and summarize our recent research results on hydrogenation properties of the Ti-Zr-Ni i-phases and related amorphous or crystal phases produced by mechanical alloying and subsequent annealing. The effects of the substitution of elements or addition of 4th element for Ti-Zr-Ni on the microstructures and the hydrogenation properties will be investigated.

Keywords: quasicrystal, hydrogen storage, mechanical alloying, Ti₂Ni, Ti-Zr-Ni

EO 04 Charge dynamics in composite systems for advanced applications

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Charge dynamics (i.e. the processes of charge generation, dissociation and collection) plays a critical role in several advanced applications based on composite nanosystems, including solar energy, water splitting, nanothermometry. In most of them, semiconducting nanocrystals exhibiting quantum confined effects (the socalled quantum dots, QDs) act as light absorbing materials, which are able to generate excitons as a consequence of photon absorption. Managing the photogenerated charges enables the exploitation of different physicochemical processes, including charge separation and collection in photoelectrochemical systems for energy conversion or tuning photoluminescence properties in luminescent nanoprobes. Key element for driving the processes to targeted applications is the modulation of composition and size of the nanomaterials, which determines the final electronic band structure of the composite systems and its functional properties. We will illustrate different examples of composite systems, targeted for specific applications. (i) "Giant" composite coreshell QDs, in which modulation of core-to-shell interface induces a single- to double-color photoluminescence; (ii) Near-infrared QDs with increased Stokes shift due to suitable electronic structure of the core and shell, to be applied in luminescent solar concentrators; (iii) Composite TiO2 mesoporous film sensitized by "giant" QDs with high charge injection from the photoexcited QD to the TiO2 anode, for excitonic solar cells and water splitting. We will discuss possible strategies to tailor the optical features of the different systems to optimize their functional properties, according to the specific application.

Keywords: exciton dynamics, composite nanosystems, solar energy, quantum dots.

EO 05

Elastic Properties of Strontium difluoride single crystal by means of Brillouin Scattering <u>B. A. Mathe^{1,2}</u>, H. Dube^{1,2}, D.M. Wamwangi^{1,2}

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The present report describes measurements of the elastic constants of SrF_2 at room temperature exploiting the elastic anisotropy of transparent bulk crystals, investigated non-destructively using Brillouin scattering techniques. In this study, an application of Reflection Induced (ΘA) scattering ($RI\Theta A$) technique is introduced. In this geometry, we can simultaneously obtain RI ΘA scattering and back scattering peaks in one frequency spectrum. Since SrF_2 is an ionic material, its elastic constants can be computed theoretically from a simple lattice model, and these computed elastic constants are compared with the experimental data, in order to examine the applicability of the theoretical model. The room temperature values of the elastic constants were obtained, in units of GPa as follows: $C_{11} = 116$, $C_{44} = 32$, and $C_{12} = 40$. The elastic constants of SrF_2 are also found to be comparable with those of the other alkaline-earth fluorides.

Keywords; acoustic phonons, elastic constants, elastic moduli, longitudinal velocity, transverse velocity

EO 06

Effects of Annealing and Pressure on the Grazing Incidence X-ray scatterings of conjugated polymer blends used in Organic Solar Cells

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This paper presents the results of an experimental study of the effects of pressure and annealing on the conjugated polymer chain configurations in poly (3-hexylthiophene) and [6,6]-phenyl C61-butyric acid methyl ester (P3HT:PCBM) blends that are used in bulk heterojunction organic photovoltaic cells (OPVs). Annealing and the application of static loads on P3HT:PCBM blends on glass substrates were investigated. Microscopy and grazing incidence x-ray scattering techniques were adopted to analyze the surface morphologies, nano-/micro-structures and the chain configurations in the conjugated polymer blends. The OPV devices fabricated resulted in the I-V characteristics that have large dependence on the changes in the nano-/ micro-structures of the polymer blends. The pressure induced polymer chain configurations that were in the direction of the applied pressure (edge-on), led to a reduced lamellae spacing between the polymer units. This increased the crystallinity in the blend and played significant role in the organic solar cell performance. The findings of the study are discussed to influence the design and control of the nano-/micro-structures and the performance of bulk heterojunction organic solar cells.

Keywords: Synchrotron x-rays scattering; grazing incidence; polymer chain alignments; solar cells

EO 07 Advanced Nanofunctional Materials for Li-ion Batteries <u>B.V.R. Chowdari</u>

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Presently used commercial lithium ion batteries (LIBs) consist of layer-type lithium cobalt oxide, spinel LiMn₂O₄ or LiFePO₄ as the cathode, graphite as the anode, and a non-aqueous Li - ion conducting solution or immobilized gel-polymer as an electrolyte¹. LIBs are extensively used in the present-day portable electronic devices and high-power applications like back-up power supplies and electric/hybrid electric vehicles. However, LIBs need to satisfy several additional criteria, namely, cost-reduction, improvement in the energy density, safety-in-operation at high current charge/discharge rates and improvement in the low-temperature-operation.Several simple and complex oxide nanomaterials are synthesized by molten salt and graphenenothermal reduction methods. These materials are characterized by Rietveld refinement X-ray diffraction, X-ray absorption fine structure, X-ray photoelectron spectroscopy, SEM, TEM, density and BET surface area methods, cyclic voltammetry, galvanostatic cycling and electrochemical impedance spectroscopy techniques. Results based on the study of binary metal oxides like MO (M= Co, Ni, Fe, Mn and Cu) and nano SnO₂ and ternary oxides Nano-MCo₂O₄ (M= Mn, Cu, Mg, Zn) will be discussed. Advantages of nano size and matrix elements on capacity values, average charge-discharge voltages, voltage hysteresis and Electrochemical performances will be highlighted.

EO 08

Questions around Electrochemical Impedance Studies of Pelletized Materials

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The transport characteristics demonstrated by solid materials are generally studied via Electrochemical Impedance Spectroscopy (EIS) on pelletized and subsequently sintered samples. This gives information about the resistance through the grains, the resistance and capacitance at grain boundaries, diffusion properties of ions through the material, relaxation effects and so on where applicable. It is well known that the sintering temperature plays a big role in these properties and many studies have been done on a range of materials looking at these effects. However, other preparation parameters are generally either vaguely reported or even not reported at all. In this work we look at the effects of using different pressures to form the pellets by isostatic pressing (a parameter often not reported), the effect of binders at different percentages and the effect of the type of electrode coated onto the pellet and the method used to form these electrodes. The size of the starting particles could also affect the properties, as will be illustrated, and has been raised in several studies but again this is frequently not reported in literature. The question of reproducibility of measurements and sample preparation is also raised. In order for us to make meaningful comparisons with literature data, we need to understand how all these parameters affect the EIS measurements and hence deduce which are critical parameters to report to allow for validation of our characterisation methodologies. **Keywords:** EIS, energy materials, sample preparation.

EO 09 Design of Materials for Advanced energy storage <u>Cengiz S. Ozkan</u>

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I will describe innovative approaches for the design and synthesis of hierarchical three dimensional graphene hybrid materials which possess characteristics including ultra large surface area, tunability, mechanical durability and high conductivity which are appealing to diverse energy storage systems. Integration of nanostructured pseudocapacitive metal oxides received a lot of attention recently due to their superior electrochemical performance. In order to realize high energy density supercapacitors, we developed a scalable method to fabricate MGM (graphene/MWNT/MnO₂) and RGM (graphene/MWNT/RuO₂) hybrid systems. The high specific/areal capacitance and extended operational voltage window of 1.5 V lead to an exceptionally high energy density of 39.28 Whkg⁻¹ and power density of 128 kWkg⁻¹. Next, I will talk about three-dimensional cone-shaped carbon nanotube clusters decorated with amorphous silicon for lithium ion battery anodes. Innovative silicon decorated cone-shaped CNT clusters on graphene (SCCC) are prepared by chemical vapor deposition (CVD) with subsequent inductively coupled plasma (ICP) treatment, followed by depositing amorphous silicon onto the carbon nanotube-graphene templates via magnetron sputtering. The seamless connection between silicon decorated CNT cones and the graphene substrate facilitates charge transfer in the system and provides a binderfree technique for preparing lithium ion battery (LIB) anodes. Lithium ion batteries based on this novel 3D SCCC architecture demonstrated fast charging, a high reversible capacity of 1954 mAhg⁻¹ and excellent cycling stability.

Keywords: Battery, Supercapacitor, Nanomaterials, Anode, Cathode
High Performance Lithium Manganese Silicate Nanoparticulate Cathode Material for Secondary Lithium Batteries

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The transition towards zero emission transportation systems such as electric vehicles, hybrid electric and plug-in hybrid electric vehicles, and the efficient storage or utilization of intermittent renewable energy sources such as solar and wind power require the design of high capacity batteries. Lithium-ion batteries have the highest energy density among all commercialized rechargeable batteries. However, tremendous efforts are being made to replace the commercially available toxic and expensive LiCoO₂ cathode material with eco-friendly, cost-effective and cell-safety cathode materials. In this regard, Lithium metal orthosilicates attract great attention as high capacity cathodes for next generation Li-ion batteries due the possibility of exchanging more than one Li-ion per redox-active transition metal ion. The electrochemical performance of lithium manganese orthosilicate (Li₂MnSiO₄), with a superior theoretical capacity of 333 mA h g⁻¹upon complete delithiation, is limited by low intrinsic electronic conductivity, thus affecting its practical applications in portable electronics and electric vehicles. This study involved a combination of hydrothermal and precipitation synthetic protocols to prepare nanoparticles of Li₂MnSiO₄. The synthesized materials were investigated using High Resolution Scanning and Transmission Electron Microscopies (HRSEM, HRTEM), X-Ray Diffraction (XRD) and Solid-State Nuclear Magnetic Resonance (SS-NMR) Spectroscopy. Electrochemical measurements were conducted using Cyclic Voltammetry (CV) and Electrochemical Impedance Spectroscopy (EIS).

Keywords: Lithium ion batteries, Charge/discharge, Orthosilicate cathode materials, scanning electron microscopy

EO 11

Synchrotron Radiation Grazing Incidence Wide Angle X-ray Scattering Studies of Photovoltaic and Battery Materials

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This presentation will cover a number of different experiments that have been carried out at Diamond Light Source, the UK Synchrotron Radiation Facility on beamline I07. This facility is dedicated to investigating the structure of surfaces and thin films using grazing incidence hard X-ray techniques. A number of different methods are available; in this presentation the focus will be on grazing incidence wide-angle X-ray scattering (GIWAXS) that has proven critical in understanding the structure of photovoltaic materials. These studies have included monitoring the growth in real time during deposition, the effect of humidity on the structure and depth dependent phase changes amongst many others. We will focus on these studies and the equipment that we have developed in order to enable high quality measurements to be recorded under realistic conditions. A recent addition to the facilities on the beamline includes a vacuum chamber to investigate the in-situ deposition of organic molecules of importance in photovoltaic cell structures. This enables pristine structures to be studied together with changes that occur with time or with exposure to gases or a humid environment. This has led to the development of a funded project to improve interactions between UK and African researchers; START (Synchrotron Techniques for African Research and Technology) is a programme funded through the UK Global Challenge Research Fund to study both energy materials and a separate strand of research to study protein structures of importance for African diseases and healthcare. The details of this project will also be presented.

Keywords: Synchrotron, Photovoltaics, Batteries, Grazing Incidence Diffraction, X-ray Scattering

Graphene based inkjet-printable electrodes for Dye sensitized solar cells

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We present a stable inkjet printable graphene ink, formulated in isopropyl alcohol via liquid phase exfoliation of chemically pristine graphite with a polymer stabilizer. The rheology and low deposition temperature of the ink allow uniform printing. We use the graphene ink to fabricate counter electrodes (CE) for natural and rutheniumbased dye-sensitized solar cells (DSSCs). The repeatability of the printing process for the CEs is demonstrated through an array of inkjet-printed graphene electrodes, with ~5% standard deviation in the sheet resistance. As photosensitizers, we investigate natural tropical dye extracts from Pennisetum glaucum, Hibiscus sabdariffa and Caesalpinia pulcherrima. Among the three natural dyes, we find extracts from C. pulcherrima exhibit the best performance, with ~0.9% conversion efficiency using a printed graphene CE and a comparable ~1.1% efficiency using a platinum (Pt) CE. When used with N719 dye, the inkjet-printed graphene CE shows a ~3.0% conversion efficiency, compared to ~4.4% obtained using Pt CEs. Our results show that inkjet printable graphene inks, without any chemical functionalization, offers a flexible and scalable fabrication route, with a material cost of only ~2.7% of the equivalent solution processed Pt-based electrodes.

Keywords: Graphene, Inkjet Printing, DSSC, Platinum, photosensitizers

EO 13 Natural products for materials protection <u>Emeka E. Oguzie</u>

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Our ongoing research project is tagged "Natural Products for Materials Protection" (NPMP), and is related to the inhibition of corrosion of iron and steel surfaces exposed to an aqueous aggressive medium by natural products. Specifically, this project focuses on the systematic investigation of some plant extracts as potential sources of benign corrosion inhibiting additives for iron and steel and involves introduction of the extract into the aqueous aggressive medium in order to bring the inhibitor into contact with the surface to be protected. This study is necessitated by the high costs and toxic nature of most common inhibitors and the need to develop a new class of corrosion inhibitors with low toxicity and good efficiency. We herein present some of our findings employing electrochemical a.c. (impedance) and d.c. (polarization) techniques to study the corrosion inhibiting effects of three tropical plant species - Moringa oleifera (MO), Mimosa pudica (MP), Dacryodes edulis (DO) on the acid corrosion of low carbon steel. Impedance measurements revealed that the steel dissolution process was under activation control and all the extracts inhibited the corrosion process by virtue of adsorption. Potentiodynamic polarization data indicate that the extracts mostly behaved as mixed-type inhibitors. The inhibitive actions of the plant extracts have been discussed on the basis of adsorption of protonated and molecular species of the extracts on the corroding steel surface. Density functional theory-based molecular dynamics (MD) simulations were performed to illustrate the adsorption process of the active species of the extracts at a molecular level and the theoretical predictions showed good agreement with the electrochemical results.

Keywords: Mild steel; Materials corrosion; Corrosion protection; Biomass extracts; electrochemical techniques; Molecular dynamics simulation.

Electrochemical properties and Effect of Deposition Cycles on the Properties of SILAR deposited Cobalt Sulphide thin films

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Dye sensitized solar cell studies based on laser dye, rhodamine 6G dye and natural dyes from *Inigofera arrecta* have been carried out by photocurrent-voltage (I-V) characteristic and electrochemical impedance spectroscopy (EIS) based on AI and Cu doped ZnO (AZO and CZO) thin film electrodes. The concentration of AI and Cu in ZnO were varied between 1-5 at.% in order to study the effect of the variation on the DSSC performance of the electrodes. The absorption spectrum of these dyes in acetonitrile solution indicates appreciable absorption in the range of 538–650 nm with a flat band peak from 538–589 nm indicating its possible use as a photosensitizer for ZnO. The I-V characteristics measured in the dark and under 80 W simulated illumination revealed enhanced DSSC performance for the electrodes with better response achieved for AZO and CZO electrodes with 2 at.% AI and Cu concentration thus, recording higher conversion efficiency and fill factor. The EIS analysis of the frequency spectra for the real and imaginary parts of the complex impedance were in good agreement with the earlier result. There are clear indication that rhodamine dye-sensitized AZO and CZO electrodes are superior to unsensitized ones in DSSC application. The remarkable enhanced properties of AI and Cu doping on ZnO were carefully studied by means of X-ray diffraction (XRD), scanning electron microscope (SEM) and UV-vis spectroscopy, and the results were in good agreement, and confirmed that AZO and CZO thin film electrodes are better for DSSC application than undoped ZnO semiconductor in alliance with rhodamine 6G dye.

Key Words: Photoelectrochemical, rhodamine 6G dye, *Inigofera arrecta*, dye-sensitized electrodes, AZO electrodes, CZO electrodes, chemical bath deposition.

EO 15

2D Materials grown on silicon as highly efficient electrodes for integrated energy storage <u>Francesca lacopi¹</u>

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In just a few years from now, several billions of interconnected "things" will aid the daily life of about 4 billion of people, leading to major improvements in the quality of life, the transport, the environment, the healthcare, and in the efficient use of resources and energy. As many of the smart "nodes" of the internet of things will require uninterrupted power, delocalized power sources with small form -factor seamlessly integrated in the IoT systems will be required. However, power sources are one of the most challenging units in terms of miniaturization and integration with silicon technologies. We have pioneered a thin film approach on silicon to obtain 2D materials with a high surface –area, such as graphenic carbon from a SiC solid source. The obtained material is a very efficient electrode for supercapacitors. We have demonstrated an all-solid-state device with high cyclability and power densities. This approach is very versatile, as it requires no transfer and no binding agents, while the electrodes can be easily patterned at the wafer-level to form interdigitated geometries. In addition, this approach can be extended to alternative 2D materials.

Keywords: 2D materials, silicon, supercapacitors

Highly environmentally stable inverted thin film organic solar cells using tri-metallic nanocomposites

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The challenges in the realization of thin film organic solar cell is low power conversion efficiency and environmental stability of the photoactive film. We have successfully synthesized and employed (Ag:Zn:Ni) trimetallic nanocomposite to address the challenges which resulted in high power conversion efficiency and extremely good life time. The nanocomposites were suspended in the solution of the active layer for the preparation of inverted thin film organic solar cell (TFOSC). The inverted device architecture of TFOSC has known for improving device stability because of its application a stable and high work function metal oxides for charge extractions. However, the incorporation of the metal nanocomposite is found to induce enhanced charge transport and significantly prolonged device stability. In this study, we are reporting the integration of trimetallic nanoparticles in the photoactive medium of an inverted thin film organic solar cells which have survived more than 90 days in ambient environment. The device characterization are discussed in terms of changes in optical, electrical and morphological properties.

Keywords: Organic Solar cell, Inverted structure, Conducting Polymers.

EO 17 Complex composition and structure materials by solution chemistry <u>Gunnar Westin</u>

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For practical application in renewable energy, complex high quality, multi-functional materials of high elemental and structural complexity in sizes down to a few nano-meters, placed in optimised hierarchical architectures are required. However, they also have to be of low cost, which most probably means solution processing with few and fast processing steps, but for its successful utilisation a detailed knowledge about the whole process from the precursor molecules, via the solution processing and heat-treatment, to the target complex materials is required which is hard to obtain. Using low temperature processes and proper precursor molecules there are great possibilities to achieve far from thermodynamically stable materials built with connection to the molecular precursor entities. Here we will describe solution processes to; complex oxides, metal and metal-ceramic composite thin- and ultra-thin films, nano-particles and sponges. We also connect the final structures to the precursors and steps in-between. A wide range of techniques were used including; XRD, IR and Raman spectroscopy, SEM, TEM, XPS and TG/DSC. Examples showing scalability of the processes will also be given.

Keywords: solution processing, thin films, oxides, metals, metal-ceramic nano-composites

Long term stability of magnetite nanofluids for solar engineering applications

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Abstract Long-term stability of magnetic nanofluids is a key requirement for their use in engineering and biomedical applications. This paper investigated the long-term stability of magnetite nanofluids for solar engineering applications. Magnetite nanoparticles were prepared via co-precipitation method. The particle size/size distribution and morphology of prepared particles were analyzed using a Scanning Electron Microscope (SEM). Magnetic nanofluids were prepared by dispersing citric acid-coated and oleic acid-coated magnetite nanoparticles in water and kerosene, respectively. The long-term stability of prepared nanofluids was analyzed using UV-Visible spectroscopy, phase contrast microscopy, and visual observations. Optical properties were measured using a UV-VIS-NIR spectrophotometer for wavelengths between 100 nm and 2500 nm. Based on visual observation, the prepared magnetite nanofluids appeared stable for more than two years from April 2014 to October 2017. These observations were confirmed by the results from UV-Visible spectroscopy and contrast microscopy analyses. The results from optical analysis showed a strong absorption in near and infrared region of the electromagnetic spectrum confirming the possibility of using the magnetite nanofluids in thermal and photovoltaic-thermal collectors.

Keywords: Magnetite nanofluids, solar engineering applications, UV-Visible spectroscopy, optical properties, long-term stability

EO 19 Green chemistry strategies for sustainable functional materials Isabella Concina

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Accessing sustainable energy applications through the use of nanomaterials calls for the development of strategies complying with the principles of green chemistry and enhancing functionality while at the same time reducing the costs for material and device production. This lecture focuses on vacuum free, cheap and scalable strategies to synthesize: i) semiconducting metal oxides (ZnO, SnO₂ and Fe₂O₃), ii) II-VI semiconductors (CdS, PbS, CdSe) and iii) plasmonic metal nanoparticles (Ag, Au, Cu) to be applied as functional materials for energy and environmental applications. Emphasis will be given to the management of critical material properties such as light management and charge transport through the tuning of material aspect. Examples of device fabrication and functional tests in the fields of solar energy conversion and photocatalysis for environmental applications will be discussed. Finally, the limits we are currently facing in these fields as materials scientists will be as well highlighted.

Keywords: metal oxides, II-VI semiconductors, plasmonic nanoparticles, solar energy conversion, photocatalysis

Combining Experimental and Computational Techniques to Understand the Solid Electrode Interphase Formation on Si Electrode in Li-Ion Batteries

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With the current surge in energy demand for electrification of transportation, developing high energy storage devices is essential. Si anode based Li-ion batteries offer huge promise in this regard by providing high theoretical capacity of 3579 mAh/g, 10 times higher than graphite anode based Li-ion batteries (LIBs). One of the major contributor to capacity fade in Li-ion batteries is the uncontrolled growth of the solid-electrolyte interphase (SEI) layer. SEI is formed due to the decomposition of electrolytes and consumes Li ions. Despite a significant amount of work on SEI, our understanding of both its formation and growth is still limited. This talk has two parts. The first one is about understanding the lithiation mechanism of the inevitable native oxide on the SI surface, identify the stable phases formed due to the lithiation and how these stable phases become part of the SEI by using Abinto molecular dynamics and X-Ray Reflectivity (XRR). The second part is studying the effect fluorinated additives in ordering of the electrode – electrolyte interface by combining XRR and Sum frequency generation (SFG) vibrational spectroscopy and how this might affect the SEI composition, morphology, and ultimatly battery perfomance. This fundamental understanding of SEI formation would enable to find better strategies for designing high-performance LIBs.

EO 21

The Development of a CSP based Milk Pasteuriser for use in rural areas of South Africa <u>J.G. Mallett</u>^{1,2,3}, M. Maaza^{2,3}w. J Perold¹ S Khamlich^{2,3}

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Currently in South Africa, there is a significant portion of the population that live in rural areas without adequate infrastructure and an unreliable electricity supply. Many of these people and communities rely on their own produce as their main source of food supply or income. Milk produced from dairy cattle is among the sources that provide large amounts of nutrition. Raw milk can however contain significant amounts of harmful bacteria which make it potentially unsafe for consumption; it also has the issue of spoiling in a short space of time if not treated properly. Pasteurisation is the process of heating milk to specific temperatures for variable periods of time; this kills the harmful pathogens of raw milk as well as increasing its life span, all without damaging the nutritional properties. However where infrastructure is not available, this heating procedure could be challenging and expensive. These issues can be eluded by making use of solar energy, a resource that is abundant in South Africa. This can be done by using the heat from solar rays to heat the milk to the necessary temperatures without the need for any electricity or other fuels. By concentrating the suns energy using Concentrated Solar Power (CSP), higher temperatures can be reached and the necessary process time can be reduced. By using a small scale parabolic trough system, solar energy can be concentrated onto a receiver tube, inside which raw milk can be pumped. The energy concentrated onto the pipe will then heat the raw milk to the temperatures necessary for pasteurization. Selective solar absorbers will also be used to coat the absorber tube to allow for greater solar absorption and reduced thermal emissions.

Keywords: Concentrated Solar Energy, Milk Pasteurization

Novel photocatalytic materials for hydrogen production

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 TiO_2 is the run-of-the-mill heterogeneous photocatalyst. It shows high activity in the UV domain, but near zero activity in the visible and IR range. Plasmonic photocatalysts constituted of metal nanoparticles exhibiting surface plasmon resonance (SPR) and a semiconducting metal oxide have been extensively investigated, because they can extend the activity of the photocatalyst to higher wavelength illumination. However, from an economic point of view, the large-scale use of such photocatalysts will be curtailed by the prohibitive cost and availability of noble metals. We propose here two strategies to reduce the amount of such metals. In the first one, we demonstrate that the activity of the photocatalyst can be tuned by exploiting whispering gallery mode (WGM) resonances expressed within the semiconductor. In the second one, we demonstrate that carbon can play a synergistic role in the development of the photocatalytic activity of an Au-TiO₂ composite plasmonic photocatalyst. Photocatalytic degradation of dyes, PEC and IPCE measurements all point toward the fact that a sandwich structure, whereby Au is sandwiched between graphene leaflets at the surface of TiO₂, gives the highest activity. However, for hydrogen production, the TiO₂@C-Au catalyst exhibits an activity which is five times greater than TiO₂@C, indicating a synergistic action of plasmonic Au NPs and graphene. Thus, although the presence of carbon can result in a significant increase of the activity of the catalyst, this increase can only be achieved if the spatial arrangement of the Au and C on TiO₂ is finely controlled. Last, we will present the use of these materials in large-scale depollution applications.

Keywords: Photocatalysis, plasmonic nanoparticles, water splitting

EO 23

Degradation of Aluminide Thermal Barrier Coating (TBC) on Inconel 713 LC used for **Compressor Turbines (CT) of Short-haul Aircrafts**

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Thermal degradation of aluminide protective thermal barrier coatings on Inconel 713LC used for CT blades of short-haul aircraft fleet was studied. The blades samples were subjected to scanning electron microscopy (SEM), energy dispersive spectroscopy (EDS), XRD and XRF analyses at the tips, airfoil, as well as the base, transverse and longitudinal, sectioned and unsectioned to investigate their role in having the blades retired from service at 6378 hours, as opposed to their preset service time of 10000 hours. It was found out that during the deterioration of the coating was greater at the tip of the blade and lesser towards the base, evidenced by cracks of the TBC at the tip. This led to severe thermal attack into the material of the blades, prevalent at the tips of the leading edge. The results further suggest that for both the transverse and cross section the tips were severely damaged compared to the airfoil and the base.

Keywords: Thermal Barrier Coating, Compressor Turbine, Short-haul aircraft, Inconel 713LC

Investigating the Suitability of Morupule Coal for Coal Gasification Technology

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Coal has proved to be a prime driver of the economy through the delivery of sustainable energy source to the industries. The widespread occurrence and abundance of coal makes it the world's principal source of energy for a wide variety of <u>end uses</u>. However, several researchers have indicated that coal combustion is a prime contributor to greenhouse emissions deteriorating the climate. This paper investigates the suitability of Morupule coal from S4, S3 and EM1 sections of the main seam for gasification technology through characterization and species transport. The characterization of coal was done by thermal analysis (Thermogravimetric Analyzer) to determine its proximate properties while numerical simulation using Ansys software was done for species transport. The samples under investigation proved to be of high ash and sulphur content, and medium volatiles bituminous parent rock, whilst species transport revealed a sufficient syngas yield per kilogram of coal for downstream processes.

Keywords: Coal, Gasification, Morupule Coal, <u>Thermo-gravimetric</u> Analyser, Ansys software

EO 25

Zinc Oxide nanorod structures grown by chemical bath deposition on a seed layer prepared by a successive ionic layer adsorption and reaction (SILAR) method <u>K. Mosalagae¹</u>, D.M. Murape¹, L.M. Lepodise¹, Z.N. Urgessa²

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Zinc Oxide (ZnO) nanorods were grown by chemical bath deposition (CBD) on glass substrates coated with a seed layer prepared by a successive ionic layer adsorption and reaction (SILAR) method. The effect of varying the number of deposition cycles for the preparation of the seed layer on the orientation, distribution and uniformity of the subsequently grown nanorods was explored. The growth conditions: growth time, temperature and precursor concentration, of ZnO nanorods by CBD method were kept constant. The CBD solution was prepared by mixing equal molar concentration of zinc acetate dihydrate and hexamethylenetetramine at 80°C for 60 minutes. The growth temperature and time were kept constant at 80°C and 5 hours respectively. The X-ray diffraction (XRD) revealed an increase in intensity of the strong diffraction peak from (002) and other low intensity diffraction peaks as the number of deposition cycles was increased. Raman spectroscopy results confirmed the presence of defects in the nanorods. The morphology of the nanorods was studied using Scanning Electron Microscopy (SEM). SEM revealed improved vertical alignment of the hexagonal wurtzite structure of ZnO nanorods as the number of seed layer deposition cycles increased. Zn and O elements were confirmed present in the nanorods by energy dispersive spectroscopy (EDS). The optical transmittance and absorbance of the nanorods was measured by UV/Vis spectrophotometer. In general, it is shown that the orientation, distribution and uniformity of the nanorods grown on such lattice mismatched substrates is controlled by the under laying seed layer. Detailed results showing these effects will be presented.

Keywords: Zinc Oxide, nanorods, chemical bath deposition, SILAR

Biotemplating Pores with Size and Shape Diversity for Li-Oxygen Battery Cathodes

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Synthetic porogens provide an easy way to create porous structures, but their usage is limited due to synthetic difficulties, process complexities and prohibitive costs. Here we investigate the use of bacteria, sustainable and naturally abundant materials, as a pore template. The bacteria require no chemical synthesis, come in variable sizes and shapes, degrade easier and are approximately a million times cheaper than conventional porogens. We fabricate free standing porous multiwalled carbon nanotube (MWCNT) films using cultured, harmless bacteria as porogens, and demonstrate substantial Li-oxygen battery performance improvement by porosity control. Pore volume as well as shape in the cathodes were easily tuned to improve oxygen evolution efficiency by 30% and double the full discharge capacity in repeated cycles compared to the compact MWCNT electrode films. The interconnected pores produced by the templates greatly improve the accessibility of reactants allowing the achievement of 4,942 W/kg (8,649 Wh/kg) at $2 \text{ A/ge}(1.7 \text{ mA/cm}^2)$.

EO 27

Exploring the $Y_xBi_{2-x}O_{\delta}$ Family for an Improved SOFC Electrolyte

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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 °C) 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 δ -polymorph of Bi₂O₃ – the highest known oxide ion conductor. Normally only stable within a high and narrow temperature range (730-824 °C), this polymorph has been exclusively studied in this work with the primary aim of stabilizing the δ -polymorph structure (Fm $\overline{3}$ m) to lower temperatures by means of yttria doping. These attempts have been successful; various Y_xBi_{2-x}O_{δ} members have been found to display the Fm $\overline{3}$ m structure at room temperature.

Keywords: SOFC, PXRD, electrolyte

EO 28 The Lyncean Compact Light Source: A Miniature Synchrotron for your Laboratory

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Synchrotron facilities around the globe are the supercomputers of X-ray science. There are more than sixty synchrotrons worldwide serving more than ten thousand researchers. The light emanating from these sources can be characterized as high flux, monochromatic, energy tunable and, in some cases, coherent. They provide a myriad of applications to thousands of researchers, but they come at a high cost requiring government support, and can take more than a decade to fund, design and construct. The Lyncean Compact Light Source (CLS) is the first commercially developed X-ray source specifically created to deliver a true home laboratory alternative to many experiments done today at the large synchrotrons. X-rays are produced via inverse Compton scattering through the interaction of low energy electrons (25 to 45 MeV) in a miniature storage ring with a micrometerperiod, high powered laser pulse (laser-undulator). Tunable, monochromatic, and high flux undulator synchrotron radiation is generated in the CLS "mini-synchrotron" due to the high repetition rate (~60MHz) of this interaction. Characteristics of the CLS X-ray beam are similar to those of a bending magnet synchrotron in terms of flux and coherence, and as such, similar applications can be performed: imaging/tomography, diffraction, scattering, and spectroscopy. The Lyncean CLS is an ideal first step for regions aspiring to build a synchrotron community. The Lyncean CLS provides a state-of-the-art tool for learning synchrotron techniques together with hands-on operation of accelerator technologies. The development and retention of a local, expert scientific beamline community can be established with a modest investment. In this presentation we will present the technology behind the Compact Light Source as well as examples of the measurements that have been made and that can be made with the Lyncean Compact Light Source.



Figure 1. Photograph of the Lyncean Compact Light Source miniature synchrotron.= **Keywords:** X-ray source, synchrotron, inverse Compton scattering

EO 29 Structure Comparison of Lithium Iron Cathode materials

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Lithium ion batteries are categorised as rechargeable batteries; this has inspired numerous developments in this research field. Lithium ion batteries convert electrochemical energy into electrical energy and the process is reversible making them suitable for energy storage systems. Having efficient and long term storage devices could possibly lead to a green and sustainable future. The cathode material remains the largest focus area for the improvement of the battery performance.² A good cathode material should include thermal and chemical stability, high capacity, affordability and low toxicity.¹ Iron containing cathode materials have shown to fit the criteria of a good cathode material and can possibly replace the existing cathode materials in certain applications. Two cathode materials have been investigated namely lithium iron phosphate and lithium iron borophosphate.

Although extensive studies have been conducted on the phosphate materials, very little is known about the borophospohates which would make an interesting comparative study. Both materials were synthesised using a hydrothermal route and were doped with different percentages of zinc. These cathode material candidates have been characterised using powder X-ray diffraction with Rietveld refinement analysis and Mössbauer spectroscopy. Since the structure and property of the materials are interrelated, it is important to understand both aspects and the electrochemical properties of these materials will be looked at next. **Keywords:** Lithium Iron, cathode, PXRD, Mössbauer

EO 30 Sulfur cathode materials for lithium–sulfur batteries Mihri Ozkan

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In this study, silica-coated sulfur particles (SCSPs) were synthesized and characterized as a cathode material for Li–S batteries. The novel core–shell structure was fabricated in a facile 2-step wet chemical synthesis. The SCSP cathode showed superior cycling stability when coupled with mrGO (mildly reduced Graphene Oxide) as an additive, improving the capacity retention after 50 cycles from 440.8 mAh/g without mrGO to 763.2 mAh/g with mrGO. The electrochemical data also shows reduced capacity fading over 50 cycles, from 12.2 mAh/g per cycle without mrGO to 8.6 mAh/g per cycle with mrGO. During cycling, SCSPs are understood to fracture and release active material (S8), and mrGO helps to contain the ruptured particles, thereby improving cycling stability. By the 50th cycle, SCSPs experienced a 318.8 mAh/g boost in specific discharge capacity with the addition of mrGO. These improvements are attributed to the polysulfide inhibiting effects of SiO2 as well as the host of benefits provided by mrGO, similar to other work. Thus, SCSPs with the addition of mrGO show great promise in the application of low-cost, high energy density battery systems for portable electronics and electric vehicles.

Keywords: sulfur, battery, cathode

EO 31 Catching the sun at low cost <u>Mmantsae Diale</u>

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Southern Africa has been recognized as a region of high solar energy collection with very little natural interferences. It is thus worth investing in collection and conversion of solar energy, making it available as electricity to millions of our communities, thus reducing poverty and the effects of climate change. This is achievable with low cost abundant materials in the region by engaging science to produce simple devices. When you walk through the countryside of South Africa there are three distinctive colours: blue, green and red. Bright blue skies are evidence of very abundant energy from the sun. Green testifies that this energy is converted and stored on a massive scale. Red comes from iron-oxide in our soil, commonly called rust. In our work, we have used fluorine doped tin oxide as substrate materials to make dye sensitized solar cells. Our dye sensitized solar cells are doped with copper nanoparticles to enhance efficiency of the devices. Rust has been used in photoelectrochemical cells to produce hydrogen from water as a method of solar energy storage. In this work, we will demonstrate our success in materials development and device fabrication to collect and convert solar energy for use when the sun comes up and when the sun goes down.

Keywords: solar cell, hydrogen, hematite, ZnO, PEDOT:PSS

Insights into the development of advanced electrode materials for rechargeable sodium ion batteries

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During the past two decades, the demand for the Electrical Energy Storage systems has increased for both portable and stationary applications, predominantly in the form of batteries. In this sense, lithium-ion batteries (LIBs) have dominated the market as offer the highest gravimetric capacity. However, owing to concerns over lithium cost and sustainability of resources, sodium-ion batteries (NIBs) have recently attracted interest of the scientific community since sodium chemistry is considered as an attractive alternative to LIBs in terms of cost, safety, and sustainability. Current research into cathode materials encompasses a wide range of different chemistries, amongst which layered oxides and polyanionic compounds stand out as the most attractive candidates. Our recent research focuses on the synthesis and extensive characterizations by means of ex-situ and in-situ measurements of low cost and environmentally friendly electrode materials for NIBs. In this work, several examples related to different cathode materials will be selected to review and discuss some aspects of our research such us:

- 1. understanding the reaction mechanisms of Na-ion electrode materials.
- 2. synthesis methods its impact in the final cost and performance of the material.
- 3. strategies to increase the operation voltage in cathode materials
- 4. strategies to improve the electrochemical performance of the material
- 5. the possible use of aqueous electrolyte

Keywords: synthesis, structural characterization, in-situ measurements, electrochemistry, Na-ion batteries

EO 33

Effects of Bending and Stretching on Composite Organic- Inorganic Trihalide Perovskite Solar Cells

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Hybrid organic- inorganic trihalide perovskite solar cells have attracted significant interest due to their unique optoelectrical properties, ease and low cost of fabrication. However, the mechanical performance of perovskite devices has not yet been fully understood. Failure mechanisms of these devices relating to stretching and bending forces have not been completely elucidated. In this paper, lead-based and tin-based perovskite solar cells on poly(ethylene terephthalate) [PET] and polydimethylsiloxane [PDMS] substrates were modeled and subjected to bending and stretching forces using finite element analysis. Preliminary results exposed PET as a more suitable substrate for bending applications while PDMS showed greater compliance for stretching purposes. Contour plots obtained showed that the relatively high modulus of elasticity and layer thickness of TiO₂ nanocrystals reduces the mechanical performance of the solar cell where flexibility is desirable. Furthermore, huge difference in elasticity between the Aluminium contact layer and the photoactive organic-inorganic material is a plausible explanation for high stress levels observed on the former in the multilayer structure. This results provide insights into the potential brittleness of these systems and their robustness for applications where flexibility is desirable.

Keywords: Perovskite, flexible, failure mechanisms, computational modeling.

Utilization of coal combustion and waste tyres pyrolysis by-products as feedstock and support for producing porous materials for energy storage applications

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Porous materials are well-know and have received significant attention in the fields of nanotechnology, material science and engineering. Even though there are several methods for producing various types of porous inorganic and carbon-based materials, there is always a need to identify innovative and cost-effective strategies that could drive down their cost of production. This talk will highlight two different strategies for utilisation of coal fly ash (CFA) in the production of low-cost zeolites and carbonaceous materials for energy storage applications. In the first instance, CFA is used as a feedstock for the production of zeolites which are then used as templates/nanocasts for producing zeolite-templated carbons. The resulting highly porous carbons are thereafter tested for hydrogen storage applications. In the second case, CFA together with its magnetic extract is utilised for the production of carbon nanofibers/tubes using waste tyres pyrolysis by-products (pyro-gas and oil) as the carbon precursor. Both strategies results in materials that are comparable to those produced from commercially available feedstocks, at a relatively lower cost. The materials are thoroughly characterized using techniques such as XRD, SEM, TGA, TEM, N2 and H2 sorption.

Keywords: Coal fly ash; waste tyres; zeolites; teolite templated carbons; carbon nanofibers/tubes

EO 35 Ab-initio simulations of photocatalysts for hydrogen production Nicola Seriani¹

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First-principles simulations based on density functional theory can provide insight into the behaviour of transition metal oxides of importance for photocatalysis. I will show how the effect of the environment can be taken into account, and how parameters relevant for materials performance can be extracted from the simulations. A detailed understanding of mechanisms acting at atomic level can be achieved for photocatalytic water splitting. Finally, limitations of this approach and future developments will be discussed.

Keywords: Hematite, titania, photocatalysis, water splitting, density functional theory

α-MnO₂/Onion Like Carbon (OLC) composite cathode material for aqueous Zn-ion battery

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Recently, aqueous Zn-ion (multivalent ion)rechargeable battery (ZIB) has a tremendous exposure with in the research world marketbecause of itslarge-scale energy storage potential applications. Moreover, Zn has various outstanding properties such as reasonable redox potential, high safety, low cost, most abundantand eco-friendly compared with the post lithium ion batteries (LIB).Zn metal as an anode delivers a high gravimetric (820 mAh g⁻¹) and volumetric (5855 mAh cm⁻³) capacities¹.The previous explorations of the cathode materials such as manganese based oxides (α - γ -MnO₂ and Todorokite-MnO₂) were used for aqueous Zn-ion batteries. However, this variety of cathode materials suffers a rapid capacity fading roughly during the initial 20 cycles, also poor rate capabilities and inadequate cycling performance². Thus, we report for the first time, the manganese oxide composite (α -MnO₂/OLC) cathode material for stable cycling with better specific capacity in aqueous based electrolyte. Herein, α -MnO₂nanorods cathode materials were synthesised via molten salt method and for the α -MnO₂/OLC composite, the appropriate amount of α -MnO₂ and OLC were dispersed using ultra-sonicator and magnetic stirrer and dried it in an vacuum oven.The electrochemistry was demonstrated using Zn-foil as anode and aqueous electrolyte of 1M ZnSO₄ with the addition of 0.1M MnSO₄. The α -MnO₂/OLC composite exhibits a high and stable capacity of ~150 mAh g⁻¹ cycled at 1C with potential window 1.0 – 1.8 V.

Keywords: α -MnO2, OLC, Molten salt method, cathode, Zn-ion battery.

EO 37

The application of remote sensing techniques for energy conservation in low-income housing units

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Domestic burning of biomass fuels remains a huge contributor to anthropogenic climate change around the world moreso in developing countries. The use of solid fuels for domestic heating and cooking causes indoor and outdoor air pollution. Carbonic fuels also contribute to greenhouse gases as well as emission of particulate matter. Exposure to particulate matter threatens the wellbeing and health of human beings. For those who reside in informal settlements and low income settlements a lot of energy is lost due to poor quality structures leading to overconsumption of an energy carrier. High expenditure on energy for poor households worsens energy poverty within low income households. The study explored how heat can be lost through the roof. A combination of air based remote sensing and in-situ measurements were used. Findings from the study were that housing units without loft insulation loose more heat through the roof more than housing units with loft insulation.

Keywords: domestic burning, indoor air pollution, low-income housing units, remote sensing

Photostability of polymer-fullerene and polymer-non-fullerene solar cells: the effect of UV on the material chemical structure and on DIO in the active layer

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Semiconductor materials are essential for the advancement of polymer solar cell technology. The design of novel materials has brought more attention to bulk heterojunction polymer:fullerene (PF) and polymer:non-Fullenere (PnF) solar cells in the past decade. A typical example is the synthesis of non-fullerene acceptors (e.g ITIC*) and of the benzodithiophene-co-thienothiophene (BDT-TT) polymers leading to power conversion efficiency (PCE) of over 10%. This work examines the effect of UV light on the photostability of PF and PnF solar cells. First, it studies the effect of polymer chemical structure on photostability of PF cells made of two classes of BDT-TT, namely, 1D polymers and 2D polymers. The polymers differ from each other only by the substituted side chains on the benzodithiophene-unit with alkoxy groups on the 1D and alkylthienyl groups on the 2D polymers. Through combined experimental techniques, the relationship between the polymer chemical structure and the UVstability of the solar cells is explored on the one hand, and on the other hand, the effect of diiodooctane on their UV-stability. Based on the polymer chemical structure, solar cells of the 1D polymers are found more stable (10-18% loss in PCE) than those of the 2D polymers (35-48% loss in PCE) over the period of study. Second, it examines the effect of the acceptors on photostability by comparing the PF cells to PnF cells. Based on the acceptor, PnF cells are found more stable (20% loss) than PF solar cells (40% loss). Finally, we postulated the mechanisms behind the observed relation between UV-degradation and the chemical structure of the materials on the one hand and the relation between UV-degradation and DIO within the films on the other hand. These findings pave the way for new materials and additives that yield efficient as well as stable organic solar cells. Notes:

* ITIC: 3,9-bis(2-methylene-(3-(1,1-dicyanomethylene)-indanone))-5,5,11,11-tetrakis(4-hexylphenyl)-dithieno[2,3-d:2',3'-d']-s-indaceno[1,2-b:5,6-b']dithiophene

Keywords: polymer solar cell, additive, UV-degradation, photostability, lifetime

EO 39

Photovoltaic properties of Cu_xAl_yS₂ thin films deposited by chemical-bath deposition. <u>Phindani Dube</u>, Albert Juma

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Cu_xAl_yS has recently gained interest as an alternative earth-abundant absorber material for thin film solar cells. Cu_xAl_yS belongs to Group I (ternary chalcopyrites) of ternary ABX₂ semiconductors, which consists of the A^IB^{III}X₂V^I compounds where A=Cu, Ag; B=Al, Ga, In; and X=S, Se, Te. Cu_xAl_yS possesses excellent qualities which make it a suitable candidate for solar cell applications; a band gap in the range 1.0–3.5 eV covering the wide spectral region from ultraviolet to near infrared, optical absorption coefficient in the order of 10⁴ cm⁻¹ and p-type conductivity. All the elements of Cu_xAl_yS are earth abundant, inexpensive and environmentally benign. Several methods have been utilized for preparing ternary chalcopyrite Cu_xAl_yS such as chemical spray pyrolysis, chemical bath deposition, spark plasma scattering, metal decomposition, iodine transport, single source thermal evaporation deposition. This work reports Cu_xAl_yS thin films prepared by chemical bath deposition, which is a low-cost, simple (ease of handling) method that produces thin films that strongly adhere to glass substrates. The sample solution was prepared with a molar ratio of Cu: Al: S =1:1:10 respectively, glass substrates were vertically immersed in a solution, after half an hour they were washed with distilled water and allowed to dry at room temperature. The concentration of the sample solution was kept constant in each cycle. The deposition temperature was kept at 50⁰ C.X-ray diffraction (XRD) analysis showed that the as-deposited films were amorphous. The Raman measurements revealed an increasing peak intensity with increase in number of deposition cycles, the optical absorption measurement showed that the films were highly absorbing with an estimated band gap energy of 2.7 eV. The absorption coefficient was found to be in the order of 10^4 cm⁻¹ for a film thickness of around 300 nm. The films also showed p-type conductivity with carrier concentrations of 10^{-21} cm⁻³. Current-voltage characteristics of ZnO/Cu_xAl_yS₂ heterojunction will also be discussed.

Keywords: Photovoltaics, Absorber, Chemical bath deposition, chalcopyrite

EO 40

Quaternized PPO/PSF Anion Exchange Membranes doped with Nanoparticles for Fuel Cell Application

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Alkaline anion exchange membrane fuel cells (AAEMFC) have been recognized as ideal candidates for the generation of clean energy for future stationary and mobile applications due to their many advantages. The key component of the AAEMFC is the anion exchange membrane (AEM). In this report, a series of quaternized poly (2.6 dimethyl – 1.4 phenylene oxide)/ polysulfone (QPPO/PSF) blend AEM were successfully fabricated and characterized for alkaline fuel cell application. Zinc Oxide (ZnO) nanoparticles were introduced in the polymer matrix to enhance the intrinsic properties of the AEM. The characteristic properties of the QPPO/PSF and QPPO/PSF-ZnO blend membrane were investigated with X-ray diffraction (XRD), thermogravimetric analysis (TGA) scanning electron microscope (SEM) and contact angle (CA). To confirm successful quaternisation, FT-IR spectroscopy and proton nuclear magnetic resonance (¹H NMR) were used. Other properties such as ion exchange capacity (IEC), water uptake, contact angle and ion conductivity (IC) were also undertaken to check if the prepared nanocomposite materials are suitable for fuel cell application. The membrane intrinsic properties were found to be enhanced by the addition of ZnO nanoparticles. The addition of ZnO nanoparticles resulted to a highest IEC of 3.72 mmol/g and a 30-fold IC increase of the nanocomposite due to its lower methanol permeability. The above results indicate that QPPO/PSF-ZnO is a good candidate for fuel cell AAEMFC application.

Keywords: Quaternized polysulfone, Polyphenylene Oxide, Anion Exchange Membrane, Nanoparticles, Fuel Cells

EO 41

Metal Organic Frameworks (MOF)-Derived Nano porous Carbon as Efficient Sulphur Host for Lithium–Sulphur Batteries

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Recently lithium–sulfur battery has drawn much attention owing to their high power density and low cost of sulphur. However efforts have been made previously to design cathode materials, but due to poor conductivity and chemical bonding of sulphur to parent material and lacuna in physical properties, restrict the materials for practical applications. In the present study we are trying to develop a dual core–shell structured Mn@S@ MOF-derived Carbon nanocomposites which will be a solution to previous problems. Metal organic frameworks (MOF) with high surface area will act as good precursor for Mn-MOF-derived carbon, which could be helpful in encapsulating sulfur and prevent its leakage from the cathode side of the battery. We anticipate that the highly porous MOF-derived carbon will be able to improve energy density, decay in capacity and increase the conductivity of the cathode material for Li–S battery application.

Keywords: MOF, Nano Porous Carbon, Sulfur host, LiS battery

Comparative performance of non-conventional Ga_{1-x} InxNyAs_{1-x} sub-junction for tandem solar cells <u>R. Ketlhwaafetse¹</u>, B Royal²

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Tandem solar cells have projected efficiencies of more than 50 % and are potential candidates for "4th generation photovoltaic devices". In order to achieve such projected efficiencies a near 1.0 eV sub-junction with good optical and electrical properties is sought. The quaternary alloy Ga1-x InxNyAs1-x has the ability to reduce the GaAs bandgap while still lattice matching GaAs. Therefore GaInNAs/GaAs junction is a logical choice for replacement of bottom Ge sub cell in the Ga0.44In0.56P/GaAs/Ge triple junction structure for efficiency enhancement [1]. The minority carrier lifetimes observed in Ga1-x InxNyAs1-x are often less than 1 ns [2], which is 500 times less than typical GaAs minority carrier lifetime [4]. The short minority carrier lifetimes result in very short diffusion lengths that make it a challenge to design the Ga1-x InxNyAs1-x /GaAs solar cells with conventional design that works well for the GaAs solar cells. Therefore a number of non-conventional designs which include; the p-i-n bulk, p-i-n MQWs and n-i-p-i, are commonly used for Ga1-x InxNyAs1-x solar cells. In this letter the relative performance of Ga1-x InxNyAs1-x /GaAs junctions' solar cells of different designs is studied. Performance parameters reported are: temperature coefficients of efficiency and dark current.

Keywords: Ga1-x InxNyAs1-x, dark current, solar cell, efficiency

EO 43 Improving the Photooxidative Stability of Organic Photovoltaic Technologies Sarah Holliday ^{1,2}, Christine Luscombe ^{1,2,3}

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Emerging solar photovoltaic technologies such organic photovoltaic (OPV) cells offer great potential for manufacturing high-efficiency, lightweight and flexible solar cells via low cost, roll-to-roll printing methods. This can be of great benefit in terms of expanding solar energy capacity globally, and especially in many regions of Africa where the level of solar radiation is high and there is a great need for low-cost solar energy solutions for rural electrification. However, several steps are still required to take OPV technology to market readiness. Specifically, the devices must combine high efficiency, low-cost and long-term stability. In recent years, significant advances have been made in improving the power conversion efficiency of OPV cells. However, some of the highest efficiency devices are also among the least stable.[1] Here we present a detailed study of the photooxidative degradation of organic photovoltaics based on two widely used benzodithiophene-co-thieno[3,4b]thiophene polymers, PTB7 and PTB7-Th. We show that both the chemical structure and the solvents used for film deposition have an important effect on active layer stability.[2] In particular, high boiling point solvent additives such as 1,8-diiodooctane (DIO) are shown to dramatically accelerate photooxidation. By replacing high boiling point solvent additives with lower boiling point additives, the photooxidative stability can be greatly enhanced without the need for high temperature or vacuum treatments, making these systems more scalable and compatible with roll-to-roll printing. This result offers a promising way forward in developing scalable, stable and high efficiency organic solar cells. The Clean Energy Institute (CEI) at the University of Washington is committed towards advancing the development of next-generation solar energy and battery materials and devices, as well as their grid and systems integration. The CEI is currently working together with the African Network for Solar Energy (ANSOLE) to build connections with African researchers working in clean energy technologies.

Keywords: Solar energy, photovoltaics, organic photovoltaics, semiconducting polymers, polymer photooxidation.

Fundamental and High Throughput Advances in Electrochemical Energy Technologies

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The electrodes in devices such as fuel cells, electrolyzers and batteries are almost invariably formed as ill-defined composites of multiple active components. Consequently, attaining a deep understanding of how the electrochemical reaction of interest proceeds, or where and how any degradation occurs is extremely challenging. To address this, some researchers have employed model geometries in which the composite configuration is precisely defined. However, as a consequence of the extreme effort involved in such studies, only a limited number of materials have been examined in this way. We describe here high throughput approaches that enable rapid evaluation of multiple materials in a precisely defined geometry. Example results are presented for (La,Sr)MnO₃, a canonical solid oxide fuel-cell (SOFC) cathode material, and for (La,Sr)(Co,Fe)O₃, a system also widely studied for SOFC cathode applications.

Keywords: oxygen reduction reaction (ORR), mixed ion and electron conductor (MIEC), electrocatalysis

EO 45 Tuning Heterogeneous Electrocatalysts for the Chlorine Evolution and Oxygen Evolution Reactions Using Atomic Layer Deposition

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The efficiency of a variety of environmentally and industrially important chemical reactions, such as the oxygen evolution reaction (OER) and chlorine evolution reaction (CER), is currently hampered by the high overpotential of heterogeneous electrocatalysts. Traditionally, optimizing heterogeneous catalysts has been difficult owing to the relatively few available tools to engineer reactant binding. We have developed a general technique to optimize the catalytic performance of heterogeneous electrocatalysts by tuning the surface properties with thin films of TiO₂. Using this method, we are able to improve the overpotential of an IrO₂ catalyst for OER and CER by 200 mV and 140 mV, respectively. In addition, we demonstrate that this effect is generalizable to a variety of materials systems. The overpotentials of an FTO catalyst were reduced by 140 mV for the CER and the RuO₂ catalysts were improved by 300 mV for OER with deposition of thin layers of TiO₂. The improvement in catalysis for each of these materials systems is correlated with a change in the surface charge density of the electrocatalyst. This work represents a breakthrough in the field of heterogeneous electrocatalysis and could allow for the optimization of catalysts for other industrially and environmentally important chemical reactions.

Keywords: catalysis, surface charge, heterogeneous, atomic layer deposition

Characterization of PbSO Thin Films by ESCA Technique for Photovoltaic Application Robinson J. Musembi

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The Lead Sulphide (PbS) thin films have been deposited by chemical bath deposition (CBD) technique at 40°C for 10 minutes. Characterization using Electron Spectroscopy for Chemical Analysis (ESCA) has revealed peaks at 137.4 – 139.3eV and 137.3 – 137.8 eV of the binding energy which are ascribed to PbO and PbS energetics, this means that the CBD-PbS is a mixed phase consisting of PbO and PbS, respectively in mixed ratio of around 1.0:3.8, we can therefore safely say that CBD-PbS is more likely PbO_zS_{1-z} with z = 0.21. On annealing the thin films in air at various temperatures, Oxygen has been observed to increase while on the other hand Sulphur is seen to decrease, the valence band is also observed to decrease on annealing. Annealing at different temperature is a useful technique for bandgap engineering of this type of material as the bandgap has been observed to vary at different annealing temperature from the bulk material bandgap of 0.43 eV to the new bandgap of 0.85 eV, this is useful for application in photovoltaic since bandgap tuning can lead to an increased conversion efficiency of a solar cell device. Preliminary test device solar cell of the type TiO₂/In(OH)_xS_y/PbSO/PEDOT:PSS/Au has been fabricated and has shown the following parameters: $V_{oc} = 0.28$ V, $I_{sc} = 7.4$ mA/cm², FF = 0.4 and conversion efficiency 0.83%. The low conversion efficiency has been attributed to interface recombination losses.

Keywords: Lead Sulphide, Thin Films, Photovoltaics, Solar Cell, Conversion Efficiency, Chemical bath.

EO 47

Nanomechanical and Morphological Characterization of solution-processed MoO₃ and MEH-PPV inter-layer for OLED applications

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In recent years, organic light emitting diodes (OLEDs) have attracted significant research interests for lighting and display applications. This is due to their relatively low cost of processing and manufacturing. Much effort has been made in the improvement of the efficiency of these devices through the optimization of the different device layers. The lifetime and reliability of these devices still remains a main issue of concern. This paper presents some studies of the nanomechanical and morphological characteristics of solution-processed molybdenum trioxide (sMoO3) and poly [2-methoxy-5-(2-ethylhexyloxy)-1,4-phenylenevinylene)] (MEH-PPV) thin films and their interface for OLED applications. The sMoO3 films, annealed at different temperatures ranging from 250 °C to 600 °C were characterized using scanning electron microscopy (SEM) and scanning probe microscopy (SPM) imaging for surface morphology and roughness studies. Fourier Transform Infrared Spectroscopy (FTIR) was used to determine the chemical binding of the sMoO3 and MEH-PPV films. Nanoindentation of the sMoO3/MEH-PPV bilayer was done to study the interfacial reliability, adhesion, viscoelastic, fracture toughness and creep properties of the bilayer. The results from this study are relevant for the design of mechanically robust systems that meet the appropriate reliability targets for OLED light and display applications.

Keywords: sMoO3, Nanoindentation, Morphology, OLED.

Structural and Magnetic Properties of Multiferroic Chromite Nanoparticle thin films and Core-shell particles

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In core-shell nanoparticles, exchange bias has been observed in ferromagnetic core/antiferromagnetic shell. Exchange bias has been an intense area of research from both fundamental and application points of view. In case of core-shell nanoparticles, EB has been observed in ferromagnetic core/antiferromagnetic shell, FM core/ferrimagnetic shell, and more recently in AFM core/FIM shell. A common feature in a field-cooled hysteresis loop for a system exhibiting EB is vertical shift along the magnetization axis and asymmetry in the magnetization lopes. The vertical shift in FC loops is attributed to uncompensated spins. There are reports of nanoparticles with core-shell morphology that exhibit EB without or negligible asymmetry in the hysteresis loops. It has been reported that the "shell" plays an essential role in stabilizing magnetism of core-shell nanoparticles and has been proposed to be crucial for applicability of future recording media. The systems under study are nanoparticles of Fe₂O₃, MnFe₃O₄, MnCr₂O₄, Cr₂O₃, Fe₃O₄, CoCr₂O₄, other core-shells and their alloys. The work seek to experimentally distinguish the individual temperature dependent magnetic responses of the core and shell. This will provide vital information about the magnetic state of the core and shell as asymmetry develops. In addition, the transverse susceptibility measurements will provide a direct estimate of the magnetic anisotropy and its evolution with temperature as asymmetry sets in. The analysis will be extended to core-shell nanoparticles with different compositions and suggests that it may be possible to selectively choose the material constituting the shell to gain control over the onset of asymmetry in a desired temperature range. The nanoparticles were synthesized by co-precipitation and sol-gel method and the core-shell were synthesized by the modified Stöber method. Various characterization such as XRD, TEM, FTIR, XPS and VSM were employed.

Keywords: Magnetic nanoparticle, Fe₂O₃@SiO₂ core-shell structure, XRD, TEM, VSM, exchange bias

NO 02

Designs, Simulation and Integration of negative-permeability meta-material based new Ultra Large Band (ULB) antennas with rejected bands

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Relationship between material structure and properties is used to tune the functionality of the device made from various material. Microelectronics for portable telecommunication systems require thin emitting or detection system such as the microstrip or patch antenna use in mobile cell phones. These low-profile planar antenna has a number of advantages over other antennas. They are their light, inexpensive, and can be integrated quite easily with many electronic components. The development of Ultra WideBand (UWB) communications systems involves the specially design antennas adapted to this technology. The antenna are often built of printed circuit board material and the substrate makes up the patch antenna's dielectric. The distance between the patch and the ground plane – the substrate or dielectric height h – determines the bandwidth. A thicker substrate increases the gain to some extent, but may lead to undesired effects like surface wave excitation: surface waves decrease efficiency and perturb the radiation pattern. In the present communication, principles of operation, impedance matching, radiation patterns, circular polarization, bandwidth, efficiency, alternative feed types, stationary wave rate, stacked patches and higher mode behavior are extensively discussed. In comparison with antennas for narrowband technologies, the antennas for Ultra wideband technology have better characteristics, namely their low power spectral density, their large bandwidth and their impulse character among others, justifying their many advantages in terms of non-interference with narrowband standards, broadband, better security in the exchange of data, strong immunity to multiple paths. The question of the coexistence of the ULB technology with the existing narrowband systems is finally addressed in the present review focusing particularly on the designs, simulations and integration of meta-material cells with negative permeability. They are two UWB monopoles with four truncated corners, one of which is powered by a co-planar waveguide (CPW) and the other by a microstrip line. Since UWB technology shares the same band with some "narrowband" systems, electromagnetic interference problems may exist. Solutions to enable these systems to coexist without disturbances are proposed. The monopoles already designed have been loaded by negative-permeability meta-materials structures SRR and CSRR types to notch the Wi-Fi 5GHz, Wi-Max 3GHz and the X bands for radio communications. In order to confirm the mastery of the narrow band filtering technique on the UWB antennas, a third butterfly-shaped ULB structure was proposed, on which three CSRR cells were printed to notch the IUT-8GHz service band and the 5GHz Wi-Fi band. A third band (4.10- 4.47GHz) was also notched.

Keywords: ultra wideband antenna, patch antenna, metamaterial, SRRs, CSRRs, notched bands

NO 03

Three Dimensional Characterization of Laser Ablation Craters Using High Resolution X-Ray Computed Tomography

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Laboratory X-ray computed tomography is an emerging technology for the 3D characterization and dimensional analysis of many types of materials. In this work we demonstrate the usefulness of this characterization method for the full three dimensional analysis of laser ablation craters, in the context of a laser induced breakdown spectroscopy setup. Laser induced breakdown spectroscopy relies on laser ablation for sampling the material of interest. Asymmetric ablation crater formation or non-ideal ablation will negatively impact the resulting spectral data acquisition. We demonstrate here qualitatively (in images) and quantitatively (in terms of crater cone angles, depths, diameters and volume) laser ablation crater analysis in 3D for metal (aluminum) and rock (false gold ore). We show the effect of a Gaussian beam profile on the resulting crater geometry, as well as the first visual evidence of undercutting in the rock sample, most likely due to ejection of relatively large grains. The method holds promise for optimization of laser ablation setups especially for laser induced breakdown spectroscopy and laser ablation inductively coupled plasma mass spectroscopy.

Keywords: Computed Tomography (CT), Ablation, Crater, Average Ablation Rate (AAR)

Patterning and Substrate effects on Coercivity for Cobalt Ferrite and Nickel Ferrite Alexandria Cruz

Alexandria Cruz

NO 05

Neutron Tunneling in Nano-Structured Systems: Isotopical Effect

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Tunneling phenomenon has been studied since the time of Sir Isaac Newton. In the case of neutron tunneling phenomenon, it is the quantum mechanics wave-particle duality which manifests itself. In this case particularly, the neutron wave-packet under total reflection condition suffers the so called frustrated total reflection as known in standard optics. More accurately, this tunneling phenomenon shows itself via sharp dips in the plateau of total reflection. The prerequisite to observe such quantum mechanics phenomenon lies within a thin film Fabry-Perot resonator configuration. This thin film Fabry-Perot resonator geometry consists of two reflecting mirrors separated by a transparent material from neutron optics viewpoint. In view of the specific neutron scattering properties related to the spin of the neutron wave-packet. As a direct proof, isotopic nickel thin films based Fabry-Perot resonator will be synthesized using the electron beam deposition under conditions such as low pressure and high vacuum. XRD, AFM, X-ray reflectometry and grazing incidence neutron reflectometry will be used to confirm the above targeted neutron tunneling phenomenon on a Ni⁵⁸/Ni⁶²/Ni⁵⁸. The results will be simulated to derive the lifetime of the tunneled neutron wave-packets. If successful, this would the first proof of engineering novel neutron optics devices for neutron research reactors based completely on isotope based nanostructures.

Keywords: Isotope, Neutron tunneling, Neutron reflectometry, Fabry-Perot resonator

NO 06

Geopolymers as potential sustainable materials for the construction industry

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Existing data show that Portland cement material production contributes ~10% to the global CO₂ emissions. Generally, ~1 tonne of CO₂ is released for each tonne of clinker produced. This is detrimental to the environment and causes global warming. In addition, ~3 billion tonnes of raw materials are required in a year for Portland cement manufacturing, which consumes a high amount of energy. Due to the above-mentioned factors, there is an urgent need to develop an alternate cost effective and environmentally friendly cement material. The geopolymerization technology is a solution. Geopolymers are inorganic polymeric materials produced by the reaction of aluminosilicates with a highly concentrated alkaline solution. The early interests of geopolymers were in development of thermal resistant materials but in recent times, research has shifted towards its use as a cementitious material. Recently, fly ash geopolymers were shown as promising binder materials alternative to Portland cement due to their comparable mechanical properties. Among the aluminosilicate sources for geopolymer production are fly ash, blast furnace slag, and metakaolin. This paper presents the mechanical properties of geopolymers formed with metakaolin mined in Abuja, Nigeria. Samples of 50x50x50mm dimensions were prepared and tested for compressive strengths. The effects of alkaline concentration and curing

temperature on the compressive strength development of the metakaolin geopolymers were studied. The results of the study revealed these geopolymers to be a potential sustainable construction material for the Nigerian construction industry.

Keywords: Geopolymers, Portland Cement, Construction Material

NO 07

The effect of N-configurations on the detection of dopamine at N-doped graphenemodified ITO electrodes

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A sensitive electrochemical method based on a nitrogen doped graphene modified indium tin oxide (NGr/ITO) electrode was developed for detection of dopamine¹⁻² (DA). N-graphene films of varying total nitrogen content and different nitrogen configurations were used to modify the ITO electrodes and then employed to investigate the electrocatalytic activity of DA using both cyclic voltammetry and differential pulse voltammetry techniques. The N-graphene films were grown at different times (2, 10 and 20 min), and XPS results showed that NGr-2 min films comprised of ~ 59.6%, ~31.2%, and ~9.17% of pyridinic, pyrrolic, and NOx-N-configurations. The NGr-10 min contained ~56.3%, ~38.1%, ~3.96% and 1.91% of graphitic, pyridinic, pyrrolic, and NOx-N-configurations; whereas NGr-20 min films were comprised of ~83.1%, ~3.5% and ~13.4% of pyridinic, pyrrolic, and graphitic Nconfigurations. The modified ITO electrodes were then labelled as NGr-2/ITO, NGr-10/ITO, and NGr-20/ITO. From the DPV studies, the linear detection ranges of DA were established to be $2 - 240 \mu$ M, $2 - 150 \mu$ M, and 4 - 40 μ M, with the estimation of the detection limits (S/N = 3) determined to be 0.131 μ M, 0.153 μ M, and 0.645 μ M at the NGr-2/ITO, and NGr-10/ITO and NGr-20/ITO electrodes, respectively. Thus, the NGr-2/ITO electrode exhibitited excellent performance for the electrochemical detection of DA. As such, the improved electrocatalytic activity towards the oxidation of DA (Scheme 1) at the NGr-2/ITO electrode was attributed to an improved π - π interaction between the pyrrolic N-configurations on the electrode surface and the hydroxyl and the amine groups on the DA molecule. Adittionally, the enhanced heterogeneous electron tranfer rate constant at the NGr-2/ITO electrode (k_s = 402.9×10⁻³ s⁻¹) versus 10.14×10⁻³ s⁻¹ and 7.923×10⁻³ s⁻¹ for NGr-10/ITO NGr-10/ITO and NGr-20/ITO electrodes was ascribed to the increased amount of basal and edge defects, as corroborated by the large defect density determined from Raman spectra. This study has provided a procedure for designing new electrochemical sensors with specific electrochemical performance.

Scheme1: Redox of dopamine to dopamine-o-quinone on electrode surface



Keywords: Dopamine, N-doped graphene, N-configurations, ITO, electrochemical sensors

Hydrothermal synthesis and gas sensing response of nanostructured La₂O₃-CuO-Co₃O₄ mixed oxides

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The unique properties of mixed metal oxides have positioned them as attractive materials for various applications such as solar cells, catalytic activities, gas sensors, biomedical and diagnostics and optoelectronic devices. Through control of composition, size and shape, it is possible to utilise their unique individual properties to obtain enhanced properties which cannot be realised with a single component. CuO and Co₃O₄ are p-type narrow band gap semiconductors whereas La₂O₃ is an n-type rare earth semiconductor with a wide band gap. These materials have individually been assessed for their gas sensing activity and have been reported to have shown some degree of useful gas sensing ability. In this study a series of CuO-Co₃O₄-La₂O₃ ternary mixed oxide nanostructures with different La₂O₃ content were synthesised via a simple, throughput and low cost hydrothermal technique followed by annealing at 500°C. The microstructure of the products was confirmed through X-ray Diffraction (XRD) and Raman spectroscopy. The morphology was examined by Scanning Electron Microscopy (SEM) and High Resolution Transmission Electron Microscopy (HRTEM). The gas sensing response was investigated by monitoring the electrical conductivity of each sample in ambient conditions and in the test gas. XRD results revealed that the pristine powders were composed of CuO, intermediate oxides (CoO_2 , $CoCuO_2$) and $La(OH)_3$. On annealing the intermediate products decomposed to monoclinic CuO, cubic Co₃O₄ and hexagonal La₂O₃ crystallographic phases. These phases were confirmed through XRD and Raman studies. Increasing the La2O3 content beyond 10 % resulted to reduced intensities of the CuO and Co₃O₄ XRD peaks meaning reduced crystallinity of the oxides. SEM and HRTEM imaging revealed formation of various nanostructures mainly composed of nanorods of various aspect ratios and nanospheres. The nanostructures showed a gas response that depended on the percentage of the La₂O₃ additive.

Keywords: nanostructures, La2O3-CuO-Co3O4, mixed oxide, hydrothermal, gas sensing

NO 09

Synthesis, Characterization and Applications of Nanostructured Copper Oxide

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Nanostructured copper oxide has attracted several research interests over the years due to their interesting optical properties and their potential use in several electronic applications such as solar cells, energy storage and gas sensors. In this work, reverse micelle microemulsions (a bottom-up approach) and high energy milling (Top-down approach) have been employed for the production of defect-free and highly defective nanocrystals. The produced defect-free nanocrystals show good crystallinity with the nanometric nature of the primary domains (20 nm – 4nm) leading to quantum confinement phenomena highlighted by photoluminescence measurements. Models have been proposed for the nanocrystal formation and growth validated by means of several techniques such as X-ray Diffraction (XRD), Scanning Electron Microscopy (SEM) and Transmission Electron Microscopy (TEM), UV-Visible and Fourier Transform Infra-Red spectroscopy (UV-Vis and FTIR). Possible energy applications have also been explored. The effect of high energy milling on the microstructure evolution was investigated using synchrotron radiation XRD line profile analysis supported by High Resolution TEM and SEM. The reduction in the average size of coherently scattering domains – and simultaneous narrowing of the size distribution - occurs in the first minutes. A proper nanocrystalline microstructure is obtained for a milling of ca. 20 min with asymptotic limit of ca. 10 nm. The reduction in size occurs at the expenses of introducing a massive quantity of dislocations in the system, reaching a limit of ca. $4 \times 10-16 \text{ m}^{-2}$.

Keywords: Copper Oxide, Microemulsions, Milling, Nanocrystals, XRD

Collimating Channel Arrays for confocal micro x-ray fluorescence microscopy at CHESS

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Confocal x-ray fluorescence microscopy (CXRF) is a variation of XRF analysis where single point spectra and 3D elemental distributions can be directly obtained from heterogeneous, un-thinned samples. In CXRF, the probe volume is defined by a pair of optics at the excitation and detection channels respectively. Virtually all implementations of CXRF prior to our work used a polycapillary lens as the collection optic, resulting a probe volume which was limited to about 10 μ m in maximum dimension at 10 keV, and which varied strongly as a function of energy and hence analyte.

Our approach is to use a novel collection optic called a Collimating Channel Array (CCA) developed at the Cornell High Energy Synchrotron Source (CHESS). CCA optics are lithographically fabricated from germanium substrates, and comprises an array of a radially spanning set of collimating channels which collect x-rays from a single source position at the focus. With this setup, the geometry of the channels defines a spatial resolution that is invariant over a wide energy range, and significantly smaller than has been achieved using polycapillaries. We have been able to achieve a depth resolution of 2µm for an energy range spanning from 1.7keV to 20keV, and our technology has been incorporated into the general user program at the Advanced Photon Source station ID 20. We will present details of the design considerations, fabrication process and characterization of CCA optics. In addition, we also illustrate the capability of CCAs in CXRF with several example applications, including studies of the lead distribution in an archaeological sample of human bone and corrosion in stained glass. We also discuss opportunities for the future, such as CCAs designed for different detector geometries to enable greater flexibility for elemental imaging and spectroscopic applications.

Keywords: X-ray fluorescence spectroscopy, 3D microscopy, Spatial resolution, Germanium

NO 11

Design of a process to produce 428L/day of silver nanoparticle infused antimicrobial paint Delight Mutonhori

NO 12

Nano technology applications, solution to mitigating global climate change in this present time

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In the Recent times, global climate change has posed a great danger to humanity. It is any identifiable change in the worldwide climate that has occurred over decades or more. In this modern time, researchers have identified Green House Gases as the cause of global climate change. Green House Gases are from natural and anthropogenic sources. The industrial revolution of 20th century to a very large extent has contributed to the warming trend. Reducing Green House Gas emission requires us to change the way we generate electricity, heat our homes and our means of transportation. These changes include generation of green energy through renewable energy sources, using green nano technologies, less carbon intensive fuels and carbon capture/ sequestration.

Key words: Global Climate Change, Green House Gases, Green Nano Technology and Carbon Sequestration.

Improved electrical conductance through direct assembly of colloidal silicon nanoparticles using electrophoresis

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Functional nanocomposite inks offer promising applications for printed electronic devices. Patterning of such inks, using electrophoresis could improve not just the structure for low cost and lightweight devices, but also significantly improve the electrical properties of such devices. In this study, we compared the electrical properties of two types of nanocomposites layers formed by dispersing milled silicon powder in a solution of acrylic binder with the subsequent colloidal form deposited by drop casting between two printed silver electrodes. The first type **A**, was drop cast colloidal composite allowed to undergo self-assembly under gravity, the second type **B**, included electrophoretic assisted deposition. The electrical conductivity for type **B** showed a 5-order magnitude improvement relative to the self-assembled layer due to particle/particle and particles/metal compaction resulting from an electric force which drives the particle to move in a preferred direction. The milled powder was earlier characterized using Transmission Electron Microscopy (TEM).

Keywords: silicon, nanocomposite, hybrid, transport

NO 14 Production and characterization of cellulose fibre cement composites Ekwe Nneka Blessing

NO 15

A new organometallic route for low temperature ALD of atomically-thin MOS₂ layers on 2D SIO₂/SI support

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Layered transition metal dichalcogenides (TMDs) such as group (IV) to (VI) metal disulfides or diselenides have emerged as a new class of 2D materials possessing a wide range of interesting electronic properties. Among them, MoS₂ and WS₂ have been widely studied as 2D semiconductors possessing a direct bandgap, and proof-ofconcept-devices such as field effect transistors, phototransistors, piezoelectric cells or chemical sensors were successfully built from mechanically-exfoliated MoS₂ or WS₂ monolayers. In order to develop new electronic devices based on these new 2D materials, numerous synthesis methods have been developed (such as hightemperature chemical vapor deposition from MoO₃ or WO₃), but very few of them meet industrial requirements in term of uniformity, integration potential, and compatibility with existing production tools. In this context, we report here ALD/MLD and CVD methods (Atomic/Molecular Layer Deposition method, see Scheme, and Chemical Vapour Deposition), based on organometallic chemistry applied to the solid surface of the wafer, for the growth of 2D MoS₂ and WS₂ crystals. The atomically-thin crystalline domains are obtained from an organometallic amorphous deposit. This original result with respect to the state of the art has been mechanistically rationalized with modelling studies on the oxide nanobeads at different annealing temperatures. This contribution will present the method, the characterization of the 2D layers (among which the first in-plane micrographs of ALDgrown MoS₂ samples) and the proposed surface coordination chemistry mechanism at hand.



Scheme: Schematic representation of an ALD and MLD approach to atomically-thin crystalline deposit on 2D support

NO 16

Structural Optical Electrical Studies of ZnO/SnO₂ core-shell structure nanocomposites formation: Field-Emission Enhancement and Sensor

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We report on simple method for the formation of transition conducting metal oxides (TCMOs) like pure SnO₂, ZnO nanoparticles, and a SnO2/ZnO core/shell nanocomposites (NCs) were prepared by chemical method. The structural, optical, surface morphology of the synthesized NCs have been characterized by high-resolution transmission electron microscopy (HRTEM), field-emission scanning electron microscopy (FESEM), Raman scattering and X-ray diffraction (XRD). The obtained pure and NCs samples are highly crystalline with a hexagonal wurtzite phase and display well-aligned array structure. A pronounced effect on increased nanorod length was found for the RTA-treated ZnO as compared to the as-grown ZnO. Analysis of XRD indicates that the (002) feature peak of the as-grown ZnO was shifted towards a lower angle as compared to the peaks of RTA-treated ZnO samples due to the reduction of tensile strain along the c-axis by RTA. Photoluminescence (PL) studies reveal that the ZnO nanorod arrays receiving RTA in an O₂ environment have the sharpest UV emission band and greatest intensity ratio of near band-edge emission (NBE) to deep level emission (DLE). Additionally, the effects of RTA on the field emission properties were evaluated. The results demonstrate that RTA an O₂ environment can lower the turn-on field and improve the field enhancement factor. The stability of the field emission current was also tested for 4 h. The gas sensing performance of the NCs films was investigated for different volatile organic compound (VOC) vapors in the temperature range from 150 to 350 °C. The gas sensing results confirmed that the SnO₂/ZnO NC film shows a high selectivity, sensitivity, good stability, and fast response time towards isopropanol at the optimum operating temperature of 300 °C.

Keywords: Metal-Oxides, SnO₂, ZnO, XRD, HRTEM, Field Emission, Sensors

NO 17 Engineering Chiral Quantum Corrals on Surfaces

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Engineering molecular superstructures on metal surfaces opens great possibilities for the control and exploration of complex nano-systems for technological applications. Of particular interest is the use of chiral molecules, such as alanine, and tryptophan, to build self-assembled nanoscale structures for the trapping of the two-dimensional free electron gas of a metal. Depending on the amino acid at hand, the reaction with the metallic surface is different. For alanine molecules, scanning tunneling microscopy, spectroscopy, and density functional theory (DFT) revealed the formation of a uniform network of hexagonal chiral pores, where each pore acts as a quantum corral by confining the two-dimensional electron gas of the Cu(111) surface state. Furthermore, each hexagonal pore acts as nanoscale tracks when excess alanine molecules were trapped at the inner perimeter of the pore, and were observed as rotating spatial states periodically moving between the six vertices of the hexagon. Contrary to this, Tryptophan molecules on Cu(111) cluster as chains to form a molecular labyrinth due to the presence of the indole group, which is a key component to tryptophan's function as a precursor for transmitting signals to the brain.

Keywords: amino acids, molecules, scanning tunneling microscopy, quantum corrals, nanoscale structures

NO 18 Catalytic soot oxidation using ceria and copper nanocomposites Eubert Mahofa

NO 19

Nano ZnO doped graphite via Agathosma betulina natural extract with improved bandgap

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This contribution reports for the first time on green synthesized Zinc Oxide graphite doped (ZnO/G) material that was fabricated and exposed to UV lamp irradiation at 250 nm for 4 hrs. The morphology and the structure of ZnO and ZnO/G were characterized by high resolution transmission electron (HRTEM) and X-ray diffraction (XRD) respectively. The Energy Dispersive spectroscopy (EDS) confirms the purity of ZnO nanoparticles with Diffuse Reflectance spectroscopy (DRS) revealing decrease in bandgap and reflectance of the irradiated composite.

Key words: Agathosma betulina natural extract, Zinc oxide nanoparticles, graphite, bandgap, and composite.

Radionuclide liquid wastes treatment of ⁶⁸Ge by graphene-based nanomaterials

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Treatment of radionuclide liquid wastes is an important step in its management and great attention has been received worldwide as radionuclide liquid wastes generated from nuclear facilities can affect humans and the environment. In the present work, new composite nanomaterials, based on graphene and graphene oxide (GO) are developed for treatment purpose. The method used for evaluation of nanomaterials retention properties was sorption experiment, being based on contact of solid material with tracer solution under defined boundary conditions (solid/solution ratio, solution composition etc.). An aqueous solution of ⁶⁸Ge radionuclide was added to the GO solution, the solution was filtered and the remaining solution was quantified by gamma spectrometry. The experiment results were the evaluated, using sorption distribution cefficient (KD) and indicated that the sorption process is more efficient with the great effect of removal of this radionuclide from the solution.

Keywords: Radionuclide liquid wastes, ⁶⁸Ge radionuclide, Graphene, Graphene oxide, Sorption

NO 21 Surfactant-free, aqueous dispersions of carbon nanomaterials <u>George Bepete</u>

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Enhanced antibacterial and Photocatalytic Activity for capping agent of Ni-doped ZnO nanoparticles star-like flower nanostructures

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Pure zinc oxide (ZnO) and nickel (Ni) doped ZnO (Ni:ZnO- NZO) nanoparticles (flower-like-structure) were successfully prepared by ethylene glycol as capping agent. As prepared ZnO and NZO nanoparticles were systematically characterized using X-ray, optical, electron microscope and antibacterial analysis. The Ni entered to ZnO lattice without altering its structure which is isomorphic substitution of NZO. The micro-Raman analysis shows the E₂(h) wurtzite structural mode appear in the both samples. Scanning electron microscope (SEM) surface images shows the aggregation of tiny crystallites of ZnO and NZO. The aggregates have definite shape of nanostars (star-like-flower nanostructures) shaped morphology and their agglomeration revealed by rough surface of each aggregate. Optical absorption study shows Ni ion-diffused into ZnO band-gap shifted towards red-shift of ZnO also narrow of energy band-gap was observed. Similarly, the red-shift observed in Raman, XRD higher-angle and enhanced bio-activity attributed well crystallinity and no secondary phase formation associated with the Ni-dopant.

Keywords: ZnO nanoparticles, XRD, SEM, DRS, Raman and Antibacterial Studies

Green Synthesis of BiVO₄ Nanorods via Aqueous Extracts of Callistemon viminalis and it's photocatalysts application

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Nowadays, the development of efficient green chemistry methods for synthesis of metal oxides nanoparticles has become a major focus of researchers. These methods are being investigated in order to find an eco-friendly technique for production of well-characterized nanoparticles. In this contribution we report for the first time, the synthesis and structural characterization of n-type Bismuth vanadate (BiVO4) nanoparticles using aqueous extracts of Callistemon viminalis as a chelating agent. To ascertain the formation of BiVO4 , X-Ray diffraction analysis (XRD), Scanning Electron Microscopy (SEM), High Resolution Transmission Electron Microscopy (TEM), Selected Area Electron Diffraction (SAED), Electron Dispersion X-ray Spectroscopy (EDS), Fourier Transform Infrared Spectroscopy (FTIR), Photoluminescence spectroscopy (PL), and photocatalysis were carried out.

Keywords: Green synthesis; Bismuth Vanadate; Nanorods; Callistemon viminalis

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Electron and ion irradiation induced structural changes in ZnO nanowires

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In this research work, wurtzite structured ZnO NWs were irradiated at different ion energies (keV to MeV), ion fluences, ions species and substrate temperatures. Structural and morphological changes were determined by means of high resolution transmission electron microscopy (HRTEM), X-ray diffraction (XRD), Raman spectroscopy and scanning electron microscopy (SEM). The study has revealed that ZnO NWs were damaged under high fluence of H and N ions. Moreover, the crystal plane spacing of ZnO NWs were reduced under N ions irradiation at 400 °C and randomly oriented crystallites embedded in wurtzite matrices appear. However, Ar⁺ ions, at the dose of 5x10¹⁶ ions/cm², manufactured uniform distributed nano-dimensional nano-holes with pore sizes of 2 to 5 nm on the entire surface of ZnO NWs under room temperature while nano-humps appear on the surface of ZnO NWs during Ar irradiation at 400 °C. Moreover, X-, Y-, II- and T-shapes welded nano-junctions of ZnO NWs by H⁺ ion beam irradiation at 400 °C were also discussed. Moreover, electron beam induced-cutting of ZnO NWs and fabricating nanoholes in ZnO NWs will be discussed. This research work will be useful for future design of ZnO-NWs based devices to be used under harsh environment. Mechanism of structural changes in ZnO-NWs by ions irradiation is explained by collision cascade effect and thermal spike model.

Keywords: ZnO nanowires, ion beam irradiation; lattice defects, Amorphization, structural stability.

Deep-space radiations like hardness of VO₂ based active smart radiation device for nanosatellites applications

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Vanadium dioxide (VO₂) is explored as an active smart radiation device (SRD) for new type of thermal control material for space craft especially in nano and micro satellites. Current space thermal control systems require heaters with an additional power penalty to maintain space craft temperatures during cold swings. Because its emissivity can be changed without electrical instruments or mechanical part, the use of VO₂ based SRD decreases the request of spacecraft power budget. As an active SRD, an ideal VO₂ based nano-coatings should have a low emissivity at low temperatures to maintain the heat, whereas at high temperatures its emissivity should be high to dissipate the additional unnecessary heat. In addition to their active thermal management properties, these VO₂ coatings must exhibit deep space radiations hardness. Whilst in outer space such coatings will be exposed to different cosmic radiation including gamma rays and Neutrons. Because these radiations interact with the material in different ways, this contribution reports on the study of VO₂ coatings properties subjected to extensive gamma rays and neutrons with typical doses encountered in space missions. The prevalent crystallographic phase after irradiation remains the monoclinic VO₂ phase but the films preferential orientation shifts to lower angles due to the presence of disordered regions caused by radiations. Raman spectroscopy measurements also evidences that the VO₂ structure is slightly affected by gamma irradiation. Indeed, increasing the gamma rays dose locally alters the crystalline and electronic structures of the films by modifying the V-V inter-dimer distance, which in turns favours the presence of the VO₂ metallic phase. From the XPS measurements of V2p and O1s core level spectra, an oxidation of vanadium from V⁴⁺ towards V⁵⁺ is revealed. The data also reveal a hydroxylation upon irradiation which is corroborated by the vanishing of a low oxidation state peak near the Fermi energy in the valence band. Similar results are observed for neutron radiations; moreover the neutroninduced multiple displacement damage causes physical alteration (coloration) on the thin films. Our observations suggest that gamma and neutron radiations induce the formation of Frenkel pairs. THz transmission measurements show that the long range structure of VO2 remains intact after irradiation whilst the electrical measurements evidence that the coating resistivity decreases with gamma irradiation and that their transition temperature is slightly reduced for high gamma ray doses. In contrast, resistivity of the neutron irradiated films increases by order of magnitude. Even though these are just some of the possible types of irradiations that are encountered in space environment, these results are very promising with regards to the potential of integration of such VO₂ films as a smart radiation device for spacecrafts.

Key words: Vanadium dioxide; Thermochromic; Irradiation; Gamma rays; Thermal shielding

Structural and Optical studies of the papilio crino Fabricius, 1792 wings

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The beautiful colour patterns observed on butterfly wings rises from the interaction of light on the periodic nanoscale structures. The replication of these colours has gained considerable attention in the biomimicry industry due to the many applications derived from such study. A combination of multi-layer interference, diffraction gratings, photonic crystals and other optical structures in several Lepidoptera species gives rise to the bright colours useful for the creation of model systems to better understand structural colours. Generally, the wings scales of the butterflies, particularly the papailioned consist of regular deformed multilayer structures that are made from alternating layers of air and cuticle which create the intense structural colours. Currently, researchers have identified the colour producing structures in several of the papilionidae species such as P. blumei, P. palinurus and P. Buddha. In recent studies, Vukusic et al. examined the scales of the P. palinurus to consist of array of concavities exhibiting two distinct colours on the edges and the incline sides. Previous studies on this species also showed that the concave cuticle air multilayer on the wings scales causes polarization rotation for blue light after double bounce from the concavity edge. One characteristic identical to these papilionidae is iridescence. The colour produced by the wing structure changes over a wide range of the human visible spectrum depending on the viewing direction. Against this background, we focus on the interaction of light on the concavity as displayed by the cover scale of papilio crino. The conspicuously large size butterfly; papilio crino, indigenous to Central and Southern India exhibit this characteristic. To our knowledge there is no comprehensive optical study on this species, hence in the present study, we show through experimental, numerical and computational modelling that the concavities are reflective as they diffractive the incident light. In the analysis, we show that the emerging colouration on the *papilio crino* is structural and is due to the combination of colours caused by multiple bounces within the concavities. In the first instance, we proceed with a quantitative study of the optical characterization.

Keywords: Scattering, Nanostructure, Lepidoptera, Multilayer, Papilionidae

NO 27

Nanospider[™] needle-free electrospinning – the technology enabling nanofiber material integration into industrial end applications

Kateřina Rubáčková

NO 28

An Initiation Mechanism of Corrosion in Low-Carbon Steel: Identified by In-Situ Transmission Electron Microscopy

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Infrastructure and pipeline corrosion present environmental and health concerns, amounting to trillions of dollars spent annually for remediation, repair, and replacement. Efforts aimed at inhibiting the onset of pipeline corrosion are challenging, due to numerous, compounding environmental and industrial parameters involved in

the onset of steel corrosion. Aqueous carbon dioxide (CO₂) conditions represent one of the most common environmental conditions to which steel is exposed, and though it is postulated that grain boundaries, material defects, and nanoscale features are likely sites for this mesa-type corrosion, adequate predictive relationships have not yet been determined. Here, we have applied a nanoscale approach to investigate the baseline corrosion pathways, formation products, and susceptible microstructures of low-alloy carbon steel under exposure to CO₂ in water. Electron transparent foils from pipeline steel coupons (1018 low-carbon steel) underwent compositional and structural mapping pre-characterization. Corrosion analysis was then undertaken using a liquid flow TEM holder after transfer of the sample foil to a microfabricated environmental cell with SiN membrane windows. Direct observation of corrosion initiation using low-dose imaging during the exposure of the steel foil to aqueous CO₂ solution directed the investigation to galvanically active nanoscale regions of the sectioned material. Local nanoscale morphologies that exhibited susceptibility to corrosion will be described. Our goal is to advance predictive capabilities for modeling low-carbon steel corrosion by CO₂ exposure in aqueous environments, and ultimately guide future corrosion prevention technologies. This work was performed, in part, at the Center for Integrated Nanotechnologies, an Office of Science User Facility operated for the U.S. Department of Energy (DOE) Office of Science. Sandia National Laboratories is a multi-mission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA-0003525.

Keywords: in-situ transmission electron microscopy, nanoscience, corrosion, steel, characterization

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Effect of Particle Size of Pozzolanic Addition on the Properties of MgO-based Cement K. Onwudiwe¹, G. Marmol² A. Onwualu³, H. Savastano⁴

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The effect of particle size of pozzolanic material addition to cement (OPC) has been found to affect the mechanical properties of the cement. The effect of the particle size variations of this pozzolanic material (rice husk ash) addition to MgO, is therefore described in the course of this work. Rice husk ash (RHA) obtained from the calcination of an agricultural waste (rice husk) as a source of pozzolanic material and amorphous silica has been used to synthesize reactive magnesium oxide, to produce MgO-SiO₂ based cement, and the effect of the different particle sizes determined. Magnesium oxide was sourced from a local supplier and the amorphous silica was obtained from the calcination of rice husk to get a silica enriched rice husk ash (RHA), which was calcined in the furnace at a temperature of 650°C for one hour to obtain the silica rich RHA and then cooled rapidly to ensure the crystallinity of the RHA to be amorphous. Effect of the particle size variation and variation in water content of the cement (60%MgO-40% SiO₂) for early and later strength of 7 and 28 days were determined by varying the particle size of the RHA at 425 μ m, 150 μ m, and 106 μ m and water to solid ratio at 0.38, 0.33 and 0.22. 50mm cube samples were cast according to ASTM C109 standard, at a cement to sand ratio of 1:3, while still varying water content. Compressive strength of the cement is low for an early strength of 7 days, with a maximum strength of 3.84MPa for a particle size of 425 μ m and an expected higher strength after 28 days since MgO based cement possesses late strength. Applications range from, sandcrete blocks, interlocks, kerbs, floorings, and for most non load bearing applications.

Keywords: OPC, MgO based cement, Pozzolanic addition, RHA, compressive strength

Structural and optical properties of MgXZn1-XO (0≤X≤0.39) nanorods grown by metalorganic chemical vapour deposition

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The effects of alloying on the *c*-axis lattice constant and the photoluminescence (PL) of $Mg_xZn_{1-x}O$ are investigated. It is found that an increase in Mg content increases the transitions related to stacking faults. The origin of the PL line broadening of $Mg_xZn_{1-x}O$ (x≤0.04) is also analyzed with respect to alloy broadening, taking into account a random cation distribution and alloy clustering. A random cation distribution is found to describe the PL line broadening in the present films quite well (at least for x ≤0.04).

Keywords: MOCVD, Mg_xZn_{1-x}O, Nanomaterials, stacking faults, alloy broadening

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Search for magnetic nanocluster formation of TM ions embedded in metal oxides

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Theoretical predictions of room temperature ferromagnetism in the wurtzite semiconductors ZnO and GaN doped with 5 at. % Mn stimulated international research effort directed towards realization of such effects in ZnO, GaN and related metal oxides and III-nitrides. While there have been several reports of observation of ferromagnetic behaviour in metal oxides doped with low concentrations of transition metal ions, the origin of the observed effects has been shown to be defect complexes and secondary effects and not the Zener model of ferromagnetism, i.e. due to exchange interaction between localized moments mediated by charge carriers. The research focus in recent years has thus shifted from intrinsic effects to extrinsic effects such as the formation magnetic nanoclusters embedded in suitable host matrices. In a search for the formation of magnetic nanoclusters in ZnO and other metal oxide substrates (Al₂O₃, MgO, SiO₂) implanted with 4 - 8 at. % Fe and other transition metal (TM) ions we have conducted a series of studies on these samples using conversion electron Mössbauer Spectroscopy and magnetization measurements. The results of our studies will be presented and discussed.

Keywords: magnetic nanoclusters, transition metal ions, metal oxides

Dependence of structural and optoelectronic properties on thickness of γ-Cul thin films deposited by vacuum thermal evaporation

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Cuprous iodide (Cul) is a p-type transparent halide semiconductor which received the earliest research interest among its family members; CuCl, CuBr, AgCl, AgBr and Agl. It has very interesting optical and electrical properties which found good use, for example, as a hole collector in solid state solar cells, an organic catalyst, organic light emitting diodes, piezoelectric transducers, among others. In this work, fabrication of gamma phase Cul thin films of high (111) orientation deposited by vacuum thermal evaporation of powders is reported. The powders were attained through cost-saving use of recycled Cu metal cuttings. The thin films were characterized through x-ray diffraction (XRD) and scanning electron microscopy (SEM). In addition, the optical and electrical properties of the thin films were also investigated. XRD revealed the formation of pure (111) highly oriented Cul phase with an increase in crystallite size and a decrease in dislocation density as film thickness increases which indicated an improvement in the crystallographic microstructure. The SEM images of the Cul thin films showed compact morphology with an increase in the large-sized particles as film thickness increased which is in agreement with XRD results. Optical investigation showed a mean optical transmittance of around 70 % in the visible region with a decreasing trend as thickness increased. There was an observed red shift on the absorption edge with thickness. All thin films also showed good electrical conductivity and the figure of merit was best at lower thicknesses. The good optical transmittance and relatively low resistivity qualify the CuI thin films as candidates for optoelectronic device applications.

Keywords: cuprous iodide, thin films, vacuum thermal evaporation, optoelectronic properties, characterization.

NO 33 Structural influence of amine and thiol surfactants on AuSe synthesis

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Colloidal nanomaterials have over the years received considerable attention due to their unique nature as well as their attractive optical, chemical and physical properties [1]. The various properties are due to several key parameters during the synthetic process such as temperature, reaction time and surfactants. The primary role of surfactants is to provide stability, to aid with solubility, to stop agglomeration and to direct growth of the nanomaterial [2]. With recent research developments there is need for novel materials with enhanced properties for use in renewable and sustainable energy technologies. Colloidal gold selenide (AuSe), a less known and not well understood metal chalcogenide is an example. AuSe crystallizes in a layered structure and exists in two phases namely; α -AuSe the metastable form and β -AuSe which is thermodynamically stable. [3]. The aim of the study was to synthesize and characterize gold selenide nanomaterials using different surfactants, one with an amine molety and another with a thiol to determine the effect these surfactants have on the structural properties of the material. Selenium powder, chloroauric acid and the desired surfactant were added together in a 3-neck round bottom flask. With the assistance of heat and under inert conditions, the mixture was subjected to strong magnetic stirring. The structural effect of olevlamine (OLA) and 1- dodecanethiol (1-DDT) as surfactants was thus investigated. From the OLA synthesis, transmission electron microscopy revealed nanobelts with varying lengths and diameters, while the results with 1-DDT showed finger-like structures. For both reactions, the presence of Au and Se. Powder X-ray diffraction patterns showed that the materials obtained were the α -phase of gold selenide, with traces of unreacted gold and unreacted selenium. The use of an amine and a thiol surfactant afforded different morphologies of the nanomaterials suggesting they have different growth-directing properties. Future studies will involve optimization of reaction conditions to afford pure AuSe samples and complete characterization of the nanomaterial.

Keywords: surfactant, amine, thiol, gold selenide

NO 34

Frequencies of a nano beam with Spring-mass Attachment, used for Tapping atomic force microscopy (TM-AFM) in tapping mode Malesela K. Moutlana

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The advent of nano technologies has refocused scientist to the application of manufacturing at molecular levels. Interest in the behavior of nano-tools has come into prominence in the past few years and is gaining more attention in a wide range of engineering sectors. The aim of this investigation is to study the motion of a cantilevered beam used in tapping mode atomic force microscopy (TM-AFM), which can be utilized in the manufacture of nano-scale structures. TM-AFM uses high frequency oscillations to remove material or shape nano structures. The nano machining structure is modeled using the Euler-Bernoulli theory and Eringen's theory of non-local continuum. The latter theory is effective at nano-scale and takes into account small-scale effects. The system is modeled as a beam with a torsionally restrained boundary condition at one end; and at the free end is a transverse linear spring attached to the tip and the other end of the spring is attached to a mass. When the linear spring constant is infinite, the free end behaves as a beam with a tip mass. When the mass is infinite, the boundary condition is that of a linear spring. When the mass is zero, the configuration is clamped-free. The motion of the tip of the beam and tip mass can be investigated to observe the tip response: displacement and force. The tip displacement frequency contains information about the maximum displacement amplitude and therefore the sample penetration depth. The force generated at the free end can be used to deform the surface of a sample and thus allow arbitrarily shaped nano structures, to be molded into desired functional forms.

Keywords: non-local effects, frequency, spring-mass

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Green Synthesis of CePO₄ Nanomaterials via Callistemon viminalis Extract <u>M. Olateju¹</u>, N. Sintwa¹, B. Mothudi¹, M. Maaza^{1,2}

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Lanthanide phosphate nanomaterials are reported to have diverse applications such as in the fields of luminescent materials, nuclear waste treatment and superhydrophobic materials. In the past decades, attention has been focussed on their preparation, characterization and application due to their very interesting unique chemical and physical properties such as very high thermal stability and low solubility in water. These unique properties can be controlled by the morphology and size of the nanomaterials which in turn can be controlled by fine-tuning parameters such as methods of synthesis. Many methods such as sol-gel have been used to successfully synthesize lanthanide phosphates in different nano-sizes and shapes. However, these methods are expensive (high temperature), involve the use of hazardous materials and lengthy synthesis times. We report for the first time the biosynthesis of CePO₄ nanomaterials using an aqueous extract from the red flowers of *Callistemon viminalis*, a plant common in certain parts of South Africa, at room temperature. There was no use of inorganic, organic solvents or surfactants in this method of synthesis making it environmentally friendly. Their structural and optical properties by electron microscopy, infrared, powder XRD and Raman are reported.

Keywords: Biosynthesis, Cerium phosphate, nanomaterial, Callistemon viminalis extract
Mechanical Properties of Metal Organic Frameworks (MOFs) and their Emerging Applications

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Metal-organic frameworks (MOFs) are a class of crystalline materials that consist of coordination bonds between transition-metal cations and multi dentate organic linkers. They are newly developed class of nanoporous materials generating considerable research interest because of their outstanding features in terms of their surface area, porosity which make them unique among the existing traditional porous materials. MOFs are potential materials for gas storage, purification and separation, catalysis and sensing applications. At present, methods are being developed for making nanocrystals and super crystals of MOFs for their incorporation into devices. In the light of their potential applications in industry and technology, the fundamental mechanical properties of MOFs need to be addressed and understood. In this paper, we briefly summarize the various methods or techniques now available for the measurement of the mechanical properties of MOFs. The emerging applications of MOFs in different fields are outlined. Finally, important challenges in the measurement of mechanical properties of MOFs such as the unavoidability of faceting and terraces on the growth surface of the MOFs, interactions between the atmosphere and the crystals etc. and the way forward are discussed.

Keywords: Porosity, surface area, elastic modulus

NO 37

Deep space radiations-like induced defects in selected smart nano-scaled carbon based materials

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Providing protection from space radiation is a major challenge for the exploration and development of space. Indeed, it is necessary to study the effects of space environment on nanomaterials and materials used in space technology to ensure safe and successful missions. Hence, the main aim of this PhD project is to investigate radiation effects on selected Carbon based nanostructured materials. More precisely, the 3 years PhD research project is geared towards investigating the induced defects by several type of ionizing and non-ionizing radiations and identify the damage mechanisms. The experiments and the modelling will be performed at several radiation facilities that stimulate secondary neutrons in the atmosphere, protons in low earth orbit and protons and heavy ions in the galactic cosmic rays spectrum that dominates the radiation fields in inter-planetary space. The radiation tolerance threshold of the various Carbon based nanomaterials will be quantified and added to the international database on space radiations hardness.

Keywords: Space material, Carbon nanotubes, Radiation, Graphene

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

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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 application at elevated temperatures the same cobalt expands more than the diamond, straining the diamond matrix and leading to premature failure of the component. 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. The leaching process reportedly results in a product with improved thermal stability and an overall improved wear resistance. A systematic investigation and evaluation of the average in-plane residual stress fields on a fatigue loaded leached PCD disc sample were undertaken. Whilst the Raman results reported a progress shift of the residual stresses from an average compressive stress state to an average tensile stress state with 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.

Keywords: Raman Spectroscopy, Polycrystalline diamond (PCD), Residual stress, Fatigue

NO 39 Nanomaterials Industrial Development Facility (NIDF): Crossing the innovation chasm <u>Mike Masukume¹, Manfred Scriba^{1*}, Vincent Ojijo¹</u>

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The Council for Scientific and Industrial Research has established the NIDF to enable industry, research entities and small, medium and micro enterprises (SMMEs) to develop and scale up high-tech materials. The focus at present is on using nanotechnology as a key enabler in polymer, cosmetics and other chemical related products in order to enhance the industries competitiveness. Nanotechnology has been considered, owing to its well published benefits that manifest due to its small, unique sizes. However, cheap imports and the difficulties to take laboratory developed products to the markets as well as the lack of testing and scale-up facilities often make it difficult for SMMEs and even large companies to start establishing new products and materials. The NIDF was thus established to assist researchers and engineers to bridge this innovation chasm between materials development and commercialization. This presentation will highlight the program objectives and offerings, innovation value chain, challenges faced including safety concerns and regulatory requirements, current projects being pursued among other things.

Keywords: commercialization, nanotechnology, innovation chasm

Tuning spherical nanostructures through spatially dependent electric confining potentials <u>Moletlanty Tshipa</u>

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Tuning nanostructures using spatially variant electric confining potentials is reported. The electric confining potentials used as case studies are the parabolic potential and the shifted parabolic potential, in spherical nanostructures. In nanostructures, electrons occupy distinct states with very specific associated energies. Electrons can make transitions from one state to the other. These processes are accompanied by absorption or emission of some energy which may involve photons, phonons or any other elementary excitations. Most of the operational principles of nanodevices rest upon the ability of charge carriers to make transitions between states. The transitions are resonant whenever the energy of excitation matches the electron's energy separation between the states, called transition energies. The energy eigenvalues were obtained by solving the Schrödinger equation within the effective mass framework. It is found that the parabolic potential enhances transition energies while the shifted parabolic potential decreases the transition energies. This imbues nanotechnology with an additional avenue of tuning nanostructures must have specific dimensions corresponding to specific energies of excitation.

Keywords: Nanostructures, electric confining potential

NO 41

Preparation and Characterization of Pd modified TiO2 nanofiber catalyst for carbon – carbon coupling Heck reaction

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Pd/TiO₂ was prepared through electrospinning of polymethyl methacrylate (PMMA) and Titanium isopropoxide (TIP) solution followed by calcination of fibers in air at 500°C. Palladium nanoparticles prepared through reduction method were successfully dispersed and supported on the TiO₂ nanofibers. Combined studies of X-ray diffraction (XRD), Scanning electron microscope (SEM) and Transmission electron microscope (TEM), indicated that the synthesized Pd/TiO₂ had anatase and Pd⁰ successfully adsorbed on TiO₂ surface. BET indicated that the synthesized TiO₂ and Pd/TiO₂ had a surface area of 53.4672 and 43.4 m²/g respectively. The activity and selectivity of 1 mol % Pd /TiO₂ in the Heck reaction has been investigated towards the Mizoroki-Heck carbon-carbon cross coupling of bromobenzene and styrene. Temperature, time, solvent and base were optimized and catalyst recycled twice. ¹H NMR and ¹³C NMR indicated that stilbene, a known compound from literature was obtained in various Heck reactions at temperatures between 100°C and 140°C. The catalyst was found to be highly active under air atmosphere with reaction temperatures up to 140°C. Optimized reaction condition resulted into 88.2 conversion and 92 % yield of *trans*-stilbene with a TON of 1993.4 and TOF value of 332.2 hr⁻¹

Keywords: Heck reaction coupling, calcination, electrospinning, Pd/TiO₂

Co-precipitation synthesis of zinc oxide nano-particles in fermented palm-wine for various applications

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In this research, an investigation had been carried out on synthesis of zinc oxide nanoparticles for various applications. Zinc Oxide nanoparticles were nanostructured by co-precipitation method using fermented palm wine. Synthesis of the zinc oxide nanoparticles were carried out by making use of fermented palm wine, zinc acetate, sodium hydroxide and Triethanolamine (TEA) as starting materials. These chemical reagents were prepared and the resulting mixture was heated under the action of magnetic stirrer for different reaction time of 1 hour, 2 hours and 3 hours. The particle size and morphology of the synthesized nanoparticles were investigated by Transmission Electron Microscope (TEM) and the elemental composition was obtained from Energy Dispersive Spectroscopy (EDS) attached to TEM and X-ray fluorescence spectroscopy (XRF). The crystal structures of synthesized nanoparticles were also observed using X-ray Diffraction (XRD). Results obtained from characterization of the nanoparticles show that pure ZnO nanoparticles with average particle sizes of 66.17nm, 117.10nm and 204.19nm were obtained for samples heated for one hour, two hours and three hours reaction times increased. It was concluded that chemically pure zinc oxide nanoparticles can be synthesized using fermented palm wine in combination with other chemical reagents.

Keywords: Co-precipitation, Palmwine, Zinc oxide nanoparticles, Synthesis

NO 43

Immiscible Polylactide/Poly(ε-caprolactone)-Containing Graphite and Graphene Oxide Biocomposites: Comparative Study

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This presentation gives an overview of the scope and issues of polylactide (PLA)/poly(ε -caprolactone) (PCL) blends and how these issues are addressed and resolved by the incorporation of lower loading (0.05 to 0.25 weight percent, wt%) graphite (G) and graphene oxide (GO) particles. The results of a locally synthesized GO, containing oxygenated functionalities presents a strong candidate for development of the advanced thermal management biocomposites. A significant improvement in the thermal stability of GO-filled PLA/PCL blends composites is observed even at high loading of poor thermally stable GO particles. However, the incorporation of highly thermally stable G particles had little influence on the thermal stability of PLA/PCL blends composites.

Keywords: enzymatic degradation, thermal, material properties

Laser-Generated Proton Beams for High-Precision Ultra-Fast Crystal Synthesis

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We present a method for the synthesis of micro-crystals and micro-structured surfaces using laser-accelerated protons. In this method, a solid surface material having a low melting temperature is irradiated with very-short laser-generated protons, provoking in the ablation process thermodynamic conditions that are between the boiling and the critical point. The intense and very quick proton energy deposition (in the ns range) induces an explosive boiling and produces micro- and nanocrystals that nucleate in a plasma plume composed by ions and atoms detached from the laser-irradiated surface. The synthesized particles in the plasma plume are then deposited onto a cold neighboring, non-irradiated, solid secondary target surface. We experimentally verify the synthesizing methods by depositing low-melting-material microcrystals - such as gold - onto nearby silver surfaces and modeling the proton/matter interaction via a Monte Carlo code, confirming that we are in the above described thermodynamic conditions. Morphological and crystallinity measurements indicate the formation of high-precision gold octahedral crystals with variable dimensions, uniformly distributed onto a silver surface with dimensions in the tens of mm². This laser-accelerated particle based synthesis method paves the way for the development of new material synthesis using ultra-short laser-accelerated particle beams and their ultimate integration into diverse applications including biology and nanomedicine.

NO 45 Deposition of multilayered iron and nickel sulphide thin films Puleng Alina Molete¹, Makwena Justice Moloto²

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A low-temperature easy to assemble chemical bath deposition (CBD) technique has been developed to deposit metal chalcogenide thin films onto various substrates like ITO, FTO and glass. Thin films of metal sulphide, like NiS and FeS, have attracted particular attention due to their ease to synthesize in the size range suitable for quantum confinement and their suitable band gap. Semiconducting NiS and FeS thin films were deposited on a glass substrate by varying the deposition parameters such as temperature and solution pH. Multi-layered thin films were deposited on a glass substrate as the co-coating enhances the optical properties and provides the uniform deposition. Single layer NiS was deposited at room temperature, pH 10 and the deposition period of 3 hours, triethanolamine was used as the complexing agent. FeS was well deposited for 6 hours at 70°C with the pH of 2.5 using EDTA as a complexing agent. Generally, the iron and nickel sulphide were prepared from their respective nickel or iron salt and the thiourea or thiosulfate as a source of sulphide ions in solution. The thin films were characterized using AFM, SEM and EDX in order to study the structural morphological properties, UV-Vis spectra showed correlation with AFM measurements as the thickness of the film increases the absorbance increases also. XRD patterns for both NiS and FeS gave amorphous features irrespective of the varied conditions. FeS showed good adherence and uniform particle size onto glass as compared to NiS. The morphology of NiS changed after the depositing it on the FeS layer.

Keywords: Chemical bath deposition, thin film, metal chalcogenide, multilayer

Synthesis of ZnS nanoparticles from Zn(II) dithiocarbamate complexes, and a study of the effect of growth time on particles sizes

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Semiconductors nanoparticles of the II-VI group have been widely studied due to their potential applications and novel properties which are uniquely different from their bulk. ZnS is an important direct wide band-gap semiconductor with low absorption coefficient in the visible range of optical spectrum. It is stable, nontoxic and has good electrical properties. These characteristics qualifies it for a wide range of applications, and has generated lot of research interest. Although different routes have been devised in the synthesis of ZnS nanoparticles, the single source precursor molecule approach which presents the entire starting compounds as a single entity is still one of the best. In this work the synthesis of hexadecylamine(HDA)-capped ZnS nanoparticles by solvothermal route using zinc(II) *N*-alkyl-*N*-ethanoldithiocarbamate as a single source precursor. By varying the growth time, the optical properties and size of the nanocrystals were studied. The as-synthesized nanoparticles were characterized using UV–vis absorption and photoluminescence (PL) spectroscopy, transmission electron microscopy (TEM), and X-ray diffraction (XRD). All the particles showed cubic sphalerite phase, and exhibited quantum confinement in their optical properties with band edge emission at the early stage of the reaction. The TEM image showed that the particles are spherical in shape, and the crystalline nature was confirmed by high resolution TEM. The good optical properties of the particles makes them a good candidate for optoelectronic devices and sensors.



Keywords: ZnS; dithiocarbamate; crystal structure; particle size

Modern synthesis of metallic nanoparticles production

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Numerous synthesis strategies have been employed for the production of metallic nanoparticles of various sizes, size distributions and shapes, including chemical reduction, electrochemical, laser ablation, pulsed wired discharged, precipitation, reverse micelles techniques, electronic beam, solvated metal ion, etc. However, these approaches have a number of drawbacks, including poor water balance, creation of environmentally unfriendly waste streams and they appear to be relatively expensive. Nanobiotechnology using plant extracts has emerged as an alternative method for the synthesis of metallic nanoparticles, because it gives an alternative "greener" way of suitably synthesizing metallic nanoparticles using natural reducing and stabilizing agents. This reviews provides an overview of methods used to produce nanoparticles and establish why biological synthesis offers potential improvements.

Keywords: Nanoparticles, synthesis, nanobiotechnology, plant extracts

NO 48

Investigating the anionic polymerization of aldehydes, promoted by strong organic bases <u>Rueben Pfukwa</u>, Justin Van Zyl, Inge Weideman, Bert Klumperman

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Polyacetals, such as poly(phthalaldehyde), and poly(*n*-butyraldehyde) are an interesting class of self-immolative polymers.¹ They have very low ceiling temperatures (*T*_c), significantly below room temperature; e.g. for PPA, *T*_c = -40 °C, however, they can be stabilized at elevated temperatures by acetate end-capping of the chain ends. When the chain end is selectively removed, or if the backbone is cleaved, by a chemical or physical trigger, the polymer chain completely depolymerizes into monomer. Polyacetals are therefore capable of responding to a stimulus, and providing an amplified response, hence there is significant interest in their application as responsive materials. Polyacetals can be synthesized via ionic (anionic and cationic) and coordinative mechanisms. Of these, anionic methods are most popular due to advances in the use of metal-free anionic polymerizations, promoted by strong organic bases, with alcohol initiators. This approach enables tailoring of end-groups, however the agreement between theoretical and experimental molar masses is not always optimum, and *D* values are often high. To enhance the appeal of polyacetals, as responsive materials, it is desirable to investigate the cause of these discrepancies, to minimize them, and improve access to well-defined polyacetals, with predictable molar masses and low *D*. In this contribution we detail our investigations into the metal-free anionic polymerization of *n*-butyraldehyde and phthalaldehyde, using strong organic bases as promoters, including phosphazene bases and 1,8-diazabicyclo[5.4.0]undec-7-ene (DBU).

Keywords: polyacetals, organic base, anionic polymerization

Influence slip and convective boundary condition on MHD 3D stretched flow of nanofluid through porous media inspired by non-linear thermal radiation

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In the present study, the main concern is to investigate the magnetohydrodynamic nanofluid flow subject to porous matrix and convective heating past a permeable linear stretching sheet. In addition, the influence of velocity slip and non-linear thermal radiation are considered. A new micro-convection model known as the Patel model is implemented for considerable enhancement of the thermal conductivity and hence, the heat transfer capability of nanofluids. Moreover, a convective heat transfer model is introduced where the bottom surface of the sheet gets heated due to a convection mechanism from a hot fluid. The numerical results of the transformed governing differential equations have been generated by using fourth-order Runge-Kutta method along with shooting approach and secant method is used for better approximation. In the present analysis, base fluids such as water and ethylene glycol and Cu, Ag and Al₂O₃ nanoparticle are considered. Results of the present investigation show that inclusion of porous matrix contributes to slow down the fluid velocity and diminution of wall shear stress (axial as well as transverse). Drag force due to magnetic field strength, slip parameter and imposed fluid suction shrinks the momentum boundary layer and up surges the heat transfer rate from the surface. It is observed that imposed fluid suction at the surface brings a noticeable drop in fluid velocity and hence belittles the thickness of momentum boundary layer whereas heat transfer rate from the surface gets enhanced. Wall shear stresses (axial as well as transverse) are not influenced by temperature ratio parameter while heat transfer rate from the surface appears to reduce upon increasing temperature ratio parameter. Convective heating up surges the wall heat flux appreciably.

Keywords: Nanofluid, MHD flow, Velocity slip, Non-linear thermal radiation, Convective boundary condition

NO 50

A Facile Microwave-Assisted Synthesis of Doped TiO₂ Nanohybrids

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The emergence of nanohybrid technology is opening a new horizon of a continuum of potential applications for TiO₂ and its hybrids. Carbon nanotube-titanium dioxide (CNT-TiO₂) nanohybrids, for example, combine the high specific surface area of CNTs and their elevated electrical conductivity with the photoresponse of TiO₂ to produce a chemically stable yet chemically active material. However, the current conventional methods used to synthesize nanohybrids are limited by low reproducibility. The application of microwave irradiation in semiconductor synthesis is receiving attention in material sciences because of its reproducibility and short synthesis times. This work reports the use of a time-efficient and highly reproducible microwave irradiation method to synthesize a nanohybrid consisting of doped TiO₂-CNT nanohybrids. Firstly, pristine and nitrogendoped nanotubes (NCNTs) were synthesized using a CaCO₃/Co-Fe catalyst in a CVD reactor and then functionalized in aqua ragia. The CNTs and NCNTs were separately mixed with titanium (VI) butoxide and NH₄OH, and the respective mixtures were placed in in quartz curvets and subjected to microwave irradiation for 20 minutes to yield TiO₂-fCNT, TiO₂-NCNT, NTiO₂-NCNT nanohybrids. After washing and drying, the optical properties of the nanohybrids were probed using photoluminescence and UV-Vis spectroscopy. The specific surface area was determined using Brunauer-Emmett-Teller (BET) N2 adoption-desorption method while the chemical composition was determined using Fourier transform (FT-IR), Raman and X-ray photoelectron spectroscopy. Crystalline phase composition was probed using XRD while transmission electron microscopy was used to determine the morphology of the nanohybrids. The nanohybrids were confirmed to consist of anatase TiO_2 and $NTiO_2$. Average crystalline size and energy band gap was lowest for the $NTiO_2$ -NCNT hybrids (~ 9 nm, 2.5 eV). XPS confirmed the bonding of $NTiO_2$ onto CNTs and the presence of N in TiO_2 and CNTs.

Keywords: Radiation microwave, doping, nitrogen, titanium dioxide, carbon nanotubes

NO 51

How to get the structure of nanomaterials: In the US and in Africa

Simon Billinge

Modern materials under study for next generation technologies, such as for energy conversion and storage, environmental remediation and health, are highly complex, often heterogeneous and nano-structured. A full understanding of the structure requires us to go beyond crystallography and to study the local aperiodic components of the structure, which is a major experimental challenge. There are recently emerging powerful experimental and theoretical developments that are bringing us close to being able to address this problem, ranging from powder to single-particle methods. I will give a personal view about the current state of affairs, highlighting what I see to be the main challenges and opportunities if these can be overcome. The most exciting developments are happening at a nexus of physics, chemistry, applied mathematics and biology and this is a rich and truly interdisciplinary activity.

NO 52

Electric Field-Induced Valley Degeneracy Lifting in Uniaxial Strained Graphene: Evidence from Magnetophonon Resonance

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Since its discovery in 2004, graphene continue to attract great attention of experimentalists, theorists and industrials. It is considered as a miracle material which can revolutionize all the technology. This two dimensional system gives rise to a rich physics when it is under a mechanical constraint. The study of strained graphene has opened the way to a new technology consisting of the strain engineering. In particular, it can offer an analogous of the spintronic effect by manipulating the valley degeneracy of its band structure. We study the role of electron-phonon interaction on the magneto-phonon resonance (MPR) spectrum in uniaxial strained graphene, under crossed electric and magnetic fields. We predict a new structure in the MPR spectrum consisting of a double peak line resulting from the valley degeneracy lifting induced by the electric field. We show that the double peak structure of MPR line is due to the different Landau level spacings in the two Dirac valleys originating from the simultaneous action of the inplane electric field and the strain induced Dirac cone tilt. This effect gives rise to a valley dependent electron-phonon interaction leading to a double peak structure in the MPR line (Figure 1).



Figure 1: Frequency shifts (a) and the broadenings (b) of the LO and the TO modes as a function of the magnetic energy for a compressive (-18%) and a tensile (18%) deformations under a uniform electric field of 5 × 106 V.m⁻¹ and for a given disorder amount 22222.

Interlayer Interaction dynamics: towards understanding controlled release in layered metal hydroxides

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Nanodimensional layered metal hydroxides such as hydroxy double salts (HDSs) can undergo anion exchange reactions releasing intercalated anions. Because of this, they have found applications in controlled release delivery of bioactive species such as drugs and pesticides. In this work, anion exchange reactions were used to intercalate guest anions into acetate HDS. Isomers of hydroxycinnamate (*i*HCn), and different exchange concentrations of hydroxybenzoate (HB) ions were used to systematically explore the effects of anion structure and preparation methods on the rate and extent of anion release in HDSs. Following intercalation and subsequent release of *i*HCn, it has been demonstrated that the nature and position of substituent groups on intercalated anions greatly affect the rate and extent of release. The extent of release was correlated to the magnitude of dipole moments while the rate of reaction showed strong dependence on the extent of hydrogen bonding within the layers. Varying the exchange concentrations of the guest HB anions resulted in different arrangements and interactions within the gallery.

Keywords: Hydroxy Double Salts, Release kinetics

NO 54

Preparation of nano-sized high purity graphite from Zimbabwean flotation concentrates

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Graphite exhibits the properties of both a metal and a non-metal, which makes it suitable for many industrial applications. The discovery that natural graphite could be a genuine contender in the graphene and anode supply chain has prompted many in the mining industry to follow the material's development with interest. It will drive the demand for high-purity graphite and promote the development of cost-effective purification technology of natural graphite. This study is conducted to utilize low grade flake A graphite flotation concentrates as nanomaterial resources. Prior to production of the nano-sized graphite powder, studies on its pretreatments were performed. An alkali roasting process, which consists of roasting with caustic soda, water washing and sulphuric acid leaching, has been found to be an effective method for graphite purification even at low roasting temperature. With this process, a flotation fine concentrate containing 888% carbon could be purified to about 99.8% carbon when roasted with 25% NaOH at 250°C and leached by 10% H₂SO₄ solution at room temperature.

Keywords: nano-sized, high purity graphite, flotation concentrates

Synthesis and thermal conductivity enhancement of silver nanowires dispersed ethylene glycolbased nanofluid

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Nanofluids are new class of conventional heat transfer fluids which could increase the efficiency of solar thermal systems to provide cost-competitive electrical energy. In this paper, ethylene glycol (EG) suspensions containing silver nanowires (AgNWs) were prepared by a simple and cost effective chemical synthesis method. Ethylene glycol (EG) was used as the base fluid and areductant, while polyvinylpyrrolidone (PVP) as structure-directing agent for the growth of Ag nanowires. Structural and morphological characterisations revealed highly crystalline three-dimensional (3D) interconnected network of Ag nanowires. The thermal conductivity measurements of AgNWs dispersed EG were conducted by using a guarded hot plate (GHP) method, in temperatures ranging between 25°C and 50°. Remarkably, enhancement up to 23% in thermal conductivity of AgNWs:EGnanofluidaged for 5h was found compared to EG base fluids. We observed a nonlinear relationship between thermal conductivity and volume fractions, and alsoexistence of a strong temperature effect on this anomalous thermal conductivity enhancement.

Keywords: Nanofluid, silver nanowires, thermal conductivity

NO 56

Synthesis and characterization of nanomagnetite by thermal decomposition

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Magnetite nanoparticles were synthesized via thermal decomposition with slight modifications. The synthesized magnetite was stabilized insitu using oleic acid/oleylamine and oleic acid/polyethylene glycol (PEG-400). The obtained nanomagnetite particles were characterized using Fourier Transform Infra-red Spectroscopy (FT-IR), Transmission Electron Microscopy (TEM), Vibration Sample Magnetometer and X-ray Diffractometry (XRD). The bidentate mode, previously observed for only oleic acid stabilized nanomagnetite was observed to change to a monodentate mode. The oleic acid/PEG stabilized nanomagnetite exhibited higher saturation magnetization at both 5K and 300K, and a larger particle size compared to the oleic acid/oleylamine stabilized nanomagnetite. Overall, oleic acid/PEG produced more crystalline particles with a smaller surface area and higher saturation magnetization. The introduction of oleylamine and PEG also resulted in an increase in saturation magnetization compared to previous reports for only oleic acid stabilized nanomagnetite.

Keywords: Nanomagnetite, Oleic acid, Oleylamine, Polyethylene Glycol

NO 57 Synthesis, Characterisation and Reactivity of Nano Au/SBA-15 catalysts for Vapour Phase Aerobic Oxidation of Benzyl Alcohol

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Highly dispersed gold nanoparticles supported on mesoporous SBA-15 catalysts were synthesised from four different methods, namely, homogeneous deposition - precipitation (HDP), micro-emulsion (ME), impregnation (IMP) and polyol (POL) and their catalytic activities were investigated for the vapour phase oxidation of benzyl alcohol to benzaldehyde. The catalysts were characterised by XRD, TEM, BET surface area, pore-size distribution, CO-chemisorption and XPS techniques. The structural data of the catalysts along with their catalytic studies indicate the presence of very small metallic Au^o species with particle size 7-8 nm, was responsible for the higher activity observed in the vapour phase oxidation of benzyl alcohol reaction. The title reaction, though industrially important, was used as a test reaction to investigate the influence of different preparation methods on the uniform dispersion of gold particles on the support SBA-15 as well as to study the catalytic performance of the Au/SBA-15 catalyst in terms of activity. Selectivity and stability over a period of reaction time. The conversion of benzyl alcohol was found to increase with decrease in the size of gold particles. Smaller gold particles with higher percentage of dispersion on the support SBA-15 had a beneficial effect on the catalytic activity. Among the four methods used for the preparation of gold on SBA-15 support, the catalyst prepared from homogeneous deposition-precipitation method showed the best performance in terms of conversion, selectivity for benzaldehyde and longer catalyst life.

Keywords: Gold nanoparticles, SBA-15, Benzyl alcohol, Oxidation and Benzaldehyde

NO 58

Nanocellulose in Catalytic and sensor applications

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We report on the isolation of nanocrystalline cellulose (NCC) produced from discarded cigarette filters (DCF). The DCF were processed into cellulose *via* ethanolic extraction, hypochlorite bleaching, alkaline deacetylation, and then converted into NCC by sulfuric acid hydrolysis. The morphological structures showed that the nanocrystals were needle-like with a mean length of 143 nm. A NCC sample was freeze-dried and showed a specific surface area of 7.78 m²/g. The crystallinity of the NCC film and freeze-dried samples were 96.77 % and 94.47 %, respectively. A novel nanocellulose/hydroxyapatite heterogeneous catalyst was used in the one-pot, two-component synthesis of triazolidine-3-one derivatives, produced from the cyclocondensation reaction

between semicarbazide and aromatic aldehyde. With the use of ethanol solvent, the products formed after a short reaction time (<30 min). The main advantages of this protocol were excellent yields (90-96%) of product, mild and environmentally friendly reaction conditions, good atom-economy, simple and fast work-up. The twelve triazolidine-3-one derivatives was characterized by ¹H, ¹³C and ¹⁵N NMR, FT-IR, and HR-MS and represent a new family of compounds containing the 1,2,4-triazolidin-3-one moiety. Finally, nanocrystalline cellulose (NCC) was used as both reducing and stabilizing agent in the formation of silver nanoparticles (AgNPs). The size and the yield of synthesized AgNPs varied over a pH range 5-10. The minimum mean AgNP diameter (4.61 nm) was observed at pH 9 while the maximum (19.93 nm) was observed at pH 5. The spherically shaped AgNPs showed surface plasmon resonance (SPR) around 416 nm. The sensitivity of the AgNPs colloids showed excellent surface-enhanced Raman scattering (SERS) substrate behaviour and was investigated using a riboflavin concentration in the range 10 – 0.00001 μ M.

Keywords: nanocellulose, hydroxyapatite, catalysis, silver nanoparticles, SERS

NO 59

Green synthesis of Europium oxide Nanoparticles by *Hibiscus sabdariffa* flower extract: Main physical and optical properties

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Nowadays there is a need to develop an eco-friendly processes, inexpensive and also which do not use toxic chemicals in the synthesis protocol in order to obtain biocompatible and harmless nanoparticles. Green chemistry approach is the eco-friendly process which has taken the researchers attention globally due to its advantages over conventional methods. This eco-friendly method have potential in transforming the inorganic metal ions into metal NPs via the bioreduction of molecules present in the particular organism. This contribution reports on the synthesis and the main physical properties of Europium (III) oxide (Eu₂O₃) nanocrystals synthesized for the first time by a completely green physical-chemistry process using Hibiscus sabdariffa natural extract as an effective chelating agent, and Europium nitrate pentahydrate (Eu(NO₃)₃.5H₂O) salts as a precursor . Eu₂O₃ nanoparticles synthesized via green chemistry process would be beneficial for the development of nontoxic, clean and environmentally friendly biosynthesis procedure. The structural and optical properties of such biosynthesis nanocrystals were analyzed by various techniques; High Resolution Transmission Electron Microscopy (HRTEM), Scanning Electron Microscopy (SEM), Electron Dispersive X-rays Spectroscopy (EDS), X-Rays Diffraction (XRD), Fourier Transform Infrared Spectroscopy (FT-IR), Raman, Ultraviolet and visible spectrometer (UV-Vis-NIR) and as well as room temperature photoluminescence (PL). The HRTEM and SEM results showed the images of small NPs formed, which indicated that the Eu₂O₃ NPs are nano-scaled with a mixed population of crystalline particles. The EDS and XRD analysis showed the grain size of nanoparticles ranged between 14 nm and 25nm, using Debye-Scherrer approximation. The luminescence properties of such cubic were characterized by an intense red emission centered at 614.8 nm (⁵D₀-⁷F₃).

Keywords: Biosynthesis, Hibiscus sabdariffa, Eu₂O₃ nanoparticles, Rare earth oxides, Luminescence

Thermodynamic Analysis of the Membrane Distillation System for Desalination of Brackish Water

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Membrane distillation (MD) is the process by which vapor passes from a feed water source of undesirable quality through a membrane to a collection region. This process is driven by transmembrane pressure difference induced by temperature difference across the membrane. MD has low power requirements as compared to other membrane water purification system such as reverse osmosis and nanofiltration, making it potentially suitable for low cost applications. This project is focusing on the need to enable effective and efficient applications of MD in communities with limited technological experience and maintenance capability in lleret, northern Kenya by incorporating economic and robust water heating and cooling mechanisms in the system. The majority of the power consumption is in the form of heat used to increase the temperature of feed water allowing for the use of solar thermal. The correlation in arid areas between water purification needs and high levels of solar irradiation make this region a perfect test bed for the system, which could be applicable across much of sub-Saharan Africa and the world.

WO 02

Crustacean derived biocomposite for decontamination of drinking water in northern Tanzania

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In Northern Tanzania, high levels of fluoride in community drinking water supply is recognized as one of the major public health concern, the problem is further ameliorated by presence E. coli and fecal coliform bacteria in surface water and shallow wells. Efforts to decontaminate the water involve mostly the use of low efficient bone char for fluoride removal without disinfecting the pathogens. To address this problem, a robust adsorbent which is capable of removing fluoride and microbes simultaneously, at lower cost and with less energy requirement and minimal diverse impact on the environment is vital. Here we highlight development of composite material developed from recycling of crustacean biomass waste from sea food industry. Chitosan polymer, isolated from prawns shell was composited with crab shell derived brushite (CaHPO4.2H₂O) to form chitosan hydroxyapatite composite. XRD and FT-IR analysis confirmed transformation of brushite phases into hydroxyapatite and formation hybrid composite. Fluoride adsorption tests were performed in batch mode to evaluate effectiveness. Defluoridation capacity of up to 3.7 mg/g in field water containing fluoride concentration of 5-30 mg/L was achieved. The best performance was observed with fluoride concentration of 10 mg/l and below. Apart from fluoride removal, the composite also reduced color tint, fecal and E coli coliforms significantly from surface water samples. The pH of the treated water was maintained around 6-9, which is recommended for drinking water.

Key words: Biocomposite; Chitosan; Hydroxyapatite; Fluoride, Microbes

Precisely designed polymer membranes for use in water purification and desalination

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Clean, potable water is both an increasingly limited resource and an important commodity for developed and developing economies. Current purification systems require significantly more energy than the thermodynamic minimum to force contaminated water through nanofiltration and/or reverse osmosis membranes, which contain a thin polyamide active layer, because these layers have uncontrolled pore sizes and torturous pathways which limits their performance. There is no obvious or systematic way to improve these membranes because they are developed and optimized empirically. Our group's research centers on a relatively new class of polymers, covalent organic frameworks (COFs), which offers great promise for controlling the porosity and composition of membranes at the molecular level since these networks form layered structures with vertically aligned pores that can be rationally designed and tuned based on their building blocks. We recently made two important discoveries that have allowed for COFs, which are typically formed as improcessable microcrystalline powders, to be incorporated into membranes: 1) that formation of these materials is catalyzed by Lewis acids (not just Bronsted acids), and 2) that robust, atomically-precise films of this material can be synthesized through interfacial polymerization. The reaction conditions for this polymerization can be modified to precisely control film thickness and obtain large surface areas. These first-generation COF films have been incorporated into NF membranes and successfully shown to enhance organic material and salt rejection in water purification studies. Current efforts aim to improve on these remarkable results by systematically varying the membrane composition by forming films with smaller actual or effective pore sizes and different linkages to enhance solute rejection.

Keywords: covalent organic frameworks (COFs), water purification

WO 04

Adsorption behaviour of mercury from aqueous solution using polymer/carbon nanocomposite

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Water pollution by mercury is of major concern to environmentalists because mercury is highly toxic to living organisms and the environment. In the present study, the adsorption behaviour of mercury on polythiophene/graphene oxide was studied. Standard characterisation techniques were used to determine the physicochemical properties of the prepared adsorbent. A sequence of batch equilibrium, kinetics and thermodynamic adsorption experiments were performed under different operating parameters to determine their effect on mercury removal. Remarkable properties consistent with adsorption performance were observed for the nanocomposite and were attributed to synergistic effect of individual components. Mercury adsorptions occurred rapidly and correlated well with the pseudo-second-order model suggesting a chemisorption process. Batch adsorption results demonstrated that process variables had significant effect on mercury removal efficiency. Langmuir isotherm model described equilibrium data adequately. The values of thermodynamic parameters such as enthalpy (Δ H), entropy (Δ S) and Gibb's free energy (Δ G) changes illustrated that the adsorption process was endothermic, rapid and spontaneous in nature. Co-ions negatively impacted mercury removal efficiency but very substantial values were still achieved. The findings of this study suggest that polymer/carbon nanocomposite adsorbents are prospective candidates for effective mercury removal from aqueous solutions.

Keywords: Adsorption; Graphene Oxide; Mercury; Nanocomposite; Polythiophene

Application of natural South African zeolite as catalyst and biomass support in an integrated photodegradation and anaerobic digestion of textile wastewater

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Anaerobic digestion (AD) is widely applied as a first step treatment technique for industrial wastewater characterised by a high organic load such as textile wastewater (TWW). The presence of an appreciable amount of biorecalcitrant organic compounds in TWW, however, hinders the hydrolysis step thus lowering the rate and efficiency of AD. A pre-treatment technique is therefore required to first reduce the biorecalcitrants contained in TWW before AD. In this study, photodegradation using titanium dioxide (TiO₂) photocatalyst was integrated with AD for the treatment of TWW containing methylene blue (MB) dye. Photodegradation was used to improve the biodegradability of the wastewater before subjecting it to AD. Natural zeolite was applied as biomass and catalyst support in a bioreactor and photoreactor, respectively, used in the integrated process. Performance of the integrated system was evaluated in terms of colour and chemical oxygen demand (COD) reduction, substrate biodegradability index and methane yield. Photodegradation pre-treatment converted the biorecalcitrant COD into biochemical oxygen demand (BOD) resulting in an improved wastewater biodegradability index from 0.33 to 1.0. In the ensuing AD process, an improved COD and BOD removal were observed. Application of zeolite as catalyst support improved COD and colour reduction by 27% and 38%, respectively, during photodegradation. In the AD process, zeolite biomass support improved COD reduction by 20% with a 3-fold increase in biogas production. Based on the methane (CH₄) yield coefficient (CH₄ I/g COD removed) of 0.044 for the integrated system as compared to 0.012 when using AD alone, the integration of the two treatment methods was found to be suitable for treatment of wastewater containing textile effluents. The natural South African zeolite having large specific surface area and good adsorption properties was found suitable for application as a biomass and catalyst support in AD and photodegradation, respectively.

Keywords: Anaerobic digestion, Methylene blue, Photodegradation, Titanium dioxide, Zeolite

WO 06

Synthesis and Surface Modification of Cellulose Nanofibrils Derived from Citrus Waste for Industrial Wastewater Treatment

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Keywords: Citrus waste, green synthesis, cellulose nanofibrils, surface modification, wastewater treatment Citrus waste biomass is underutilized and generally of low economic value even though it contains components such as cellulose, which can be used to produce high value-added products like cellulose nanocrystals and cellulose nanofibrils. The aim of this study was to synthesise cellulose nanofibrils using a green synthesis route and to tailor their surface properties to enhance their ion adsorption capacity. Alkali pre-treatment and acid hydrolysis were used to purify and enhance the fibrillation of the cellulosic material and a ball milling machine was used to reduce the particle size of the treated cellulose. The synthesized cellulose nanofibrils were tailored using a modified version of the enzymatic phosphorylation method and were used to remove heavy metals from synthetic wastewater. The cellulose nanofibrils were characterised for their crystallinity, composition, morphology, particle size and functional groups using X-ray diffraction (XRD), scanning electron microscopy (SEM), transmission electron microscopy (TEM) and Fourier transform infrared spectroscopy (FTIR). Pre-treating the cellulose enhanced the material's fibrillation by breaking down connections between lignin and carbohydrates which resulted in reduced energy consumption during the mechanical process. The results also revealed that tailoring the surface of the cellulose nanofibrils by introducing phosphate groups onto the cellulose nanofibrils improved their ion adsorption capacity and their ability to simultaneously remove multiple metal ions from synthetic wastewater. The study showed that decreasing the energy consumption during the synthesis of cellulose nanofibrils and modifying the cellulose nanofibrils to improve their ion adsorption capacity could be

considered an environmentally and economically beneficial process for converting citrus waste to high valueadded bio-adsorbents.

WO 07

Charged Polymer Complexes for Membrane Applications

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While the design and synthesis of water filters has been the focus of a significant amount of research, there is still a need for easily processable and versatile materials for membrane fabrication. One such available materials system is based on polyelectrolyte complexes. In these complexes, polyanions and polycations form electrostatic rather than covalent bonds that are stable in most solvents. Current polyelectrolyte processing techniques such as layer by layer deposition are not scalable for industrial applications. In this work, a rapid quenching method induces a bi-phase separation within these complexes forming a desired porous structure much faster than current techniques. Additionally, simple changes in the processing chemistry allow for these membranes to be used in a wide suite of applications. Cross-sectional SEM was used to understand the driving factors behind pore formation. Furthermore, solvent stability measurements were taken using the quartz crystal microbalance. Finally, performance characteristics in a range of filtration and ion exchange applications were assessed.

Keywords: Water, Membranes, Polyelectrolyte Complexes

WO 08

Bimetallic Immobilized Hyperbranched Polymer embedded on a Polysulfone Membrane for removing Organic pollutants in water

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Reductive degradation using bimetallic nanoparticles has emerged as a promising alternative for decontamination of emerging organic pollutants present in water. Polychlorinated biphenyls (PCBs) forms part of persistent organic pollutants (POPs). These compounds are insoluble in water and due to their lipophilic nature, they are likely to have a great affinity to fat-rich tissues. Thus, they tend to accumulate, persist and bioconcentrate in living organisms at higher trophic levels. Health effects caused by PCBs include endocrine disruption in human beings. Furthermore, due to their stability, these compounds may take several years to degrade. Therefore, this study seeks to develop a catalytic membrane for the degradation of PCB-153 from synthetic water samples. This study describes the preparation, characterization and application of a polysulfone (PSf) composite membrane prepared by embedding hyperbranched polyethyleneimine (HPEI) polymer and Fe/Pd bimetallic system on a commercial PSf membrane support for the removal of PCB-153 from water. The nanoparticles were immobilized onto the membrane using the co-complexation method. The morphology and physicochemical properties of the membranes were evaluated using Atomic Force Microscopy (AFM), Scanning Electron Microscopy (SEM) and Transmission Electron Microscopy (TEM) coupled with Energy Dispersive Spectroscopy (EDS). The size of the Fe/Pd nanoparticles ranged from 44 nm to 77 nm as confirmed by AFM analysis. Moreover, AFM analysis revealed that the surface roughness of the membranes increased from 6.54 nm to 22.77 nm upon HPEI loading. EDS mapping analysis gave evidence that the Fe and Pd nanoparticles were uniformly distributed in the membrane matrix. Hence, the Fe/Pd bimetallic system was successfully fabricated within the PSf/HPEI membrane. The catalytic activity of the PSf/HPEI-Fe/Pd membranes will be evaluated against PCB-153. The analytes will be tested using gas chromatography coupled with mass spectrometry (GC-MS).

Keywords: Co-complexation, Fe/Pd bimetallic nanoparticles, Hyperbranched polyethyleneimine (HPEI), Polychlorinated biphenyl (PCB)

Sustainable water treatment technology for rural/urban communities

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Ceramic water filters are promising household water treatment technology (HWTS) and are proven to be capable of removing waterborne pathogens, removing other chemical contaminants and reducing turbidity in drinking waters. In this paper, processing approach of this economical water filtration technology will be presented along with a combined experimental and analytical modelling. Statistical analysis performed on flow rates, mean flow rates (in the first hour) and permeability values had been highlighted. The flow rate values (in the first hour) for the six ceramic water filters were found to be between 1.4 - 3.0 L/hr with corresponding permeability values for a range of micro- and nano-scale pore sizes. The statistical variations in the flow rates and effective permeabilities were elucidated along with the potency of a multiple ceramic water filter system for scale-up studies in serving communities

Keywords: Water filtration, Ceramic Water Filters, Flow rate, Hydraulic Conductivity, Permeability

WO 10

Preparation of hyperbranched polyethyleneimine(HPEI)-cysteamine intergrated thin film composite membranes for heavy metal removal

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In this study a nanofiltration (NF) thin film composite (TFC) membranes were prepared for the removal of cadmium (Cd⁺²) from waste-water. Membranes were prepared via an interfacial polymerization (IP) using hyperbranched-polyethylenimine (HPEI), trimesoyl chloride and cysteamine. The membranes were characterised using Fourier transform infrared spectroscopy (FTIR), scanning electron microscope (SEM), atomic force microscope (AFM), contact angle, batch adsorption, dead-end filtration. Anodic stripping voltammetry (ASV) and inductive coupled plasma-optical emission spectroscopy (ICP-OES) were used to analyse the samples during adsorption. FTIR confirmed formation of TFC. At constant transmembrane pressure of 900 kPa the pristine PES and 8% HPEI/PES membranes exhibited flux of 191.10 L / h cm² and 32 L / h cm² respectively. AFM revealed an increase in membranes surface roughness with an increase in HPEI loading. The unmodified membrane possesses lower surface roughness of 4.9 nm and 107,5 nm for PES/HPEI modified membrane. Consequently, inducing adsorption capacity. SEM further confirmed the formation of compact membrane structure after IP. The water contact angle of the pristine PES was 85.88°, however after HPEI grafting the contact angle decreased to 26° for PES/HPEI due to tertiary amine groups in HPEI. Indicating that the hydrophilicity of PES increases with an increase in concentration of HPEI. During batch experiments, Cd⁺² adsorption data showed a decrease in the current peaks of ASV from 1.212×10⁻³ to 6.606×10⁻⁴ (I/mA) and 1.212×10⁻³ to 1.025×10⁻³ (I/mA) for both PES/HPEI and pristine PES membrane respectively. When pH of Cd⁺² was adjusted from acidic medium to basic, the current peak changed from 4.071×10⁻³ to 0 after 20 min adsorption with PES/HPEI. This is due to deprotonation of amine groups that attract positively charged Cd⁺² or metal precipitation in basic solution. Adsorption data showed that the adsorption capacity of PES/HPEI membrane for Cd⁺² is higher than that of pristine PES.

Keywords: Cadmium, Nanofiltration, Thin film composite, Hyperbranched polyethyleneimine, Anodic Stripping Voltammetry.

Electrophoretic Deposition of TiO₂ Thin Films for Photocatalytic Degradation of Organic Pollutants in Water

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In this study, electrophoretic deposition (EPD) technique was used to deposit titanium dioxide (TiO₂) thin films on conducting glass substrates for application in photocatalytic degradation of organic pollutants in water. Phenol was used as a model pollutant. The EPD suspension related parameters and deposition conditions were first optimized for good quality film deposits. The suspension stability and deposition conditions that result in good adherence of TiO₂ particles to the substrate with homogeneous film coatings, is ethanol, a TiO₂ solid loading of 4.0 wt%, a 0.2 wt% iodine concentration in the solvent and a deposition voltage of 20.0V in a time of 3.5 mins. The photocatalytic activity of TiO₂ thin films decreases exponentially with the ultraviolet light (UV) illumination time and it is also dependent on film thickness, and sintering temperature of the TiO₂ thin films. Highest rate of photocatalytic activity is observed at an optimal film thickness of 95.0 \pm 2.0µm sintered at 300.0 °C. The implications of these results are discussed for design of inexpensive waste water purification systems for light industries as well for semi urban small communities.

Keywords: Electrophoretic deposition, Titanium dioxide, Photocatalysis

WO 12

Downscaling the conventional iron barrier technology to safe drinking water <u>Togue Kamga F.^{1,2}</u>, Noubactep C.³, Woafo P.^{*1}

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Fe⁰ filters have been demonstrated to be efficient for the removal of both microbial and chemical contaminations. Due to the volumetric expansive nature of iron corrosion, the inter-granular space (pore space or porosity) is gradually filled with precipitated iron corrosion products. Eventually this might lead to a clogged system (porosity and permeability loss). Permeability loss is the main negative factor on the sustainability of Fe⁰ filters. Metallic iron-based filters (or Fe⁰ filters) have a great potential for decentralized safe drinking water provision. However the whole effort to estimate the long-term performance of Fe⁰ filters should be reconsidered since the whole literature on metallic iron (Fe⁰) for water treatment is based on the false premise that Fe⁰ is a reducing agent. Accordingly, Fe⁰ oxidation by water has been wrongly considered as a side reaction. This work deals with the filtration of aqueous contaminant in a Fe⁰ scale down permeable reactive barrier consisting of iron particles mixed with sand particles. PRB technology is well known as a promising environmental remediation technology which media are mainly zero valent iron (ZVI), organoclays, natural zeolites etc. Here, the rate of flow, porosity loss and concentration of contaminant at the exit of the barrier are obtained using respectively the Darcy law, our model of porosity loss developed and the equation of solute transport in the iron barrier. Effects of the proportion of iron particles on the contaminant removal efficiency and the life service of the barrier are analyzed.

Keywords: Iron wall; Permeability loss; Volumetric expansion; Water treatment; Zero-valent iron

Removal of Selected Pharmaceuticals from Wastewater using Electrospun Argema mimosae Silk Fibroin Nanofibers

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Pharmaceuticals and/or their metabolites have been detected in wastewater, surface water (including rivers, lakes and coastal waters), groundwater and drinking water (Ortiz de García et al. 2013). The presence of several pharmaceutical groups in aquatic environment even at extremely low concentration levels can result in adverse effect such as antibiotic resistance or the disruption of hormonal functions in the body (Halling-Sorensen et al. 1998). The knowledge of the presence of pharmaceuticals in the aquatic environment has drawn the attention of researchers, policy makers, water management authorities as well as the general public. There are several conventional wastewater treatment technologies which have been developed, however, most of these methods fail to effectively remove pharmaceuticals, while others are not environmentally friendly. Various adsorbents such as carbon nanotubes, activated carbons, clays and others have been used for the removal of pharmaceuticals in wastewater treatment processes, but they have limitations like high costs for large scale application and toxicity associated with some of them (Rossner, Snyder, and Knappe 2009).

Silk fibroin has abundant functional groups providing potential sites for adsorption of pharmaceuticals for water treatment. Furthermore, silk fibroin allows for surface modification and functionalization making it an attractive material to explore as a potential adsorbent (Li et al. 2012). From preliminary experimental data, degummed silk fibroin showed effective removal efficiency for selected groups of pharmaceuticals. Therefore, due to the unique properties of nanofibers, such as; large specific surface area, high porosity, small pore size, high thermal and electrical stability and mechanical strength (Greiner and Wendorff 2007), this study focused on developing a method for the efficient removal of selected pharmaceuticals using electrospun nanofibers from *Argema mimosae* silk fibroin.

Keywords: Argema mimosae, nanofiber, pharmaceuticals, silk

WO 14

Optimization of magnetite nanoparticle and pine cone based nanocomposite synthesis for water treatment

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Water treatment materials are continuously being improved in a bid to increase water remediation efficiency and lower treatment costs. Natural materials are an ideal option due to their biodegradability and environmental friendliness. The use of biomaterials in water remediation has gained interest due the availability and low cost of biomaterials. Biomaterials however suffer drawbacks since they lack mechanical strength and porosity required during water treatment operations. Nanomaterials on the other hand possess high mechanical strength and surface areas which are ideal for water treatment operations but also suffer drawbacks presented by their small sizes which make their separation from treated water costly and they lack the functionalization required to sequester pollutants especially heavy metals. In this work magnetite nanoparticles, synthetic parameters were optimized for the remediation of chromium contaminated water. The synthesis parameters were optimized following one factor at a time design to identify the conditions that resulted in particles which had the highest chromium sorption efficiency. The parameters modified were the amount of co-precipitating agent, temperature, and precipitation duration. Pine cone powder, a natural biosorbent was used to prepare a nanocomposite with magnetite. During the composite preparation, the effect of biomass amount on the sorption efficiency was also monitored. With an increase in the amount of precipitating agent, temperature and time, the sorption efficiency increased to an optimum level and decreased with further increments. The incorporation of pine cone powder and magnetite in the nanocomposite resulted in improved adsorptive properties compared to magnetite and pine cone powder when used separately. The presence of pine cone improved the surface properties of magnetite nanoparticles by reducing agglomeration hence improving surface areas.

Keywords: chromium, magnetite, nanomaterials, nanocomposite

WO 15

The use of NF membranes for rejection of nickel (Ni), copper (Cu) and palladium (Pd): A hope for mine effluent treatment

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Recovery of precious metals from synthetic samples containing Pd, Cu and Ni ions with an application of membrane technology from chlorides metal salts were studied. Three commercial membranes (NF90, NF- and NF270) were employed for rejection of metals species and charged solutes. Firstly, charged solutes (NaCl and MgCl₂) were both employed for characterizing (NF) membranes in terms of water and salt permeability. A 1 ℓ capacity dead end unit was used and the solutions were constantly stirred at 500 rpm to homogenize the sample (feed). It was found that NF270 (highest permeate flux) membrane, performed above lowest void sizes (NF90 and NF-) with rejection of 98% for Mg²⁺ than Na⁺ with 95% rejection for 20 ppm solution at 5 bar during pH 2.0. The highest recovery value of 94% was observed on NF- for Cu²⁺ and Ni²⁺ at 5bar. Pd²⁺had a major decrease on membrane rejection reaching the lowest retention of 17% at 20bar. The pH, pressure and concentration had an influence on the retention behavior of metals on membrane surface material. Metals have high rejection capacity of being removed from wastewater using nanofiltration membrane technology.

Keywords: Nanofiltration, Mining effluent, Polymeric Membranes

WO 16

Design and fabrication of polymer layered silicate nanocomposites for water purification Mbui Damaris¹, Andala Dickson², Abong'o. Deborah¹ & <u>Mmbaga. John¹</u>

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Zeolites employ the principle of surface adsorption of toxic heavy metals in remediation of polluted water. Zeolite and cellulose-acetate nanocomposites were fabricated in this study using a combination of melt blending and solution mixing. The nanocomposites were optimized for heavy metal adsorption using spiked Lead and Cadmium solutions. Fourier Transform Infrared Spectroscopy, Scanning Electron Microscopy, Energy Dispersive X-Ray Spectroscopy and Powder X-Ray diffraction crystallography were used for physical characterization. Fourier Transform Infrared spectra showed a reduction of the hydroxyl peak for cellulose acetate and that of the residual silanol group for zeolites symbolizing bonding during nanocomposite formation. Scanning Electron Microscope results showed an increase in voids with zeolite loading in the nanocomposites, a useful characteristic of good adsorbents. Powder X- ray diffraction crystallography results showed a reduction in 2 theta values for the nanocomposites due to penetration of the polymer into the silicate lattice e.g. zeolite 2 theta peak at 7.44[°] reduced to 7.09[°] in the nanocomposites signifying an increase in crystal lattice d- spacing from 11.88Å to 12.47 Å. It was also noted that a maximum of 98.87% of Lead ions were adsorbed using 20% zeolite nanocomposite while 85.30% of Cadmium ions were adsorbed using 40% zeolite nanocomposites. The timedependent adsorption experiments for both heavy metals in solution favoured a pseudo second order kinetic model. Contact time experiments were conducted with intervals of 5, 10, 20, 40 and 75 minutes under neutral pH. The Langmuir Isotherm showed the best fit for both metals with R² values of 0.985 and 0.996 for Lead and Cadmium ions respectively implying that the adsorption process was chemisorption. The zeolite-cellulose acetate nanocomposites can be applied in heavy metal removal from water and could be up-scaled and commercialized into membrane or granular based domestic water purification platforms. Keywords: Zeolites, nanocomposites, adsorption, characterization

Poly(vinylidene fluoride) ultrafiltration membranes incorporating catalytic Metal Organic Frameworks for degradation of dyes in water

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There's a hype associated with water stable Metal Organic Frameworks (MOFs) in water treatment due to their high porosities and specific interactions with adsorbate and the possibility that their catalytic properties could be utilised to degrade toxic compounds or pollutants. The textural properties of MOFs, and particularly their often large porosity, are frequently regarded as one of the main drivers for using MOFs for organic contaminants adsorption and catalysis from aqueous solutions. Nevertheless, the textural parameters are believed to be playing a minor role as controlling factors of the adsorption mechanism. The pore window size of the MOF is not even compared to that of the pollutant, it is the molecular size of the organic contaminant to be removed that has to be similar or larger than that of the MOF pore windows. The ability of MOFs to degrade organic contaminants from water sources is another option for water purification. Degradation is advantageous over adsorption because MOF will be ready to be reused, no sorbent regeneration step, and organics are not required to be eliminated. This study describes the preparation and characterisation of MOF-2, and preparation of graphene oxide (GO)-MOF-2 composite. Composites of 1 % weight and 9 % weight were found to be more stable in water and were continued for the study. Composites of different concentrations were used as fillers for membrane preparation using PVDF as a basis of the membrane, PVDF/[GO/(MOF-2)_{0.9}]_{0.25/0.5} and PVDF/[GO/(MOF-2)0.1]0.25/0.5, where 0.25/0.5 indicate the loading of 0.25 wt% and 0.5 wt% for the preparation of 50 wt% of the membrane. The physicochemical properties and morphology of membranes were evaluated using FTIR, water contact angle (WCA), Scanning electron microscopy (SEM) coupled with Energy Dispersive Spectroscopy (EDS). FTIR confirmed the expected functional groups, and WCA showed that membranes with low concentration of the composite, PVDF/[GO/(MOF-2)0.1]0.25/0.5, had improved the hydrophilicity of PVDF than those with higher concentration of the composite, SEM revealed surface morphology and EDS indicated the amount of elements which were present in the membrane. Membranes were applied in photo degradation of dye stuff, Methyl range and Congo Red, water flux, rejection of dye stuff, and fouling studies.

Key words: MOFs, dye stuff, composite membrane, water flux, rejection, fouling studies

WO 18 Biosorption of Hg²⁺ from aqueous solutions by *Cladophora sp* alga immobilized in calcium alginate beads: a continuous flow study

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Biosorption is emerging as a technology for the remediation of water impacted by toxic elements. Mercury is one of the most elements found in the environment due to its propensity to bioaccumulate and biomagnify in living organisms and thus cause severe human health disorders. Algae are one of the most extensively used biosorbents for the removal of toxic elements from water because they are highly abundant, have high surface area to volume ratios and high adsorption capacities. However, their fragility and tendency to swell and block columns limits their application in continuous flow operations. Hence, they are often immobilized in solid supports like alginates to overcome this challenge. In this study, the efficiency of *Cladophora sp* alga immobilized in alginate beads for the removal of mercuric ions from unitary and multi-elemental aqueous solutions using a continuous flow mode was evaluated. *Cladophora sp* alga was modified by entrapment in alginate beads and characterized using Fourier transform infra-red spectroscopy (FTIR), Braunner-Emmet-Taylor (BET) analysis, scanning electron microscopy (SEM) and Thermogravimetric analysis (TGA). The effects of bed height, flow rate and inlet metal concentration on the efficiency of the biosorption system were also investigated. The breakthrough behavior of the biosorption column was assessed using the Adams-Bohart, Thomas and Yoon-Nelson methods. Optimal metal removal was achieved at a solution pH of 5, bed height of 7 cm, flow rate of 2 mL min⁻¹ and inlet metal concentration of 2 mg L⁻¹. The experimental data also fitted the Thomas Model for

different values of bed height, flow rate and inlet metal concentration implying that under the conditions studied, the biosorption of mercury by *Cladophora sp* alga immobilized in alginate beads followed pseudo-second order kinetics. The results obtained in this work could serve as groundwork for the adaptation of this biosorption system for large scale water treatment operations.

Keywords: biosorption, mercury, remediation, Cladophora sp, algae, immobilization

WO 19

Enhancing the photocatalytic degradation of selected chlorophenols using Ag/ZnO nanocomposites

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Chlorophenols are among the priority listed water contaminants due to their estrogenic, mutagenic or carcinogenic health effects. The Ag/ZnO nanocomposites were synthesized, characterized and tested for photacatalytic degradation of chlorophenols in water. The synthesis was done using zinc nitrate hexahydrate (ZnNO₃. 6H₂O) precursor and sodium hydroxide (NaOH). Silver nitrate (AgNO₃) was added to ZnO and reduced with sodium brohydride to produce the silver nanoparticles within the ZnO structure. The silver content was varied from 1, 3 and 5wt% for optimisation. The nanocomposites were characterised using ultraviolet - visible spectroscopy (UV-Vis), photolumniscence (PL), x-ray diffraction (XRD), fourier transform infrared spectroscopy (FTIR) and transmission electron microscopy (TEM). The nanocomposites were tested for their photocatalytic properties on 2- chlorophenol (CP), 2,4- dichlorophenol (DCP) and 2,4 6- trichlorophenol (TCP) in water. The UV-Vis results showed that, as the amount of silver was increased a gradual slight red shift was observed. The XRD patterns for Ag/ZnO exhibited peaks that were characteristic of the hexagonal wurzite structure and peaks characteristic for Ag appeared at 38.24°, 44.37°, 64.67° and 77.58° corresponding to (111), (200), (220) and (311) reflection planes. STEM results showed the presence of Ag in ZnO with ZnO appearing as rods shapes. The EDX elemental analysis confirmed the presence of Ag in the Ag/ZnO nanocomposites with no contaminants peaks. On testing the nanocomposites for phohotocatalytic degradation of chlorophenols, addition of Ag to ZnO improved degradation of the chlorophenols compared to the pure ZnO.

Key words: Ag/ZnO, precipitation, photocatalytic degradation, chlorophenols

WO 20

Potential Wastewater Purification Nanosystem Based On Renewable Polymers

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Botswana is one of the countries that have adopted the emerging and promising nanotechnology for wastewater purification. Pollutants ranging from heavy metals, bacteria, effluents and dyes have been removed from wastewater and other environmental settings using nano sized materials owing to their merited antibacterial and photocatalytic properties. Metallic nanostructures are most suitable for photocatalytic and antibacterial applications. Their limitations including recombination of the photogenerated e⁻/h⁺ pair, inefficient photon absorption in the visible light region, and leaching have resulted in partial or incomplete pollutant degradation. Metal-polymer nanocomposite exhibit elevated optical, electrical, thermal and mechanical properties as compared to bare metallic nanomaterials. This study presents the development of an efficient, economic and environmental friendly system, which is a vital endeavour to the bionetwork of environmental and water system

mitigation. Oil palm empty fruit bunches were used during in-situ solution casting process for the synthesis of an efficient Ag/ZnO-cellulose based nanocomposite. Different analytical techniques which includes; X-ray diffraction (XRD), scanning electron microscopy (SEM) equipped with energy dispersive spectroscopy (EDS), UV-vis-NIR spectroscopy as well as the Fourier transform infrared spectroscopy (FTIR) were used for sample characterisation. The nanocomposite was tested for photocatalytic activity by monitoring the degradation of a probe organic pollutant, cationic dye methylene blue (MB) under direct solar irradiation. The antibacterial activity of the nanocomposite was tested against *E.coli, S.aureus* and spore forming *B. subtilis* using Agar diffusion method. The photodecomposition capacity of the nanosystem was monitored by removal of aqueous methylene blue (MB) under direct solar irradiation. Ag/ZnO-cellulose based nanocomposite showed excellent photocatalytic activity against MB and also exhibited strong activity against the growth of *E.coli, S.aureus* and *B. subtilis*. The enhanced activities are attributed to the synergic contribution between Ag and ZnO as well as the role played by cellulose.

Keywords: Cellulose-based Nanocomposite, Antibacterial Activity, Photocatalytic Activity

WO 21

Heterogeneous Fenton's degradation of methylene blue by activated carbon-iron oxide composite: Kinetics study & mechanism

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Advanced oxidation processes (AOPs) are processes that involve the production of highly efficient hydroxyl radicals for the degradation of organic pollutants. One of these AOPs is heterogeneous Fenton oxidation process. In this paper, one step synthesis was adopted, were an agricultural waste pine cone was used as a source of carbonaceous materials and iron chloride hexahydrate as an activating agent and source of iron oxide, for the synthesis of activated carbon-iron oxide composite via microwave at 600 W at different amount of iron precursors. The catalyst was characterized by EDX, XRD, and XRF.

The catalysts were also tested on the Fenton oxidation of methylene blue at a temperature of 27°C. The pseudofirst, pseudo second order kinetic and Langmuir-Hinshelwood models were fitted to the data. The mechanism of Fenton's oxidation is known to depend entirely on the decomposition of H₂O₂ catalysed by the iron oxide species producing radicals that promote degradation of the pollutants. To confirm the degradation mechanism, the % degradation was measured in the absence and presence of radical scavengers, such as isopropanol which acts as a scavenger for hydroxyl radicals and benzoquinone that acts as a radical scavenger for superoxide radicals. The addition of scavengers at the beginning of the experiments resulted in a decrease in the degradation of methylene, and it was also observed that the decrease in methylene blue degradation was higher for experiments were isopropanol was used as compared to benzoquinone, suggesting that the hydroxyl radical are more active as compared to superoxide radicals. However in the degradation of MB, decolorization of MB it does not mean the complete mineralization to nontoxic molecules. MB is blue in color and leuco MB (LMB), the reduced form of methylene blue is colorless. LMB it can be converted back to MB, hence it should be confirmed that the decolorization of the MB it is not due to the formation of LMB. It was observed that methylene blue was degraded to smaller organic acids.

Keywords: methylene blue, degradation, pseudo-first, pseudo-second order, Langmuir-Hinshelwood model

Bio-adsorbent from avocado peel for removal of As³⁺ and Cd²⁺ from water

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The water pollution is the worldwide problem that affects everyone hence this study investigates the adsorption of As(III) and Cd(II) by using natural adsorbent from avocado peels. The natural adsorbent from avocado peels is saponified by NaOH in order to increase the OH groups on the surface of the adsorbent which in turn increase As(III) and Cd(II) adsorption on avocado peels. The functional groups found on the avocado peels were characterised by FTIR, SEM, EDS and BET. The batch extraction method was applied in adsorbing As(III) and Cd(II) from standard solutions and real water samples. The arsenic(III) and Cd(II) determination were done separately by using anodic stripping voltammetry (ASV) after optimising the following adsorption parameters, pH, adsorbent mass, analyte concentration, contact time and temperature. The adsorbent has a good stability because it was applied separately for arsenic(III) and Cd(II) adsorption for more than 8 times and the same results were obtained . The avocado peels displayed a great potential as an adsorbent because after adsorption the current signal in 20ppb As(III) standard decreased from 7x10⁻⁵ to 2x10⁻⁵ μ A while Cd(II) in 10 ppm standard solution decreased from 3x10⁻⁶ to 5x10⁻⁶ μ A. The concentration of the analytes in real water sample after adsorption were also confirmed by using ICP-OES.

Keywords: avocado peels, adsorption, arsenic(III), cadmium(III), anodic stripping voltammetry

WO 23

Syntheses of metal organic framework composites for removal of nitrophenol in wastewater and electrocatalytic hydrogen evolution reaction

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Experts have long warned of the dangers that increasing atmospheric carbon poses to the planet leading to shortage of clean water; from general environmental change all the way through to melting polar ice caps, floods, tsunamis. Now, a collaboration of nanotechnology research group at University of Limpopo (NanoRG@UL), South Africa, could be set to develop a solution. Metal organic framework (MOF) composites, developed by NanoRG@UL, and has already been applied in hydrogen evolution reaction (HER) energy and water purification as part of waste to profit studies. These could be a breakthrough in tackling climate and water challenges due to ability of MOF to store, separate and capture carbon as it is released into the air and also to remove contaminants in water. "This collaboration is another exciting validation of MOFs potential to address energy and water problems," says NanoRG@UL Senior Lecturer, Dr KD Modibane. "It is important for us to harness the power of MOFs for large scale applications that solve real problems. It is hoped that this research will expedite our efforts to put University of Limpopo on the map as a hub for MOF based innovation, and also as leading players in the fight against climate, energy and water challenges." Hence, this present work is on the syntheses and applications of MOF composites for water treatment and HER (**Figure 1**).



Figure 1: Cyclic voltammetric curves during HER and SEM image of resulted p-Nitrophenol/MOF composite from wastewater

Keywords: Metal organic frameworks, Composite, Water treatment, Hydrogen evolution reaction

WO 24

Green synthesis of PVDF nanofibres decorated with biocidal Ag nanoparticles <u>Lebea Nthunya</u>¹, Bhekie Mamba¹, Arne Verliefde², Sabelo Mhlanga^{1*}

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This study was aimed at developing polyvinylidene fluoride (PVDF) nanofibres decorated with silver (Ag) nanoparticles (NPs) synthesized using a greener process. AgNPs with diameters between 20 - 30 nm (see the synopsis below) were produced using one pot synthesis where apple extract was used as a reducing agent. These NPs were mechanically mixed with PVDF solution and electrospun to produce biocidal PVDF nanofibres. The resulting biocidal nanofibers were characterized using SEM, XRD, UV-Vis, and TEM for determination of surface morphology as well as the formation and dispersion of the NPs. The biocidal nanofibres were tested for their efficacy on Gram +/- bacteria for the determination of their ability to prevent biofilm formation in water purification. SEM images confirmed the formation of uniform structures of the PVDF nanofibers (average diameter = 311 ± 85). XRD and UV-Vis results showed the presence of Ag NPs and the differences in reduction plasmon resonance due to different concentrations of the Ag precursor. The uniform Ag NPs occurred at a lower concentration of the precursor. The antibacterial nanofibres were observed to effectively inhibit the growth of the bacteria.



Synopsis: A schematic representation of the formation of Ag NPs, their deposition on PVDF nanofibres and their inhibition on bacterial growth.

Keywords: Green synthesis, PVDF nanofibres, Silver nanoparticles, water purification

Investigation of Antibacterial and Fouling Resistance of Silver and Multi-Walled Carbon Nanotubes Doped Poly(Vinylidene Fluoride-co-Hexafluoropropylene) Composite Membrane

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Clean drinking water availability is a major problem for developing countries. Membranes technology has become a popular filtration technique and plays a significant role in separation of unwanted constituents such as organic and inorganic pollutants. Herein, the study has focused on the preparation of poly(vinylidene fluorideco-hexafluoropropene) (PVDF-HFP) doped with multi-walled carbon nanotubes (MWCNTs) and silver nanoparticles. The nanocomposite membrane were prepared by a phase inversion method, and characterised by Thermogravimetric analysis, Fourier transform infrared spectroscopy and scanning electron microscopy. The results indicated an increase in porosity, swellability and water content of the PVDF-HFP membrane with the addition of MWCNTs and/or Ag nanoparticles, showing an improved hydrophilicity. The 1.5 wt % MWCNTs/PVDF-HFP composite membrane showed good desalination and fouling resistance rates, which correlates with a low water contact angle. The membranes were also used to filter contaminated water with *E. coli* (ATCC 25922) wherein they demonstrated high microbial load reduction and high antibacterial activity.

Keywords: Composite membranes; multi-walled carbon nanotubes; PVDF-HFP; fouling resistance; antibacterial activity

WO 26

Application of magnetic Fe₃O₄@Mg/Al- layered double hydroxide (LDH) nanocomposite as an adsorbent for ultrasound assisted solid phase microextraction of trace metals in water matrices

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A new method was developed for the determination of trace Cd, Cr, Pb, Co, Ti, and Ni in environmental water by inductively coupled plasma–optical emission spectrometry detection after ultrasound assisted solid phase microextraction (UADSPME). The magnetic Fe3O4@Mg/Al-layered double hydroxide (LDH) was used as adsorbent. The magnetic nanocomposite was prepared by low saturation coprecipitation in the dispersed Fe₃O₄ suspension. The nanoadsorbent was characterized using FTIR, TEM, XRD, SEM and EDX. Furthermore, the magnetic nanocomposite can be easily separated from the aqueous solution by an external magnet before and after adsorption process. Effective experiential parameters controlling the performance of the microextraction process, such as the adsorbent amount, extraction time, eluent concentration and pH were optimized using central composite design. Under optimum conditions, the developed method displayed relatively low limits of detection and quantification, good repeatability (intra-day precision) and reproducibility (inter-day precision). Lastly, the developed method was successfully applied for extraction of Cd, Cr, Pb, Co, Ti, and Ni at trace levels from analytes in environmental water samples.

Keywords: Magnetic nanocomposite; trace metals, environmental matrices

Chemical Oxidation Of Macadamia Activated Carbon Through Impregnation By Inorganic Acids For Enhanced Cr(VI) Adsorption

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Macadamia activated carbon (MAC) was impregnated with different concentrations of sulphuric acid or phosphoric acid or nitric acid and heated in a muffle furnace to improve the structural characteristics of the adsorbent for enhanced Cr(VI) removal. Alteration of surface structural characteristics was confirmed by Fourier transform infrared spectroscopy, scanning electron microscopy and thermogravimetric analysis. The chemical oxidation of ACs increased the surface oxygenated functional groups. Adsorption of Cr(VI) was carried out by varying parameters such as contact time, pH, concentration and adsorbent dosage. The optimum operating conditions for the adsorption of Cr(VI) were pH 1 and pH 4, contact time 120 min, adsorbent mass 0.5 g (0.3 g) and Cr(VI) concentration 25 mg.L⁻¹. The results showed that the *Macadamia*–based AC can be used efficiently for the treatment of chromium containing solutions as a low cost alternative compared to commercial AC and other adsorbent reported. The results showed that treated MAC performed better that untreated MAC, signifying the effect of secondary treatment on enhanced removal of pollutants.

Keywords: Adsorption, chromium, Macadamia, modification, mineral acids

WO 28

Modeling and Simulation of the Adsorption Process of Fluoride to the Surface of Porous Clay-Hydroxyapatite Filter

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Fluoride is known to have both beneficial and adverse effects on humans, depending on the total intake. Chronic exposure to excessive fluoride may cause toxic damage to osseous tissues, which manifests as dental and skeletal fluorosis. Therefore it is necessary to reduce the concentration of fluoride in our drinking water so as to make it safe for consumption. This paper presents an artificial neural network model (ANN) for the prediction of fluoride adsorption capacity to the surface of a porous clay-hydroxyapatite (C-HA) filter. Effective parameters such as fluoride concentration, ratios of clay to HA, temperature, and contact time are studied to optimize the conditions for maximum removal of fluoride. The amount of fluoride adsorbed on to the surface of the porous clay-hydroxyapetite filter is found to increase with increase in each of these parameters except for temperature. Hence, the ANN model shows close agreement with experimental studies for fluoride adsorption efficiency on clay-hydroxyapatite composite under different conditions. Therefore, results from this work provide a predictive system for determining the effectiveness of Clay-HA as fluoride adsorbent.

Keywords: Adsorption, porous clay-hydroxyapatite filter, artificial neural network, feed forward neural network.

Use of Diatomaceous Earth (DE) Wastes for Nano-Porous Composite Membranes in Water Purification Systems

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The outbreaks of water-borne diseases are a common occurrence in developing countries and has claimed millions of lives in the recent years despite the many water purification approaches in use. This is because most of these water purification systems are inefficient in removal of all pathogens especially viruses from drinking water. Furthermore, the DE wastes have not found direct application in science. Thus, the wastes pose a challenge to DE industries. In this work, the nanomaterials of diatomaceous earth (DE) wastes and activate carbon are employed in the design of efficient and effective water filtration membranes capable of eliminating pathogens and viruses from water. The DE wastes and activated carbon raw materials were ground to the range of 86.0 nm to 200.0 nm. The DE wastes were characterized in terms of chemical analysis. They were found to contain 89% silica and a total flux content of 11.0% (4.14% of Al₂O₃, 3.88 of CaO, 0.85% of K₂O, 0.19% of MgO and 5.10% of Na₂O) making it a suitable material for water filter membranes. The samples for the filter membranes were fabricated from a mixture of DE and activated carbon in various ratios and fired at 1000 °C. The pore size of the finished filter was in the range of 22.0 nm – 150 nm. The mechanical strength of the filter membranes was enhanced by use of plant derived binders ("mrenda") thereby increasing the filter flow rate without compromising on its structural reliability.

Keywords: DE wastes, Nano-porous Composite Membrane

WO 30

PES/quaternized-PES blend anion exchange membranes for use water purification: Investigation of the polymer compatibility and properties of the blend Monaheng L. Masheane¹², Bhekie B. Mamba¹, Arne R.D. Verliefde², Sabelo D. Mhlanga^{1#}

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The polymer blend method is the most common and simple method used to modify membrane properties such as the surface charge density, mechanical and thermal stability. The compatibility between the polymers is an important factor affecting the structure and properties of blend membranes. Polyethersulfone (PES)-based anion exchange blend membranes were prepared from quaternized-PES (Q-PES) and N-Methyl-2-pyrrolidone (NMP) casting solutions with water as coagulant *via* non-solvent-induced phase inversion. The compatibility of the membranes was investigated through the thermodynamics while the membrane formation was determined using cloud point technique. The properties of the membranes were investigated using AFM, contact angle measurements and SurPASS Electrokinetic Analyzer. The results indicate that the PES/Q-PES blend system was partially compatible, thus leading to instantaneous demixing (**Fig. 1**). The ion exchange capacity and the swelling of the membranes were also investigated. The roughness and the surface charge density increased with increasing addition of Q-PES while the total surface energy decreased. The IEC increased with the addition of Q-PES while the swelling decreased.

Keywords: Ion-exchange, compatibility, membranes, quaternized-polyethersulfone

Employing valorized waste remains for the effective removal of toxic ions from

wastewater

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In this work, eggshell waste remains which is abundant, easily available, cheap and environmentally friendly waste material in Botswana was rejuvenated by subjecting it to a simple green procedure, then applied as an adsorbent to clean wastewater through the removal or reduction of common toxic ions that usually exist in wastewater. To improve the adsorbing capacity of the powder material, a simple environmentally friendly sample pre-treatment procedure that involved optimally washing (7 times) the waste powder material with an environmentally friendly, weak organic acid, vinegar, of a low concentration of 12.67% was employed. Minitab software was employed for the simultaneous optimization of factors that affect sorption studies. Initial ion concentration, sorbent dose, contact time and solution pH were found to be 27.14 mg/L, 74.21 mg/L, 67.43 min and 7.75 respectively. Employing the optimized conditions, the valorized waste remains exhibited high percentage removal efficiencies toward the selected ions from raw wastewater samples ranging from 68.93% to 95.77% with %RSD < 2 for n = 3. Fourier transform infrared spectrometer spectra of the waste powders displayed multiple functional groups such as amines, carboxylic, hydroxyl, and carbonyls which are well known to bond well with ions through hydrogen and oxygen bonding as well as ion exchange. The X-ray diffractogram and the Raman spectrograph reflected the presence of calcite within the eggshells waste, which has excellent ion exchange ability for both cations and anions. The valorized waste material efficiency was demonstrated by removing hazardous ions commonly found in wastewater.

Keywords: Waste remains, Eggshells, Wastewater, Valorization, Inorganic ions

WO 32

Conducting polymer composites for the adsorption and reduction of toxic hexavalent chromium in water

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Mining, electroplating, tanning, textile and other industries produce wastewater containing high concentrations of toxic hexavalent chromium, Cr(VI). The release of Cr(VI) into water sources is a serious concern due to its high toxicity to humans and animals and high mobility in the environment. Therefore, industrial wastewater must be treated prior to discharge into the environment to ensure Cr(VI) levels are well below the maximum allowable limits prescribed by water quality standards [2]. Conducting polymers such as polypyrrole (PPy) and polyaniline (PANI) have been widely studied as adsorbents for Cr(VI) removal from water due to their ion-exchange properties and inherent ability to reduce Cr(VI) to less toxic Cr(III). In this study, conducting polymers were modified by incorporating suitable dopants and magnetic nanoparticles to improve their Cr(VI) adsorption capacity and impart other properties important for water treatment applications. Polypyrrole/2,5diaminobenzenesulfonic acid (PPy/DABSA) composite and magnetic polypyrrole-polyaniline/iron oxide (PPy-PANI/Fe₃O₄) nanocomposite, were synthesized by in situ oxidative polymerization methods. The composites were characterized using various techniques including FTIR, SEM, TEM, TGA, XRD, XPS and VSM. Batch adsorption studies were carried out to evaluate the performance of the conducting polymer composites for the removal of Cr(VI) from aqueous solution. The PPy/DABSA composite and PPy-PANI/Fe₃O₄ nanocomposite both showed high Cr(VI) adsorption capacities. Both composites selectively removed Cr(VI) from aqueous solution and could be used for up to 3 cycles without any loss of adsorption capacity. Conducting polymer composites were shown to be promising adsorbents for the remediation of industrial wastewater containing Cr(VI).

Keywords: polypyrrole, polyaniline, adsorption, reduction, chromium

Dual-Functional Ultrafiltration SiO₂ PSf/PVA Membrane for Simultaneous Removal of disinfection by products

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The disposal of industrial effluents containing dyes in wastewater streams is a serious environmental concern due to their synthetic origin and complex molecular structure making these compounds difficult to biodegrade. In this work, dual functional PSf/PVA membranes modified by incorporation of SBA-15 or ZnO nanoparticles were fabricated for the removal of Congo dye in aqueous solutions using a dead end set up. The removal mechanism of the dye molecules was through the adsorption and rejection. The highest dye removal capacity (53.5%) was achieved by PSf/PVA/ZnO (0.5) membrane. The removal capacity of the membranes decreased and also during reusability studies. The highest removal capacity obtained at the second cycle was 31.1 % and 3.7% removal was obtained during the third cycle. This study sheds the new light in fabricating reusable, ultrafiltration membranes for the removal of dyes in aqueous solution.

Keywords: Dual-functional membranes, ultrafiltration, removal of Congo dyes

WO 34

Adsorptive removal of Cr(VI) and V(V) ions using clinoptilolite modified with polypyrrole and iron oxide nanoparticles

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Clinoptilolite modified with polypyrrole and iron oxide nanoparticles (Cln-PPy-Fe₃O₄) nanocomposite as a potential adsorbent for Cr(VI) and V(V) was prepared via polymerization of pyrrole monomer using FeCl₃ oxidant in aqueous medium in which clinoptilolite-Fe₃O₄ nanoparticles were suspended. The structure and morphology of the prepared adsorbent was analysed with the Fourier transform infrared (FTIR), field-emission microscope (FE-SEM), energy dispersive X-ray (EDX), high resolution transmission electron microscope (HR-TEM) and X-ray diffraction (XRD). Batch adsorption studies were performed to test the ability of the adsorbent to remove Cr (VI) and V (V) ions from aqueous solution. The sorption kinetic data fitted well to the pseudo-second order model and isotherm data fitted well to the Langmuir isotherm model. The maximum adsorption capacity determined from the Langmuir isotherm increased from 344.8 to 434.8 mg/g and 65.0 – 74.9 mg/g for chromium and vanadium respectively, as the temperature was increased from 25°C to 45°C. Thermodynamic parameters revealed that the adsorption process is spontaneous and endothermic in nature.

Keywords: Clinoptilolite; chromium; vanadium; nanocomposite; adsorption

Fabrication of macrovoid-free polyethersulfone/sulfonated polysulfone/o-MWCNT support UF membranes with improved mechanical strength, antifouling and performance properties

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Herein, we report on the successful incorporation of multi-walled carbon nanotubes (MWCNTs) onto polyethersulfone/sulfonated polysulfone (PES/SPSf) ultrafiltration (UF) membranes via non-solvent induced gelation phase separation method. MWCNTs were first prepared using a nebulized spray pyrolysis of toluene and ferrocene mixture at elevated temperatures. MWCNT were ideally grown on a silicon wafer substrate and around the walls of the quartz tube. Microscopic studies show that the outer diameters of MWCNTs measured from ${\sim}10$ nm to 14 nm. The MWCNTs produced were further purified and oxidised by mild acid treatment to aid their chemical interaction with PES/SPSf matrix during UF membrane preparation. Thermal stability analysis revealed that the oxidised MWCNTs (O-MWCNTs) undergo complete thermal degradation and no catalyst residues were detected after 600 °C, while Raman spectroscopy data indicates a reduction in lattice distortion due to the absence of impurities. PES/SPSf membranes containing different loadings of O-MWCNTs (0; 0.005; 0.01; 0.03, 0.05 and 0.1 wt%) were prepared by a non-solvent induced phase separation method. Investigations show that the inclusion of O-MWCNTs in the PES/SPSf polymer blend did not distort the sponge-like morphology as commonly reported for hydrophilic additives such as OMWCNTs. Furthermore, membrane hydrophilicity, permeability, mechanical strength and antifouling properties were found to improve after incorporation of O-MWCNTs. Our results therefore demonstrate that macrovoid-free PES/SPSf/O-MWCNT supports are a promising membrane material with superior antifouling properties and mechanical strength properties.

Keywords: carbon nanotubes, nebulized spray pyrolysis, non-solvent induced gelation phase separation, membranes

WO 36

Adsorptive removal of toxic organic and inorganic cations from solution using novel facile magneto-carbon black-clay composite adsorbent <u>Paul N. Diagboya^{†,*}</u>, Ezekiel D. Dikio[†]

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New magneto-carbon black-clay composite adsorbents derived from feldspar clay, acorn (*Quercus robur*) fruit pericarp have been developed for efficient removal of both organic (methylene blue- MB) and inorganic (Cd(II)) pollutants from aqueous solutions. The facile composite adsorbents prepared in a one-pot process using two varying mass ratios of clay to carbon black of 0.5:1 (BMF-0.5) and 1:1 (BMF-1) exhibited higher cation exchange capacity (CEC) than any of the starting adsorbents. The rates of MB removal were faster than for Cd(II) ions in both composites, and consequently, faster equilibrium (30 and 120 min, respectively). The pseudo-second order kinetic model described the adsorption data better suggesting that the removal mechanism for these cationic species onto the composite adsorbents majorly involved electrostatic interactions. Surface adsorption (\geq 56 %) accounted for the bulk of cations removal on the BMF-0.5 composite, while adsorption on pores or within various partitions was dominant (\geq 54 %) on the BMF-1 adsorbent for both cations. The BMF-0.5 and BMF-1 adsorption equilibrium data fit the Langmuir type adsorption isotherm implying that adsorption of both cations occurred on adsorption sites having equal affinity for these cations and with the formation of only monolayer on adsorbent surfaces at equilibrium. Cd(II) was more adsorbed than MB on the adsorption capacities of BMF-0.5 and BMF-1 for both cations were approximately 14 and 16 mg/g, respectively. Pre- and post-adsorptive IR spectra study suggested

that the positions of active interactions between the cations and the adsorbents involved surface functional groups such as the -OH, $-COO^-$, and -C-N groups. The composite adsorbents could be reused more than three times without significantly losing the cation adsorption efficiency. Thus, this magneto-carbon black-clay composite is a promising adsorbent for removal of organic and inorganic pollutants from water.

Keywords: Waste biomass; Feldspar clay; Magnetic adsorbent; Methylene blue; Cd(II); Water treatment

WO 37

Quaternary imidazolium-modified montmorillonite clay for disinfection of water <u>Phumelele Kleyi</u>,¹ Suprakas Sinha Ray,¹ Arjun Maity¹

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Although 91% of the global population now has access to clean drinking water, 663 million people still remain without safe water sources; such as unprotected wells, springs and surface water. Fifty percent of this population lives in sub-Saharan Africa. Lack of piped water supply in this population means that water is consumed untreated and the consequence is high risk of exposure to waterborne diseases. Capacitating households with tools to treat and safely store drinking water would reduce the risk of exposure to waterborne diseases and hence improve their health. Therefore, there is a necessity for research efforts to focus towards the development of affordable and user-friendly household water disinfection technologies. Nanoclays are naturally occurring nanomaterials that, when organically-modified, can be used for various applications; such as rheological modifiers in packaging, as additives in paint, ink and cosmetics, as carriers and drug delivery systems as well as for water treatment. Disinfectant nanomaterials were synthesized by modification of montmorillonite clay using quaternary imidazolium cations containing various alkyl chain lengths. The nanomaterials were characterized using various techniques including TGA, XRD and TEM. The disinfectant nanomaterial containing the octyl chains displayed excellent disinfection of water samples (distilled, borehole and river) inoculated with E. coli. Investigation of the mechanism of inactivation using TEM revealed rupturing of the cell membrane after contact with the nanomaterial. Therefore, the quaternary-modified montmorillonite clay can be used for development of a household water filtration device.

Keywords: montmorillonite, quaternary imidazolium, disinfection, E. coli

WO 38

Hyperbranched polyethyleneimine-multi-walled carbon nanotubes (HPEI/MWCNTs) polyethersulfone (PES) membrane incorporated with Fe-Cu bimetallic nanoparticles for water treatment

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The contamination of freshwater systems by pesticides such as 2,4,6-trichlorphenol (TCP), hexachlorobenzene (HCB) and endosulfan is a key environmental problem. These compounds are stable and bio-accumulate in the environment, thus making it impossible to be removed from water systems. Pesticides have been detected in South Africa water systems and these mainly emanate from agricultural activities. HPEI is a highly branched cationic dendritic polymer. Its main role in this study was to assist in the dispersion of multi-walled carbon nanotube (MWCNTs) and Fe-Cu bimetallic nanoparticles. HPEI was covalently attached to MWCNTs via an amide bond to form HPEI-MWCNTs nanocomposite. Fe-Cu bimetallic nanoparticles were synthesized via the polyol method to form HPEI/MWCNTs/Fe-Cu. The HPEI/MWCNTs/Fe-Cu was blended with a polyethersulfone (PES) membrane via phase inversion and evaluated for the removal and degradation of 2, 4, 6-Trichlorophenol (TCP). The morphology and physiochemical properties of the membranes were characterised using scanning electron microscopy (SEM), contact angle analysis and water flux measurement. The sorption capacity of the membranes

was evaluated using liquid chromatography-mass spectroscopy (LC-MS). The modified membranes (HPEI/MWCNTs/Fe-Cu/PES) were more hydrophilic ($39.27^{\circ} \pm 1.25$) compared to the pristine PES membranes ($55.70^{\circ} \pm 3.27$). Generally, the flux was found to increase with increasing operating pressure up to 300kPa. The modified membranes exhibited high TCP removal rate of 99% as compared to pristine PES which exhibited 58%.

Keywords: 2,4,6-Trichlorophenol, Hyperbranched polyethyleneimine, Multiwalled carbon nanotubes, bimetallic nanoparticles, polyethersulfone ultrafiltration membrane

WO 39

Effect of the cobalt oxide nanoparticles size on the fenton catalytic activity

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Textile dyes releases largest groups of organic compounds that are found frequently in trace quantities in industrial waste water .When these compounds are discharged to the environment without prior treatment, they can cause destructions to the ecological balance in the environment because of their carcinogenic properties towards human being and animals. Methylene blue is a coloured compound which is used in dyeing and printing textiles and is a common water pollutants. Due to its toxicity human intervention is required to develop methods towards eliminating dyes from wastewater before discharging to the environment. Hence this study aims to degrade this compound by the Fenton reaction with hydrogen peroxide oxidation. Cobalt oxide nanoparticles were prepared using precipitation-oxidation method with cobalt acetate, sodium hydroxide and a combination of hydrogen peroxide and oxygen as oxidizing agents and were used as a catalyst for the oxidation degradation of methylene blue.The XRD diffraction pattern showed that the cobalt oxide phase of the nanoparticles is cubic Co_3O_4 . The size of the nanoparticles decreased with an increase in the amount of H_2O_2 added and the shape was found to be cubic as determined by TEM. The catalytic properties of the obtained Co_3O_4 nanoparticles were investigated on the degradation of methylene blue. It was found that the rate of reaction increases with a decrease in the nanoparticle size due to larger surface area of the smaller nanoparticles. However, the rate per surface area decreases as the nanoparticle size increases.

Keywords: cobalt oxide, catalytic degradation, Fenton reaction, oxidation

WO 40

Visible-light-induced BiVO₄ semiconductors for efficient wastewater treatment Chhabilal Regmi^a, and Soo Wohn Lee^a*

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A visible-light-driven metal and non-metal doped BiVO₄ photocatalysts were synthesized using a facile microwave hydrothermal method. The nominal amount of metal as well as non-metal doping exhibited the excellent photocatalytic activity for varieties of water pollutants, including ibuprofen and p-amino salicylic acid (pharmaceutical), *Escherichia coli* (bacteria), and green tides (phytoplankton). The strategically modified BiVO₄ sample exhibited better performance than pure BiVO₄ in visible light. Moreover, the first principle calculation on metal doping (Ni, Cu, Fe) revealed that doping in the desired side either vanadium or bismuth gives the most stable configuration of the synthesized samples with the formation of an in-gap energy state and oxygen vacancies. The in-gap energy state and the oxygen vacancies serve as an electron-trapping center that decreases the migration time of the photogenerated carrier and increases the separation efficiency of electron-hole pairs, which are responsible for the observed efficient photocatalytic, anti-bacterial and anti-algal activity of the samples. Similarly, the increased in the density of states at the valence band maximum on phosphate doped BiVO₄ improves the charge separation efficiency which is also responsible for enhanced photocatalytic activity. These properties thus suggest potential applications of metal and non-metal doped BiVO₄ as a multifunctional material in the field of wastewater treatment.

Keywords: metal and non-metal doped BiVO₄, First principles calculation, Ibuprofen, p-amino salicylic acid, *Escherichia coli*, *Chlamydomonas pulsatilla*

WO 41 Novel Macadamia nutshell powder grafted with 1,5-diphenyl-carbazide for enhanced removal of Cr(VI) from aqueous solution

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Chromium is considered among the hazardous metals for human health. It is generated from steel production, leather tanning and electronic components. The most common forms of chromium are trivalent chromium Cr(III) and hexavalent chromium Cr(VI). Cr(VI) is highly toxic and harmful to environment and humans. Agricultural waste materials such as Macadamia nutshells are currently receiving more attention for removal of Cr(VI). However, they have low adsorption capacity when used in their raw form. Therefore, this study investigated the modification of Macadamia nutshells to increase their adsorption capacity. On that note, Macadamia nutshell powder was treated with three different concentrations of hydrogen peroxide separately to remove extractable compounds and improve the pore structure of adsorbents. The peroxide treated powder was further grafted with 1.5'diphenylcarbazide reagent. 1.5'diphenylcarbazide is a chromogenic reagent used in Cr(VI) colometric analysis and in this study it was envisaged that its incorporation to the adsorbent surface will enhance Cr(VI) removal and selectivity. All the prepared materials (peroxide and grafted) were characterized by Fourier transform infrared spectroscopy (FTIR), Brunauer-Emmett-Teller (BET), scanning electron microscope (SEM) and the CHNS analyzer and evaluated for their Cr(VI) removal abilities by investigating numerous parameters such as the effect of initial pH, concentration, contact time, adsorbent mass, and co-existing ions. Optimum parameters were pH 1, 100 mg/L, 2 h and 0.2 g. Grafting of 1.5' diphenylcarbazide on the surface of Macadamia nutshell powder improved its performance for the removal of Cr(VI). The concentration of adsorbed Cr(VI) was determined by ultraviolet visible spectrophotometric method while that of total chromium was ascertained using flame atomic absorption spectroscopy.

Keywords: Activated carbon, amination, Macadamia, chromium(VI), adsorption, reduction

AO 01

Silk Fibroin-Based Edible Coatings to Control Crops' Post-Harvest Physiology

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The reinvention of structural biopolymers into technical materials has enabled the design of biomedical and optoelectronics devices with unique and compelling properties that can serve at the interface between the biotic and the abiotic worlds. For example, we have previously shown the use of silk fibroin bioinks as detector for E. coli contamination to enhance food security. Silk fibroin, in fact, is an edible and biodegradable protein extracted from B. mori cocoons that can be engineered in several formats ranging from films to particles, foams and gels. By exploiting silk fibroin essential properties (i.e. polymorphism, conformability and hydrophobicity) it is possible to design a water-based protein suspension that selfassembles in nano- to micro-meter thick membranes upon dip coating. The so formed thin films modulate mass transport (e.g. O_2 and CO_2 diffusion and water vapor permeability). This is possible by controlling protein polymorphism (i.e. formation of random or beta-sheet structures) during and post material assembly. Here, we show how silk materials can be used as an edible coating to preserve food freshness and mitigate spoilage. In particular, silk fibroin coatings with an increased beta-sheet content decrease O_2 and CO_2 diffusion in crops, effectively reducing oxidative stresses and cell metabolism. The control of silk fibroin polymorphism also allows to reduce loss of weight due to dehydration in several crops, including cassava roots, grapes, berries, bananas and tomatoes. The water-based processing and edible nature of silk fibroin makes this approach a promising alternative for food preservation with a naturally derived material. In the context of this presentation, we will also compare silk fibroin coatings with other natural alternatives as shellac, chitosan and zein based coatings.

Keywords: biopolymers, silk fibroin, spoilage, food loss, food waste, food security

AO 02 Synthesis and application of paraffin wax-surfactant dispersant composite particles in oil spill remediation

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Oil spills are major community, environmental and occupational health disasters because they can adversely affect the health of plants and animals in the ecosystem. To minimize the impact of oil spill on the environment, different remediation strategies such as chemical dispersants, in-situ burning, mechanical containment and collection and oil spill sorbents are adopted. Chemical dispersant is one of the most widely used remediation strategy in minimizing the impact of oil spills on the environment. However, indiscriminate application of dispersant to subsea and surface oil spills coupled with aqueous solubility of the formulated liquid dispersant results in significant amount of dispersant not coming into contact with the oil and wasted. To increase dispersant efficiency and reduce toxicity, water insoluble paraffin-wax particles containing surfactant as chemical dispersant were synthesized and their application in oil spill remediation examined using the baffled flask test. The results from the study showed that the dispersion effectiveness of the paraffin wax-surfactant composite particles were dependent on the surfactant-to-oil ratio (SOR), solubility of the matrix material (paraffin wax), crude oil type, salinities of sea water, mixing energy and the particle size of the dispersant composite particles. The dispersion effectiveness of the dispersant composite particles were compared with that of solubilized dispersant. For light crude oil, the dispersion effectiveness of the dispersant composite particles at higher SOR was almost the same as that of the solubilized dispersant. However, for heavy crude oil, the dispersion effectiveness of the solubilized dispersant was higher than that of the dispersant composite particles at higher SOR. The results from this study show the potential of dispersant composite particles to replace solubilized dispersants in oil spill remediation, and as a result eliminate the environmental complications associated with the use of solvents in formulating traditional liquid dispersants.

Keywords: Oil Spill Remediation, Dispersant Composite Particles, Chemical Dispersant, Toxicity, Paraffin-wax
Scoping study on Kenyan food quality and safety and waste management

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The aim of this study was to map out the relevant existing projects and initiatives on food quality and safety in Kenya; identify key issues and challenges and unmet needs in the sector; and propose and assess options in these areas. Food quality and safety initiatives in Kenya can be divided into the following categories: (i) projects supported by government and international development partners; (ii) research-driven projects; (iii) projects supported by regional bodies; and (iv) industry-supported initiatives. Challenges include low levels of on-farm and post-harvest mechanization, inadequate access to financial services, poor transport infrastructure, biological hazards, non-conducive government policies, high cost of farm inputs, unfavourable international trading rules and environmental challenges. Another area that also featured is the issue of wastage especially at the retail markets where huge quantities of fresh produce is discarded daily because it has been mishandled. From the Porter's Diamond Analysis and consultations with stakeholders several key issues have emerged which can form the basis for intervention through support and partnership both with the private sector, government agencies and government. These include (i) supporting firms to embrace appropriate Quality Management Systems from the farm to the market in order to improve productivity and quality; (ii) capacity building food handlers, especially in retail markets where post-harvest losses are highest; (iii) aggregating farmers into cooperatives in order to improve their access to markets without going through brokers (iv) establish a Quality Control Laboratory as a National Centre of Excellence in KIRDI to provide technical support to processors who cannot afford to establish their own quality control facilities or cannot meet the costs charged by commercial analytical services or other government agencies. Waste management can be tackled by utilizing appropriate packaging, storage and transport facilities and utilizing waste products for energy generation.

Keywords: Food Quality, Safety, Waste Management

AO 04

Micro-nanoencapsulated *Bacillus thurinigiensis* with a pH triggered release mechanism for the efficient bioprotection of brassica crops

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Bacillus thuringiensis (*Bt*) based formulations have been widely used to control lepidopteran pests in agriculture and forestry. One of their weaknesses is their short residual activity when sprayed in the field, due to their poor stability when exposed to sunlight. In this work, we have encapsulated *Bt* using only components which are harmless and compatible with agricultural processes. The colloidosome capsule is constituted of a thin shell of polymer which is opaque, so as to protect the active ingredient from sunlight, impermeable and insoluble when pH < 8.5. Above this pH, which corresponds to the midgut pH of the targeted lepidopteran pests, the capsule is dissolved, and *Bt* is released. The encapsulation process, which is based on a solvent-destabilization of a Pickering emulsion formed by pH-sensitive polymeric nanoparticles, fully preserves the bioactivity of *Bt*. Trials targeted the cabbage looper (*Trichoplusia ni*, T. ni (Hubner) that attacked brassica plants grown in a controlled environment as well as in the field. They demonstrated that the encapsulated *Bt* lifetime is significantly prolonged in comparison to non-encapsulated *Bt*. Thus, the use of colloidosomal microencapsulated formulations is a promising strategy for the development of environmentally acceptable pesticides for agriculture systems.

Keywords: Nanoencapsulation, Pickering emulsion, controlled release, biopesticide

Synthesis of a Chitosan Nano Polymeric Slow Releasing Fertilizer: A Novel Approach of Improving Agricultural Productivity

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Nanotechnology is an emerging technology with a potential to increase agricultural yield by taking advantage of the novel properties of nanomaterials. Nano-encapsulated conventional fertilizers help in slow and sustained release of nutrients over an extended period of time. This research work focuses on the synthesis of a slow releasing fertilizer nanocomposite using a wet chemical method which also involved nano-encapsulation of a conventional Nitrogen, Phosphorus and Potassium (NPK) fertilizer and zinc oxide nanoparticles. The product was characterized using Fourier Transform Infrared Spectroscopy (FTIR) for chemical composition, Powder X-ray Diffraction for particle size analysis and Scanning Electron Microscopy (SEM) for surface morphology. A phosphate test was done to test the slow releasing effect of the nano polymeric fertilizer compared to the regular fertilizer. Based on the results obtained the nano polymeric fertilizer showed the slow release of phosphate from the encapsulated fertilizer whilst the regular fertilizer showed that the phosphate content was released early on from the start and was quickly exhausted. A phosphate leaching test conducted for a period of 50 minutes for the conventional NPK and nano composite fertilizer showed a leached phosphate concentration of 0.008 mol/dm³ and 0.002 mol/dm³ respectively. The current research work has the ability to transform the agricultural industry and increase crop yield.

Keywords: Agriculture, Nanotechnology, Slow Release Fertilizer, Productivity

AO 06 Bio-based nanostructures for food applications M.A. Cerqueira, <u>L.M. Pastrana</u>

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The development of structures at nanoscale has been pointed as one of the most promising areas once they can help developing healthier foods while increasing food safety and reducing cost production. The applications at laboratorial but also at industrial scale of new and high performance materials have exponentially increased in the last two decades. These nanostructures can be used not only to improve food processing, change chemical and physical properties of materials but also as a way to encapsulate and delivery functional compounds. They been proposed as a way not only to improve safety and quality of foods but also for the development of new food products, where several bio-based structures' properties showed to be influenced at nanoscale. Some of the examples are: the interpenetrating biopolymer networks and gelation processes where micro- and nanoscale domains can be used to predict mechanical and rheological behaviour at macroscale; the use of nanostructures such as nanoemulsions, nanohydrogels and nanocapsules, to encapsulate, protect and delivery functional compounds, improving stability and bioavailability; and also the enhanced functionalities of packaging materials by the use of nanotechnology, aiming the development of active and intelligent packaging materials.

Despite all the advantages and opportunities generated by the use of nanotechnology in food industry several challenges rise, being the regulatory aspects and the consumer behaviour (facing the use of new technologies in foods) the aspects that most alert the food industry. The main stakeholders in the food chain should work together to increase the acceptance of nanotechnology-based products and thus reduce the risk perception associated with nanotechnology in foods. The scale-up of the nanosized structures using bio-based materials is still under development when compared with petroleum/synthetic-based ones and should be fostered by the research institutions in collaboration with the companies.

Keywords: nanotechnology, food grade, safety, quality, nutrition

"Programmable" Ecosystems: Engineered Environments for the Study of Plant Environment Interactions

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The necessity of understanding the role of the abiotic and biotic environment on the development of plants and ecosystems is challenged by a lack of tools capable of providing simple and controllable model systems with which to test hypotheses. While biology has made great strides in the implementation of sophisticated methods for the characterization of the various -omics, relatively little has been done to improve and standardize the tools available for the growing of plants in controlled environments. Our group has created a set of integrated tools to allow the scientific community to generate completely customizable environments with which to conduct plant biology and plant ecology experiments. In this talk I will describe a strategy for the design of model ecosystems for plants and their microbiome in which the ecosystem composition, connectivity, and stimulation can be programmed and dynamically controlled. We will show how engineered flows in these systems allow for the quantitative and dynamic control of the effective signaling distances between organisms (down to the μ m scale) in cm-scale networks of cm-scale habitats that combine the control, modularity, and connectivity of microfluidics with the simplicity and low cost of Petri dishes. We believe that the versatility of these systems could be of great utility for the study of unusual growth conditions or for the understanding of ecosystem evolution in closed environments.

Keywords: ecosystems, signaling, model systems, microfluidics, microbiome

AO 08 Fostering the usability of PHA to the biodegradable packaging sector Luis Cabedo

AO 09

The effect of EG and its synergistic effect on the thermal conductivity, flammability and properties of Polybutylene succinate

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In the past decades, the development of composites has achieved a significant progress for environmental protection together with government regulations in some countries. The composites are usually manufactured with biodegradable polymers as matrix host and conductive fillers or flame retardant fillers as enhancement phase. Poly (ε -caprolactone) (PCL), poly (lactic acid) (PLA), poly (butylene succinate) (PBS) and poly(3-hydroxybutyrate-*co*-3-hydroxyvalerate) (PHBV) are most commonly used as matrix phase of composites, amongst which PBS particularly attracts increasing commercial interest. PBS is polymerized from butanediol and succinic acid, which are available from bio-based renewable resources.



Figure 1 PBS and its production route

Due to the chemical constitutions of the PBS, it is easily flammable and has low thermal conductivity, which hinders PBS applications further. Expanded graphite is blended with PBS to improve both thermal conductivity

and flammability resistance of the biopolymer. The flammability resistance is improved further with the addition of both EG and clay in the PBS matrix. The properties of (PBS/EG and PBS/EG+clay) were also investigated by using techniques such as **SEM, DMA, XRD, TGA and Rheometer**. The storage modulus (Figure 2) of PBS increases with the addition of EG with the modulus increases more with its synergy with clay.



Figure 2 Storage modulus of PBS and its composites with EG and clay

Keywords: flammability, expanded graphite, clay, nanocomposites, polybutylene succinate

AO 10 Target-Molecule-Triggered Release Technology for Smart Fertilizers <u>Tsae, P.K¹</u>, Zhang, X.¹, Derosa, M.C.¹

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Small, synthetic single stranded oligonucleotides (ssDNA/ssRNA) known as aptamers are capable of binding noncovalently to their target molecules with high affinity and specificity. Aptamers display attractive properties such as ability to assume various shapes as a result of their tendency to form helices and single stranded loops as well as their conformational change upon target binding. Such properties can thus be exploited and applied in targeted delivery systems for purposes of controlled release. For instance, release of nutrients to crops is one application that can benefit from triggered release technology. With population increase, which has consequently resulted in a decline in available cultivable land and increase in demand for food, as well as inefficient nutrient use by crops, increased use of fertilizers which have both economic and environmental impacts, there exists a need for development of smart fertilizers that could help address these issues. Thus a smart fertilizer would be one from which the release of nutrients is synchronized to crop demand for that nutrient, thereby increasing nutrient use efficiency. Delivery of payload can be achieved by employing hybrid polyelectrolyte microcapsules as carriers that respond to external stimuli. Previous studies have demonstrated the ability of aptamers encapsulated within polyelectrolyte microcapsules to retain their target binding properties resulting in payload release. In this work, the possibility of an aptamer polymer tape causing global conformational change as a result of cooperative folding within microcapsules and subsequently releasing payload is being investigated as proof of concept work for future applications in smart fertilizer technology as well as being compared to other controlled release technologies being used in our laboratories.

AO 11 Controlled release of urea from chitosan microspheres prepared by emulsification and crosslinking method

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Encapsulation of urea was performed in chitosan microspheres via emulsification followed by cross-linking with genipin, a natural cross-linker. The microspheres were prepared by varying different parameters, e.g., concentrations of chitosan, urea and cross-linker. The effect of these parameters on urea loading (%), urea content (%), entrapment efficiency (%) and release rate was studied. Higher amount of chitosan (1.0 g) and cross-linker concentration (0.75 mmol/g of chitosan) produced entrapment efficiencies of 99.0 and 78.5 %, respectively. Release rate was found to be dependent on the concentrations of urea, chitosan, cross-linker and temperature of the release medium. Higher concentration of loaded urea enhanced the release rate, whereas higher concentrations of chitosan and cross-linker reduced it. Higher temperature of the release medium improved the release rate. It was found that water uptake (%) increased through the increase of concentrations of urea and chitosan and decrease of that of crosslinker. Fourier transform infrared (FTIR) spectroscopy indicated the incorporation of urea in the chitosan microspheres. There was no significant interaction between chitosan and urea as evidenced by FTIR study. Surface of the urea-loaded microspheres appeared coarser and rough compared to that of unloaded microspheres as revealed by scanning electron microscopy.

Keywords: Microencapsulation, slow-release, chitosan, fertilizer, entrapment efficiency, release rate

AO 12 Corn Fibres-Polymer Composites

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The cultivation of corn has increased significantly due to increasing production of biofuel worldwide. As the results massive amounts of corn stalk residues are generated not only in South Africa, around the world. Instead of burning corn stalk residues and the remains in the field after harvest, researchers have found a way to add value to agrowaste through value added products by developing robust biocomposite materials with specific applications in automotive sector and packaging, to mention a few. Corn fibre reinforced composites have received increasing attention as a result. The key drivers for this trend is due to rising environmental awareness, ecological concerns and new legislations, respectively. Corn fibre-reinforced composites have many advantages over traditional glass fibre such as availability, lighter weight, environmental friendliness, recyclability and they can be turned into plastics, fabrics and fibres, respectively. However, the poor adhesion between corn fibre and matrix is commonly encountered problem in these fibre reinforced composite materials. To overcome this problem, specific physical and chemical treatments were suggested for surface modification of fibres by investigators. Comprehensive research on recent corn fibre reinforced composites is cover

Keywords: Corn fibre, Biocomposites, Agro-waste, Environmental awareness

Novel Agriculture Support System Using Plant Bioelectric Potential and Gas Sensor Response

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The artificial plant cultivation facilities such as plant factories have been in practical use for several decades for ensuring a stable amount of clean, safe and high quality agricultural production of vegetables, flowers, and fruits. However, these facilities have problems with high costs and operating expenditures, because they need to maintain a stable and complete environment control system that includes air conditioner, a feed nutrient solution line, and sensing devices for control. Therefore, various studies have been carried out to investigate how to control the optimal environment for growing plants, reducing costs and improving the productivity of cultivation.

In our previous work, we focused on the plant bioelectric potential response, which is generated by ions inside the plant cells and related to physiological activities, as a low-cost and a highly sensitive evaluation technique for an agriculture support system. Such measurement for detecting signal from plant directly is one of the methods of the so called SPA technique, which means Speak Plant Approach.

In this study, we measured and compared the potential and the response signal of a Non-Dispersive Infra-Red (NDIR) type of CO₂ gas sensor. These results showed that the plant bioelectric potential responses are correlated with the physiological activities, such as a respiration and a photosynthetic rate. Although the NDIR type gas sensor has a high sensitivity, it is an expensive equipment and not convenient for practical use at the farm. It is also necessary to observe the influence of other gas components such as ethylene which is one kind of the plant growth hormones. In addition, we employed a silicon carbide field effect transistor (SiC-FET) device as an ethylene gas sensor to evaluate fruit ripening. Eventually, we aim to develop a novel agriculture support system which combines the plant bioelectrical potential and FET gas sensor response.

Keywords: Plant bioelectric potential, Plant factory, Fruit ripening, SiC-FET gas sensor

MO 01 Development of palladium selective reagents and materials

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The technological importance of Platinum Group Metals (PGMs) in catalysis and many important industrial synthetic processes has established their place as the most sought after rare metals of the modern age. Due to the low natural abundance of these precious metals and the complex processes required for their refining, research into the development of low cost and highly selective resins has become increasingly important. Herein, adsorption and separation of Pd(II) from Pt(IV), Ir(IV) and Rh(III) by silica micropartcles functionalized with triethylenetetramine (TETA), 2-(2-aminoethylthio)ethanamine (NSN), 2-(2-(2-aminoethyl)ethylthio)ethanamine (NSSN), by continuous column studies is reported. The functionalized resins were characterized by microanalysis, SEM-EDS and FT-IR. Palladium selectivity of the sorbent materials was achieved by stripping of rhodium, iridium and platinum chlorido species with 0.5 M of NaClO₄ in 1 M HCl while [PdCl₄]²⁻ was eluted with 3% w/v thiourea. The desorption efficiency of the functionalized silica resins were in the order S-NSSN (23.85 mg/g) > S-NSN (12.70 mg/g) > S-TETA (4.97 mg/g). The extraction patterns on the sorbent materials were explained by considering the coordination chemistry of the ligand with [PdCl₄]²⁻ and ionic interactions of [PtCl₆]²⁻, [RhCl₃(H₂O)₃] and [IrCl₅(H₂O]⁻.



Keywords: column studies; coordination; ionic interactions; silica microparticles; palladium selectivity

MO 02

Safe Mining Strategies to Reduce Hazards Associated with Artisanal Mining in Nigeria

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The current status of the Nigeria mining sector presents an immense opportunity for economic growth and development. It currently accounts for 0.02% of exports, 0.3% of national employment and contributes 0.5%, an estimated \$2.0 billion to the nation's GDP which is still low in comparison to global trends for the sector. Over 90 % of mining activities in the country are carried out by Artisanal and Small-scale Miners (ASM). Up to 75 % of this is carried out illegally. Although, Artisanal and Small-scale Mining (ASM) is an important part of the Nigerian mining sector which has the potential to raise internally generated revenue and enhance foreign exchange earnings, create employment, reduce poverty and encourage Foreign Direct Investment (FDI). These potentials have remained unaccomplished as a result of unregulated practices, weak polices and inadequate training, non-existence of large scale mining and low technology input. This paper identifies and classifies mining hazards in Nigeria, examines the legal and regulatory framework required to address mining hazards and contributes towards improving mining environment, increasing the country's GDP and foreign exchange reserves. This was achieved through a critical review of the documented experiences of miners and evidences of hazards. Chemical hazards, mechanical injury, physical hazards, social or psychological hazards related to organization in the work place are forms of hazards that were identified. The enforcement of legal and regulatory framework and adoption of the globally recommended safe mining practices is critical to address the threatening mining hazards in Nigeria and Africa continent. This will create huge market for indigenous miners and minerals processors and increase the contribution of mining to the country's GDP from the current 0.5 % to about 15 %.

Keywords: Safety, mining methods and hazards (MMH), artisanal and small scale mining (ASM), mining law and acts

MO 03

Solidification cracking susceptibility of type AISI 430, 436, and 439 ferritic stainless steels David Konadu^{1,2}, Pieter Pistorius²

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The susceptibility to solidification cracking of a non-stabilized Titanium and Niobium stabilized ferritic stainless steels was investigated using a self-restraint Houldcroft method. Autogenous bead on plate gas tungsten arc welding with three different welding speeds of ~6 mm/s, ~3 mm/s, and ~1 mm/s was employed on the samples. The welded samples were characterized using optical and scanning electron microscopy with EDX. During the welding of 6 mm/s, all the steels cracked with the highest length being the Nb and the non-stabilized was the least. The optical metallography showed columnar grains in the weld zone. The non-stabilized ferritic stainless steel did not crack at a welding speed of ~3 mm/s whilst the Nb and Ti stabilized steels cracked. The microstructures of the steels also revealed columnar grains in the weld zone. Only the Nb stabilized steel cracked at a welding speed of ~1 mm/s whereas the others did not crack. The metallography of the steels were curved columnar grains. SEM fractographic studies of all the cracked steels showed that the hot cracks were inter-dendritic. The EDX elemental analysis of all the cracked surfaces revealed the elements Nb, Ti, Mn, Si, Al, and Mn to be associated with the solidification cracking compared to the stabilized steel.

Keywords: Houldcroft, ferritic stainless steel, gas tungsten arc welding, microstructure

MO 04 Leveraging People, Process, and Data to Advance the Large-scale Deployment of Sustainable Structural Materials Esther Obonyo

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The innovative design and synthesis of transformational building materials can significantly advance efforts directed at catalyzing economic development at the regional scale through narrowing the global adequate housing gap. Building materials account for one-third of the total cost of construction. Thus, transformational use of sustainable building materials would result in significant financial benefits by reducing construction costs while also enhancing the optimal use of scarce materials in more sustainable and durable building systems. There is a broad scope for attaining these ecological and money-related performance targets through novel and innovative use of building materials. In a comprehensive analysis done by the World Economic Forum categorized the existing material sciencedriven opportunities into: 1) incremental improvements regarding traditional materials and existing characteristics; 2) syntheses of new material combinations with additional multi-functional characteristics, and; 3) radical innovations in materials with entirely new functionalities (World Economic Forum, 2016). These vast opportunities for innovation have attracted a lot of attention from researchers across the globe. This notwithstanding, the existing market-ready building materials cannot be deployed easily in a low-income context at scales matching the existing needs. This paper explores possible solutions challenge. Although the focus is largely on the design and use of masonry system, the overarching research and development question is applicable to the most if not all construction materials – what sort of science is required to yield knowledge that can be translated into disruptive technologies that move the needle with respect to addressing pressing societal problems such as providing adequate shelter at scale in a sustainable manner? The empirical data presented in the main body of the discussion is based on work done by the PI in previous NSF-funded efforts has focused on investigating strategies for optimizing the performance of both fired and unfired structural clay bricks in East Africa.

Keywords: Affordable Housing, Sustainable Materials, Systems Thinking

MO 05

The relationships between grain orientation, deformation-induced surface roughness and taylor factor in an AISI 436 ferritic stainless steel

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In order to meet the growing demand for higher strength, coupled with adequate formability in steels, modern-day *steel engineering* has led to a number of alloy steels being developed and hence being tailor-made to meet different requirements. In this study, a ferritic stainless steel AISI 436, with a chemical composition ranging from 0.013 - 0.017% C, 17 - 17.4% Cr, 0.9 - 1% Mo and 0.4 - 0.5% Nb, was investigated in order to correlate its surface roughening behavior during deep drawing to texture. The observed roughening of this steel, and in some cases tearing and/or cracking during deep drawing reported in industry has since suggested that not only texture, but grain size and grain distribution also influence the drawability of the steel. Hence, both evolution of texture and grain size and distribution after thermomechanical processing, cold working and annealing have been the subject of investigation

in this work. Two industrial trials at a commercial steel plant in South Africa, intermediate annealing rolling (IR) and direct rolling (DR), were followed in the rolling of 436 from which samples for the study were obtained. The mapping of texture to surface roughness was then achieved by analyzing the samples, after incremental uniaxial tensile deformation using Optical Microscopy and EBSD. The results obtained proved that an increase in flow lines (surface roughening) was more evident in the DR samples as compared with the IR samples, and became more severe with an increase in plastic deformation. The presence of the *cube texture* combined with grain clustering and/or texture banding in some instances encouraged surface roughening. The IR samples had a more homogeneous γ -fibre texture and less surface roughening. In general, the Taylor factor (TF) was found to be higher and more homogeneously distributed in IR, hence, the improved surface roughening.

Keywords: Deformation, Ferritic stainless steel, Taylor Factor, Texture, Surface Roughness

MO 06 "Value Addition...Some Thoughts..." Josephat Zimba

The concept of value addition for Africa's vast mineral resources is one of the most discussed topics, and probably the least understood too. This presentation discuses some broad thoughts on the issues of value addition, the opportunities, possible approaches and constraints. This presentation is not meant to be a scientific presentation with objectives, experimental procedures, results, discussions and conclusions. Rather, it is a summation of thought provoking ideas on value addition, some which go against the grain of current thinking, from which the audience can draw their own conclusions and map the way forward on value addition within their own unique boundary conditions.

MO 07

Effect of lignin-degrading enzymes on the decomposition of large aromatic hydrocarbons: Coronene as a surrogate for powdered activated carbon

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Lignin-degrading enzymes such as lignin peroxidase (LiP), manganese peroxidase (MnP) and laccase, are known to degrade aromatic hydrocarbons by cleaving the C=C and C=O bonds in materials like coal and powdered activated carbon (PAC) which are sometimes used as surrogates for the carbonaceous matter in refractory gold ores. However, these substrates have complex molecular sizes and structures, making it difficult to adequately quantify the effects of the enzymes. Accordingly, coronene ($C_{24}H_{12}$) was selected as a surrogate for the larger hydrocarbons because it represents the smallest approximation to graphene sheets. It was anticipated that by using this simpler aromatic carbon, it would be easier to characterize and make inferences about the effects of biodegradation on materials like PAC. A 10 mg coronene (97%) sample was contacted with 20 mL of the cell-free spent medium (CFSM) collected after the fungus *Phanerochaete chrysosporium* was cultured for 3 days in a 1% glucose medium. Enzyme activity assays of the CFSM indicated the presence of 1.12 mU/mL LiP and 20.62 mU/mL MnP. After coronene degradation, the solid residue collected was washed with ultrapure water and dried under vacuum before characterization. Fluorescence spectrometry determined that the 20 mL CFSM containing 22.4 mU of LiP and 414.4 mU of MnP degraded 1.36 mg of coronene by the 3rd day of treatment. This led to the production of some water-soluble aliphatic compounds which increased the acidity of the liquid phase residue. Furthermore, FTIR and ¹H-NMR showed an increase in the aliphatic functional groups C-H, C=C-H and carbonyl C=O relative to the C=C in the solid phase. The

coronene residue and PAC residues from our earlier work exhibited similar changes in structure after CFSM treatment, with the exception of the pH change, indicating that both substances might have followed C=C bond cleavage pathways for aromatic carbon degradation by lignin degrading enzymes. The PAC residues were additionally characterized by N_2 adsorption experiments. It was observed that the specific surface area was significantly decreased after the enzyme treatment and this change was ascribed to the destruction of the microporous structure to form larger pores. However, analysis of the coronene residue by XRD showed that the layer structure was progressively compressed, the CFSM treatment resulting in a decrease in the d-spacing of the slits. This observation illustrates that it is possible that not all the micropores in the PAC residue were enlarged but that some might have become inaccessible through compression. Further tests on the suitability of coronene as a surrogate for PAC will be conducted, including Au(CN)₂⁻ uptake, but, based on the currently available data, it can be concluded that coronene can serve as a useful surrogate for larger, insoluble aromatic hydrocarbons.

Keywords: Coronene, Lignin-degrading enzymes, Phanerochaete chrysosporium

MO 08 Effect of concrete quality on the sensitivity of the chloride conductivity test to salt concentration and capillary voltage Mike Otieno

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This study assessed the robustness of the chloride conductivity test with respect to the effect of concrete quality on its sensitivity to selected test parameters. Experiments were carried out to assess the sensitivity of the test to changes in (i) concentration of the NaCl solution, and (ii) variation of capillary voltage. Concrete test specimens were made using three w/b ratios (0.40, 0.50 and 0.60) and three binder types (CEM I 52.5N, PC), 70/30 PC/FA and 50/50 PC/GGCS). The results show that concretes with high chloride conductivity index (CCI) values are generally sensitive to changes in concentration of NaCl solution and capillary voltage across the test specimen. For such concretes, the CCI increases with increase in capillary voltage, and decreases with decrease in salt concentration.

Keywords: Chloride conductivity, durability index, chloride resistance, sensitivity

MO 09

Exploration of local Cellulosic fibers, Modification and potential use for the local Industry <u>Ndebombuya Mokaloba¹</u>, Venkata P. Kummola²

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Presently, there is an ever-increasing demand for newer, stronger, stiffer, yet lighter-weight, environmental friendly (biodegradable) materials in the fields such as aerospace and automobile for non-structural applications. This array of advanced materials include polymer composites and nanocomposite materials. An interesting alternative for reinforcing soft polymeric matrices with short fibers is the use of cellulose fibers, which show remarkable reinforcing effects in plastics such as polypropylene. This has led to extensive research and development efforts in the composites fields as they offer properties superior in strength and modulus. These materials are now being rapidly utilized in industries, and they have become the forefront of research and development activity. The principal reasons for using natural (cellulosic) fibers stem from are several attractive properties such their economic

feasibility, enhanced sustainability, good specific mechanical properties, and desirable aspect ratio for good performance after melt-processing. Plants such as sisal, flax, and napier grass provide important fibers in terms of quality and commercial use. The proposed study investigates the extent of commercial exploitation of cellulosic fibers for beneficiation, particularly by the automotive industry; for non-structural and low-strength interior applications within the SADC economic region. The scale of application of natural fibers by the automobile industry indicates minimal uptake, which translates to further avenue for industrialization. Chemical pre-treatment time, solution concentration and fiber extraction technique have profound influence on the manufacturing cycle time and final product quality. The characteristics of the resultant composite profiled against equivalent material systems in Ashby material property charts exhibited suitability for light, low strength and low flexure applications.

Keywords: Cellulosic-fiber, Composite, Chemical modification, Sisal, Napier grass

MO 10

Compressive strength of compressed earth blocks stabilized with calcium carbide residue and rice husk ash

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The mankind has used earth as early as the beginning of civilization to build shelter. Today, we still witness the existence of thousand years old earthen structures, in their many different construction forms. In the modern construction, the society perceives this natural material as either a material for the poor or having low performance. Since the past half-decade, attempts have been made to improve this perception. By compressing earth into a regularly shaped mold, a modern form of Adobe, Compressed Earth Block (CEB), is formed. Additionally, depending on the quality of the earth, Portland cement and/or lime are mostly used as chemical stabilizing agents to further improve their performance. This paper presents the progress made in improving the properties of CEBs using two main by-product materials: Calcium Carbide Residue (CCR)/Lime and Rice Husk Ash (RHA) available in Burkina Faso. Particularly, this study sought to understand how the addition CCR and its controlled substitution with RHA affect the compressive strength of CEBs. Raw materials are processed and their physico-chemical and mineralogical properties are characterized. The CEBs are formed by addition of varying fractions of CCR and CCR/RHA to the earth and cured in ambient conditions until the testing age (45 days). It is revealed that the addition of 15 wt.% of CCR:RHA in 7:3 ratio imparts extra 60% of compressive strength, i.e. 6.6 MPa, with respect to 2.5 MPa when CCR is used alone. This improvement is related to the pozzolanic interactions between CCR with the clay fraction in the earth and the RHA. It implies that these CEBs can be used in construction of load bearing walls of two-storey housing. Further studies will investigate the hydro-thermal performance and durability of these CEBs in the Sahelian context.

Keywords: Earth, by-product, CEBs, Compressive strength

MO 11

Advanced XRD analysis of samples on modern multipurpose diffraction platforms – looking beyond simple powder diffraction

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Powder X-ray diffraction analysis has traditionally been applied to mineralogical/material science samples for decades in order to identify and quantify the minerals in various types of rocks. Recent developments in the field of XRD like the emergence of modern multi-purpose diffraction platforms and the development of 2-dimensional detectors, result in a variety of new applications suitable for the characterization of materials. In the presentation we will introduce several new applications, such as phase distribution mapping and computed tomography, and show how the combination of multiple analytical approaches can improve our understanding of the properties and the formation materials/rocks. The presentation will cover basic explanations of the various techniques and show several examples. In addition a case study will be presented showing the successful combination of powder diffraction, microdiffraction and CT analysis to characterize a meteorite sample.

Keywords: X-ray diffraction, CT analysis, mapping

MO 12

Influence of Laser Processing Parameters on the Surface Quality of 316L

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Surface quality of metallic components has a huge influence on the wear, fatigue, and eventually service life of the part. Scanning of high-energy laser beams on metal powders during the layer-by-layer melting and solidification process of Selective Laser Melting (SLM) method of additive manufacturing has been determined to affect the mechanical characteristics and surface integrity of the sintered product. Some of the major processing parameters that have potential influences on final material properties, and can affect the quality of the finished product have been identified as laser power, scanning speed, and layer thickness. These parameters also influence the surface characteristics and quality of the engineered components. This study focuses on the effect of the processing parameters on the surface characteristics. Surface morphology, material defects such as pores, voids, cracks; melt pool formation, and chemical elements distribution on 316L stainless steel samples were investigated. Increased laser power resulted in enhanced surface quality for all samples, whereas higher scanning speed led to detrimental defects, discontinuity, pores and cracks on the surfaces. High energy density was found to result in wider melt pools and improved surface texture. Statistical analysis showed that laser power has more effects on the melt pool developments. Chemical element distribution throughout the melt pools revealed carbon and oxygen concentration at melt pool boundaries, which ultimately would induce cracks and balling effects in overlapped regions.

MO 13

Addressing Africa's development challenges through use of waste materials in concrete Sunday Nwaubani

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"Waste" they say, is "Wealth" nowadays. Construction has proved a good avenue for utilizing various forms of waste materials, in a rational and sustainable way, to minimise the use of energy-intensive materials. The use of waste is also rapidly becoming a newly emerging supra-disciplinary field in most parts of the world where the use of industrial wastes like fly ash, granulated steel slag, silica fume, waste fibres etc., in construction has become very popular since the last half of the 20th century. Other forms of industrial wastes are also re-used even for more sensitive applications on soils to upgrade soil texture. E.g., waste from bauxite refining (red mud) is known to be extensively re-utilised. These concepts are yet to take tangible hold in Africa, despite the huge resources available.

This talk provides a brief overview of the potential viability of waste products and other natural and locally occurring materials in African regions that can be applied as partial substitution of cement and aggregates in concrete. It will describe methods of producing structural grade concrete products with waste mixes that yield compressive strengths above 30 MPa (general structural use) in 28 days to evidence the potential of waste materials use as economically viable alternatives to conventional concrete. The Speaker believes that greater use of such waste materials, sourced from African countries, will reduce the high cost of cement, contribute to reduction of virgin mineral consumption and will promote environmental preservation as well as much desired resource efficiency in African countries.

Keywords: Sustainable construction, waste materials, concrete, African development, construction materials.

MO 14

Effect of lignin-degrading enzymes on the decomposition of large aromatic hydrocarbons: Coronene as a surrogate for powdered activated carbon

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Lignin-degrading enzymes such as lignin peroxidase (LiP), manganese peroxidase (MnP) and laccase, are known to degrade aromatic hydrocarbons by cleaving the C=C and C=O bonds in materials like coal and powdered activated carbon (PAC) which are sometimes used as surrogates for the carbonaceous matter in refractory gold ores. However, these substrates have complex molecular sizes and structures, making it difficult to adequately quantify the effects of the enzymes. Accordingly, coronene ($C_{24}H_{12}$) was selected as a surrogate for the larger hydrocarbons because it represents the smallest approximation to graphene sheets. It was anticipated that by using this simpler aromatic carbon, it would be easier to characterize and make inferences about the effects of biodegradation on materials like PAC. A 10 mg coronene (97%) sample was contacted with 20 mL of the cell-free spent medium (CFSM) collected after the fungus *Phanerochaete chrysosporium* was cultured for 3 days in a 1% glucose medium. Enzyme activity assays of the CFSM indicated the presence of 1.12 mU/mL LiP and 20.62 mU/mL MnP. After coronene degradation, the solid residue collected was washed with ultrapure water and dried under vacuum before characterization. Fluorescence spectrometry determined that the 20 mL CFSM containing 22.4 mU of LiP and 414.4 mU of MnP degraded 1.36 mg of coronene by the 3rd day of treatment. This led to the production of some water-soluble aliphatic compounds which increased the acidity of the liquid phase residue. Furthermore, FTIR and ¹H-NMR showed an increase in the aliphatic functional groups C-H, C=C-H and carbonyl C=O relative to the C=C in the solid phase. The

coronene residue and PAC residues from our earlier work exhibited similar changes in structure after CFSM treatment, with the exception of the pH change, indicating that both substances might have followed C=C bond cleavage pathways for aromatic carbon degradation by lignin degrading enzymes. The PAC residues were additionally characterized by N₂ adsorption experiments. It was observed that the specific surface area was significantly decreased after the enzyme treatment and this change was ascribed to the destruction of the microporous structure to form larger pores. However, analysis of the coronene residue by XRD showed that the layer structure was progressively compressed, the CFSM treatment resulting in a decrease in the d-spacing of the slits. This observation illustrates that it is possible that not all the micropores in the PAC residue were enlarged but that some might have become inaccessible through compression. Further tests on the suitability of coronene as a surrogate for PAC will be conducted, including Au(CN)₂⁻ uptake, but, based on the currently available data, it can be concluded that coronene can serve as a useful surrogate for larger, insoluble aromatic hydrocarbons.

Keywords: Coronene, Lignin-degrading enzymes, Phanerochaete chrysosporium

MO 15

Adsorptive Recovery of Auro-Dicyanide Anions from Aqueous Solutions using Activated Carbon-Magnesium Oxide (C-MgO) Nanocomposite as Adsorbent

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The reprocessing of tailings or gold mine waste dumps to extract gold has become an attractive proposition for mining houses worldwide because of the availability of gold which was not easily recovered using old technologies. This study seeks to exploit the novel properties of nanostructured materials in enhancing gold extraction from gold mine tailings. The beneficiation of slimes or tailings involved taking samples for mineralogical studies, synthesis of a novel adsorbent medium (nano C-MgO) prepared by using both chemical and mechano-synthesis methods, oxidative pre-treatment of flotation concentrates, cyanidation and final recovery of the precious metal from solution in a Carbon in Column (CIC) system. The nanocomposite adsorbent was studied by powder X-ray Diffraction (XRD) for structural analysis, Field Emission Scanning Electronic Microscopy (FESEM) for surface morphology, Energydispersive X-ray spectroscopy (EDX) for elemental analysis and Fourier Transform Infrared (FTIR) spectroscopy for chemical structure analysis. The Brunauer-Emmett-Teller (BET) Surface Area Analysis procedure was employed to determine the total specific surface area of the nano-adsorbent. Representative tailings samples of 100-500 g were obtained for different analytical investigations using a riffle splitter. The tailings grade was analysed using the Atomic Absorption Spectroscopy (AAS) technique and was found to be an average of 0.5 g/tonne. A comparative Pseudo-Equilibrium test showed that the novel C-MgO nano adsorbent had an average of 84% recovery against 70 % for convectional activated carbon. The average crystalline size of 4.5 nm for the majority of MgO nanoparticles was obtained using the Image J software. FESEM confirmed that nano MgO was porous in nature and highly agglomerated. EDX exhibited the successful synthesis of the nano-composite product. This work shows that the nano-adsorbent also presents a huge potential for application in the conventional processes for gold adsorption.

Keywords: Gold; Adsorption; Nano-adsorbent; Beneficiation, Value Addition

MO 16 Technologies for sustainable roads infrastructure development Stainless Steel Manufactured Components by Selective Laser Melting (SLM)

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It is recognized that achieving many, if not all, of the Sustainable Development Goals and the 2030 Agenda for Sustainable Development requires success in sustainable transportation in all its varied forms. In African and other developing countries there is a severe underdevelopment of transportation infrastructure. Roads are sparse; they are mostly unpaved or if paved poorly constructed; and they receive little or no regular and necessary maintenance. Familiar states of roads include frequent pothole occurrence, deep ruts, waterlogged in the wet season and blinding dustiness in the dry seasons. These conditions are not only economic inhibitors; they are also safety and health hazards. Effective solutions are needed. Recently the Vice president of Ghana has promoted concrete roads as the preferred cost-effective long-term solution to road building. Is it? In this presentation we explore various technologies. We discuss, in particular, an ongoing engagement with highway and road building authorities in West Africa to explore latex-modified soil stabilization technology. This technology offers a way to modify the properties of the soil in place by mixing in an appropriate latex formulation. No new aggregate material is brought in for the road base. The type and amount of latex depends on the characteristics of the soil determined from a suite of standard soil tests/analyses. We discuss these facets as well as the potential of the technology to make it a time and cost-efficient way to build roads sustainably. Lessons learned in this engagement have been insightful. **Keywords**: Sustainable development; latex; soil stabilization

MO 17

Minimising the risk of thermally induced cracking in mass concrete structures through suitable materials selection

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The hydration of cement is an exothermic reaction which generates around 300 kJ/kg of cement hydrated. In mass concrete structures such as dams and large foundations, this heat of hydration causes a significant rise in temperature in the internal sections of the concrete. If thermal gradients between the internal sections and the near-surface zone of the concrete element are sufficiently large, the thermal stress can cause cracking of the concrete. This cracking may cause functional and/or structural problems in the operation of the structure. In order to minimise the potential for such cracking, it is necessary to minimise the rate and amount of heat that is evolved, particularly during the early period of the hydration process. This can be achieved by design engineers and concrete technologists through judicious selection of concrete-making materials.

This paper presents the observations and results obtained over a number of years from adiabatic testing of concretes, computational modelling of temperature development in large concrete structures and direct temperature measurements in actual structures, with a view to understanding the effects of concrete-making materials on temperature development in concrete. The paper considers the effects of different types of Portland cement, fineness of grinding and the addition of supplementary cementitious materials on the rate and amount of heat evolved during hydration. Furthermore, using a maturity approach to computational solution of the Fourier equation for heat flow, the paper shows the effects of different aggregate types on the development of time-temperature profiles in large concrete elements.

Atomistic insights into the Electrochemical Reduction of Carbon Dioxide on Transition Metal Clusters from First Principles Investigation

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The electrochemical reduction of carbon dioxide continues to be of great interest for renewable energy. Materials in the sub-nanometer to nanometer regimes exhibit enhanced activity and selectivity for hydrocarbons as products. Here, we present a series of sub-nanometer mixed copper-nickel clusters and gold clusters with diameters of ~20 nm for the electrochemical reduction of CO₂. First principles studies in conjunction with thermodynamic and kinetic theories provide an in-depth understanding of the reduction mechanism on cluster systems. Our results show that several factors play a role in the selectivity and onset potential for the electrochemical reduction of CO₂ including cluster spin multiplicity, cluster composition and size. We find that not only does size contribute to the selectivity of products but also the availability of open metal-sulfur sites on the Au-cluster surface plays a key role. These results aim to promote clusters and cluster assemblies as materials as catalysts with application to related electrocatalytic processes that are of technological and environmental interest.

Keywords: Clusters, CO₂, Electrochemistry

CO 02

Computational Studies on Transition Metal Catalysts for CO₂ Conversion to Hydrocarbon Fuels

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Waste CO₂ could be transformed into useful forms like CO, a feedstock in the Fischer-Tropsch process for the production of long chain hydrocarbons fuels or directly hydrogenated into methane. Despite the energetic challenges with CO₂ transformations, Fe and Ni are known active sites for CO₂ conversion into CO, thus surface modifications of iron with nickel could enhance the process of CO₂ dissociation. We have employed spin polarized density functional theory calculations to perform extensive mechanistic studies of CO2 reduction into CO and methane on the most reactive Fe (111) surface and also explored nickel deposition and CO₂ dissociation on the low Miller index surfaces of iron i.e. Fe (100), (110) and (111). Dissociation was also considered on the same surfaces coated by a monolayer of nickel. CO₂ chemisorbs on all three bare facets and binds more strongly to the stepped (111) surface than on the open flat (100) and close-packed (110) surfaces. Compared to the bare Fe surfaces, we found weaker binding of the CO₂ molecules on the Ni-deposited surfaces as well as reduced surface work function on only the predominant (110) facet. The trends in dissociation energy barriers were observed to follow that of the surface work functions, however, the instability of the activated CO₂ on the Ni-covered surfaces will result in CO₂ desorption on the nickel doped iron surfaces as seen on Fe(110). The reverse water gas shift reaction on iron (111) will proceed via the carboxylate intermediate while methanation is formed via the formate intermediate, as such modified iron surfaces (e.g. by nickel deposition) favouring weaker CO₂ binding will favour methane formation and hinder CO formation on the surface.

Keywords: Reverse water gas shift reaction; Sabatier reaction; Ni-doped iron; metal deposition; Surface workfunction alterations

Investigation of the hydration and structure of model lipid membranes

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We have done a significant amount of work in which we have carried out a series of simulation studies to investigate the hydration of the head groups and structure of various model bilayers representative of lung surfactants, brain cells and red blood cells. In this talk I will summarise these studies, and compare our results to those obtained from the neutron diffraction experiments carried out by our collaborators. Additionally, I will briefly discuss how disease affects these properties in the case of brain and red blood cells. Finally, I will discuss a recent investigation of how environmentally sensitive fluorescent dyes interact with model membranes, and show how the molecular scale properties of the dyes observed from simulation link to their fluorescent properties.

Keywords: Molecular dynamics simulations, lipid membranes, brain cells, red blood cells

CO 04

Spiking Neural Network Architecture Development Towards the Design of a Scalable Neuro-Inspired System for Complex Cognition Applications

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Artificial neural networks (ANNs) research activities are inspired by how information is dynamically and massively processed by biological neuron. Conventional ANNs research have received wide range of applications including automation but there are still problems of timing, power consumption and massive parallelism. Spiking neural networks (SNNs) being the third-generation neural networks can be applied in the areas of image and speech recognition, sound processing and healthcare services (cancer detection). Hence, it attracts greater number of researchers' attention due to its timing concept, which defines its closeness to biological spiking neural networks (bio-SNNs) functions. Spike timing plays important role in every spiking neuron and proves computationally plausible than other conventional ANNs. The real biological and distinct neuron timing and spike firing can be modeled artificially using neuro dynamics and spike neuron models. Spike timing dependent plasticity(STDP) learning rule also incorporates timing concepts and is suitable for training SNNs which describes a general plasticity rules that depend on the timing of pre- and postsynaptic spikes. This paper presents a software implementation of a spiking neural network based on the Leaky Integrate-and-fire (LIF) neuron model and STDP learning algorithms. In addition, we present a novel hardware design and architecture of a lightweight neuro processing core (NPC) to be implemented in a packet-switched based neuro-inspired system, named NASH. The NASH architecture uses LIF neuron model and reduced flit format size that solves the problems of timing and high-power consumption. Software evaluation shows that our network tested 94% accuracy with MNIST datasets of handwritten digits.

Keywords: Spiking Neural Network, Leaky Integrated-and-fire, Scalable, Network-on-Chip(NoC), STDP.

CO 05 Anharmonic Phonons in Cuprite

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We report an extremely large anharmonicity of optical phonons in cuprite, Cu₂O. Phonon dispersions were measured at 10, 300, and 700 K by rotating a single crystal in the ARCS spectrometer at ORNL. Ab initio calculations of harmonic phonons accounted for the dispersions at 10 K. At 300 K, however, large broadenings of phonon energies made it impossible to use harmonic or quasiharmonic interpretations. The broadening was calculatedfrom the cubic anharmonicity using the stochastic Temperature Dependent Effective Potential method (quasiharmonic phonons in an anharmonic potential), but the experimental broadening was considerably larger than these calculations. Results will be compared from ongoing ab initio molecular dynamics calculations and experimental phonon linewidths with full background corrections. Cuprite is stable to a temperature of 1503 K, but the phonon spectrum at 700 K is so broad that it may not be interpretable with phonons. Implications for vibrational entropy will be discussed.

Keywords: inelastic neutron scattering, anharmonicity, vibrational entropy, ab initio molecular dynamics, phonons

CO 06

Beyond Li-ion: Computational Modelling Studies on Stability of Li-S-Se System

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Recent rechargeable batteries are mainly based on conventional lithium intercalation chemistry, using lithium transition metal oxides as cathode material with typical capacities of 120-160 mA.h/g. The low energy density and/ or high cost of these cathode materials have limited their large scale production and application in Li ion batteries. Exploration of new cathode materials is consequently necessary to realise more efficient energy storage systems. Lithium sulphur cells have a promise of providing 2-5 times the energy density of Li-ion cells, however, they suffer poor cycling performance. Improvements that are effected by using Li/SeSx system in different electrolytes have been reported. In the current study we employ computational modelling methods to explore stability, structural and electronic properties of discharge products formed in the Li/SeSx battery, which has potential to offer higher theoretical specific energy and remedies the challenges that Li-S battery encounters. First principle methods were used to calculate thermodynamic properties of Li2S and Li2Se, which agreed with available experimental results. A cluster expansion technique [4] generated new stable phases of Li/SSex system and Monte Carlo simulations determined concentration and temperature ranges in which the systems mix. Interatomic Born Meyer potential models for Li2S and Li2Se were derived and validated and used to explore high temperature structural and transport properties of mixed systems.

CO 07 First principle calculation of direct and indirect phase transition of the early transition metals carbonitrides: Ti, Zr and Hf

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We performed static and dynamical structural phase stabilities of the early refractory carbonitirides based on first principles calculation in the framework of generalized gradient approximation. The calculations shows that induced postulated zinc blende structure is stable however the cesium chloride is not as there was appearance of soft modes in the phonon spectra, which prevents the formation of this crystal. Comparing the indirect phase transition pressures, the nitrides are found to be relatively smaller relative to the carbides. The electronic structure calculation also indicates that, the carbides of the zinc blende structure shows semiconducting behavior whilst that of the nitrides remains metallic, however, the cesium structure of all the carbonitrides were metallic with strong hybridization at the gap region.

CO 08 Computational modeling as a complementary and predictive tool in materials science research <u>George Amolo</u>

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With the recent scenario of affordable computers with large RAM and storage capabilities as well asthe availability of high performance computing facilities, research in materials science using simulations has rapidly grown. The research focus has now gradually shifted from fundamental science investigations to properties of materials that have applications in environmental preservation, search for as well as adoption of alternative fuels and green energy at large, health, among others, which have an expected impact on the quality of life. Our group in Kenya has in the last few years worked on hard materials for cutting and sharping in industry as well as materials for energy conversion and materials for electronic applications. In particular, we have investigated hardness in Transition Metals Carbides and Nitrides (TMCNs) and extended to other indicators such as shear modulus, rigidity and brittleness; metal electrode contacts on diamond surfaces for diamond electronics; metal hydride materials for applications in hydrogen fuel storage and the electronic structure of the interface of dye/TiO2 in dye sensitized solar cells (DSSC), among others. Highlights of the finding of these cases and recent advances are provided. These examples, among others, are provided to show how computational modeling richly supports experimental work and yet can also be used to provide useful information that may not directly be accessible to experiments.

Simulation Of Gravimetric Capacity, Structural And Electronic Properties Of Vanadium Disulphide

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Materials play very important role in the technological advancement of lithium-ion batteries. In this work, the stateof-the-art *ab initio* method based on density functional theory was used to investigate the adsorption of lithium ions on layered vanadium disulfide. The adsorption energy, structural and electronic properties were computed using both the local density approximation and the generalized gradient approximation for comparison. The preliminary results indicate that single-layered vanadium disulfide is a candidate anode material for lithium-ion batteries with enhanced gravimetric capacity.

Keywords: DFT, VS₂, Batteries.

CO 10

Computational modelling study of pyrite surfaces and adsorption of xanthates, dithiophosphates and dithiophosphate onto pyrite

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Computational modelling methods were employed to investigate pyrite surfaces, and the effect of water molecule on the three typical thiol collectors (xanthate, dithiocarbomate and dithiophosphate) interactions at the pyrite surfaces. The calculated surface energies for {100}, {110}, {111} and {210} showed that {100} surface is most stable whereas {110} is the least stable. Morphologies of pyrite indicate predominance of the {100} facets and limited presence of others. The adsorption results suggest that the interactions of thiol collectors are via their S atoms bonding with the surface Fe atoms, indicating that the Fe atom participates in the bonding interaction. The analysis of density of states (DOS) suggest that thiol are composed of the S 3p orbital, indicating that the S 3p orbitals are very active. In addition, the DOS of S atom with a single bond is the same as the S atom with a double bond, indicating that the two S atoms in the thiol group have similar chemical reactivity, which may be ascribed to the conjugation effect of a pi bond. The presence of water molecule has an obvious effect on the electron distribution, covalent bonding and reactivity of surface atoms and consequently influences the interaction between the collector and mineral surface. These results agree well with the flotation practice.

Keywords: pyrite, surface, water molecule, thiol collector, adsorption

Effect of transition metals clusters on the electronic and magnetic properties of MoS₂

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Using first-principles calculation, we carried out a systematic study on the effect of transition metal (TM: Ti, V, Cr, Mn, Fe, Co, Ni) dopant lattice separation and clustering on MoS₂ monolayer as potential spintronics, catalytic and optoelectronics material. The electronic and magnetic properties changed both as a function of the TM ion dopant and lattice separation. The calculated binding energies indicate that it is possible to introduce TM ions into the lattice of MoS₂. The calculated clustering energies shows that TM ions exhibit dispersive distribution void of cluster formation in MoS₂ lattice. Generally, there is a reduction in the electronic band of doped MoS₂ compounds with a consistent red shift in the absorption spectra. The calculated redox potentials of H₂O splitting lie properly astride the valence and conduction bands for Cr doped MoS₂, indicating that this material is a potential photocatalyst. Increasing the atomic separation of the co-doped compounds strongly favors the anti-ferromagnetic configuration with increase in the overall magnetic moment. This theoretical investigation provides further insight into the application of TMDCs as ultra-thin spintronics materials. These ordered monolayer TMDCs could lead to designing effective advanced solid state materials with improved performance in various areas.

Keywords: Dft, Electronic, Optical, Photocatalysis

CO 12 Computational Studies of NaMn₂O₄ and MgMn₂O₄ polymorphs Lethole N.I, Ngoepe P.E.

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Spinel lithium manganese (II) oxide (IV) (LiMn₂O₄) has been intensively studied as a positive electrode for rechargeable Li-ion batteries due to its abundance in the earth crust, low toxicity, and high theoretical capacity of 148 mAh/g. However this material has been reported to suffer from severe capacity fading, particularly at high temperatures during the charge/discharge process. This drawback makes the material incompetent for commercial application, though many attempts were made to improve its capacity sustainability. Recently, preliminary studies have shown that NaMn₂O₄ and MgMn₂O₄ have great potential for use in Na-ion and Mg-ion batteries. However, little has been reported on the physical and chemical properties of these compounds. In this work, we perform first principles calculations to investigate the structural, thermodynamic, electronic and mechanical properties of spinel NaMn₂O₄ and MgMn₂O₄, particularly the lattice constants, heats of formations, band structure, density of states, elastic constants and phonon dispersion curves. Calculations have been performed within DFT+U method as implemented in the Vienna Ab initio Simulation Package code. The calculated lattice constants are in good agreement with the experimental data to within 3 %. The phonon dispersion curves showed negative vibrations along high symmetry lines in the Brillion zone; a condition for instability. Furthermore, new stable structures were extracted from the negative vibrations of the phonon dispersion curves.

Keywords: thermodynamic, phonon dispersion curves, voltage profiles

Effect of pressure on structural, mechanical, dynamical and electronic properties of ReSe2:A theoretical investigation

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Effect of pressure on structural, electronic, mechanical, and Dynamical properties of ReSe2 has been investigated using the first-principles calculations. These calculations are based on density functional theory and were performed using the generalized gradient approximation with the empirical van der Waals correction. The calculated lattice parameters ReSe2 under effect of pressure are consistent with the available experimental values upto 9.03 GPa, which motivated us to explore the stated properties beyond the 9.03 Gpa limit. The lattice parameters and volume of ReSe2 decrease with the increasing pressure whereas the total enthalpy increases. The mechanical properties are predicted using the Voigt-Reuss-Hill approximation from which there is an inverse relationship between volume and pressure implying that as we subject ReSe2 to large pressure the material becomes somehow more compact due to reduced inter-atomic distance hence increase in magnitude of elastic coe_cients as well as bond strength. The Dynamical instability was investigated by computing the phonon frequency to check for imaginary modes. ReSe2 is dynamically stable below 40 GPa. The band gap was estimated using the Perdew-Burke-Ernzerhof (PBE) and modi_ed Becke{Johnson potential, which con_rmed that as pressure increased, the band gap decreased in almost a linear manner.

CO 14

Numerical Insight on the Early Stage Growth of an Isolated Metal Nanoparticle

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Nowadays, supporting metal nanoparticles have attracted much interest due to their fascinating physio-chemical properties and potential application in fuel cells, sensors, catalysis, magnetic data storage devices and among others. One of the interesting issues from engaging physiochemical properties of supporting nanoparticles is to understand their nucleation and growth mechanism in order to get a good control of their structural and morphological parameters. Although studied for decades, however, the full details are still out of reach. In this presentation, we will first review the classical theory of nucleation and growth and secondly present our recent finding and theoretical development on the growth of an isolated metal nanoparticle using a combined experimental (linear sweep voltammetry, chronoamperommetry and FESEM) and Time dependent Multi-Ion Transport and Reaction Model (TD-MITReM). In this presentation we focused on the numerical approach. The use of such a model and simulation tool allows studying nanoscale electrochemical deposition as a whole, without the need to assume a dominant growth mechanism such as diffusion or kinetic control. The simulation results reveal that the existing theory of nucleation and growth is only valid for some specific conditions. Some of the findings will be discussed in this presentation.

Keywords: Finite element method, Multi-Ion Transport and Reaction Model, nanoscale nucleation and growth, kinetic control, diffusion control Theme: Computational Materials Science.

CO 15 Effect of Confinement on the Structure and Dynamics of Hydrogen Bonding: Role of the Instantaneous Surface

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Many industrial processing operations involve the spreading of a liquid on a solid surface and controlling the wetting of one material by another is of crucial importance in such applications as adhesion, coating and oil recovery. It is thus quite important to understand the structural and dynamical properties of liquids that come in contact with them to achieve the desired functional properties. Using molecular dynamics (MD) simulations, we investigate the structural and dynamical properties of water molecules in a slab of water in contact with model polystyrene surfaces of varying polarity. Our investigation is mainly focused on understanding the dynamics of hydrogen bonding at the interface and how it is correlated with the wetting property of a surface. We find that the density of water molecules and the number distribution of hydrogen bonds as a function of distance relative to an instantaneous surface exhibit a structure indicative of a layering of water molecules near the water/PS interface. Our results indicate that the polarity of the surface dramatically affects the dynamics of the interfacial water molecules with the dynamics slowing down with increasing polarity. The results from the model polystyrene surface also reveal that the lifetime of interfacial hydrogen bonds between water molecules that do not form hydrogen bonding with the substrate does not depend on the polarity of the substrate.



Keywords: Interface, hydrogen bonding, relaxation, diffusion

CO 16

Molecular dynamics simulations of the structural and dynamic properties of Pyrite (FeS₂) nanoparticles

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Nanoparticles (NPs) have been the area of active research in the recent years due to their unique material properties, which distinguish them from the bulk materials. NPs have attracted the attention of researchers in the fields of materials science, physics and chemistry. They have enhanced structural and physical properties, which make them desirable to a wide range of industries. Pyrite (FeS₂) at a nanoscale is considered to be one of few materials for photovoltaics capable of bridging the cost and performance gap of solar batteries. It also holds promise for energy storage applications as the material for high-performance cathodes. Computational modelling technique, molecular

dynamics (MD) was performed to provide atomic or molecular level insights of the structural and dynamics of FeS_2 NPs. NPs of different sizes were considered. The effect of temperature on different sizes of NPs are analysed in a form of structural and dynamic properties; namely Radial Distribution Functions (RDF's), energy and diffusion coefficient. The temperature associated with the melting transition and stability increased with an increase in the nanoparticle size.

Keywords: Pyrite (FeS₂), Nanoparticles, Molecular Dynamics

CO 17

Computational study of anatase TiO₂ nanotube as an anode material for lithium ion batteries <u>M. Gandamipfa</u> and P. E. Ngoepe

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In lithium-ion battery, graphite is a widely used anode material, but it has some disadvantages as compare to anatase TiO_2 nanotube anode such as electrical disconnection, structural deformation, and initial loss of capacity. The choice of the anode material is very important for an effective development of a high energy density batteries and the use of high capacity electrode materials (anode & cathode) is an essential factor. The anatase TiO_2 nanotube anode is a material that conducts electric current and they do not expand to more than three times their volume during charging and then shrink again during discharge. Given these exciting properties, it becomes necessary not only to synthesize such solid-state and molecular systems but also to model their properties at an appropriate size and time scale. In this work we study anatase TiO_2 analogues (bulk and nanotubes) in an effort to understand how the DFTB+ potentials influence structural parameters and electronic properties. Our structural and electronics parameters are in good agreement with the experimental results.

Keywords: TiO₂, DFTB+ potentials.

CO 18

First-principles studies of chromium line-ordered alloys in a molybdenum disulfide monolayer <u>N.F. Andriambelaza¹</u>, R.E. Mapasha¹, N. Chetty^{1,2}

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Density functional theory (DFT) calculations have been performed to study the thermodynamic stability, structural and electronic properties of various chromium (Cr) line-ordered alloy configurations in a molybdenum disulfide (MoS₂) hexagonal monolayer for band gap engineering. Only the molybdenum (Mo) sites were substituted at each concentration in this study. For comparison purposes, different Cr line-ordered alloy and random alloy configurations were studied and the most thermodynamically stable ones at each concentration were identified. The configurations formed by the nearest neighbor pair of Cr atoms are energetically most favorable. The line-ordered alloys are constantly lower in formation energy than the random alloys at each concentration. An increase in Cr concentration reduces the lattice constant of the MoS₂ system following the Vegard's law. From density of states analysis, we found that the MoS₂ band gap is tunable by both the Cr line-ordered alloys and random alloys with the same magnitudes. The reduction of the band gap is mainly due to the hybridization of the Cr *3d* and Mo *4d* orbitals at the vicinity of the band edges. The band gap engineering and magnitudes (1.65 eV to 0.86 eV) suggest that the Cr alloys in a MoS₂ monolayer are good candidates for nanotechnology devices.

Keywords: density functional theory, *ab-initio* simulation, electronic structure, two dimensional materials, molybdenum disulfide.

African School on Electronic Structure Methods and Applications (ASESMA) - Building African Networks for Computational Materials and Biological Sciences

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The African School on Electronic Structure Methods and Applications (ASESMA) is a series of workshops held every two years in different Sub-Saharan countries, designed to foster a collaborative network for research and higher education within Africa. Participants are drawn from across the continent through a competitive process, and the lecturers and mentors are outstanding scientists from across the world including Africa. ASESMA is sponsored for the years 2010 to 2020 by the International Union of Pure and Applied Physics (IUPAP) as a joint mission of the Commissions on Physics Development, Computational Physics, Physics Education and the Structure and Dynamics of Condensed Matter, and it is supported by the International Centre for Theoretical Physics, the National Research Foundation in South Africa, the U.S. Liaison Committee for IUPAP, the American Physical Society and as well as a number of international organizations and industries. The core guiding principle is that computation makes it possible for world-class research to be done with modest investment, and it is an essential part of education for the future. The skills acquired are useful for teaching at the university level and are transferable to other disciplines. The participants are the teachers who will educate future generations of Africans! The focus of ASESMA is computational methods and applications of electronic structure, chosen because it is an important field that is narrow enough to build up a network for joint work and collaboration, yet broad enough to span the range from fundamental physics to applications in materials science, chemistry, biology and many other fields. In each workshop participants learn the basic theory and computational methods with hands-on computing, and each participant is involved in a project in an area of current research that can be continued after the school. The main applications are to materials that are crucial for many areas of technology, including solar energy and the vast reserves of minerals and materials mined in Africa. The important need now is for funding for research, for ASESMA participants to attend meetings, and for short visits to international institutions that are all essential for scientists to participate fully in the global community.

ASESMA has shown that it is possible to build a network across sub-Sharan Africa with world-class research. It already is expanding to involve more chemistry and materials science, and the next school will be an introduction into biological systems. These are steps toward fulfilling the vision of building African Networks for Computational Materials and Biological Sciences.

CO 20

Investigation of Two-Dimensional (2d) Graphene-Like Layers as Potential Safe Anode Material for Li-Ion Batteries.

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New technologies such as portable electronic devices, implantable medical devices, hybrid electric vehicles (HEV) and electric vehicles (EV) rely on the availability and cost of batteries that are safe, have long cycle life, high power and high energy density. Li-ion batteries (LIBs) have over the past presented themselves as a suitable candidate due to their flexibility and high energy density over other types of batteries. Rechargeable Li-ion batteries typically use carbon (graphite) as anode materials. These graphite anodes have two problems: 1) the formation of a solid-

electrolyte interface in the first charging cycle and 2) the possible formation of dendritic filaments of Li that could lead to short circuit in the cell. These problems hinder their applications in areas where safety is the number one priority. In this work we suggest two-dimensional materials, namely Graphene, Phosphorene, hexagonal-Boron Nitride (h-BN) and graphene-like Silicon-carbide (SiC) layers as alternative anode materials. We have performed first principles numerical simulations to study the structural, electronic and electrochemical properties of these candidate materials. The computed properties are been compared with available experimental results. The goal is to determine if any of these materials can be a safe replacement for Graphite in the anode of LIBs.

Keywords: DFT, Li-ion batteries, Graphene, Phosporene, h-BN, SiC

CO 21 Catalysts for African Development and Advancement [CADA] Omololu Akin-Ojo^{1,2}

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The twin problems of electricity shortage and limited access to clean drinking water in Africa can be solved by the development of catalysts. Abundant catalysts that can facilitate the splitting of water into hydrogen gas (and oxygen gas) are required as well as cheaper catalysts that can be used in fuel cells to produce electricity by the oxidation of hydrogen. An important by product of the fuel cell is clean water from the combination of hydrogen and oxygen. Thus, even dirty water can be used to produce electricity and clean water. While platinum and platinum-ruthenium alloys work as catalysts in fuel cells, they are costly and cheap and abundant alternatives are needed. The goal of this work is to understand the mechanism of action of these expensive catalysts as a guide to developing alternative cheap and abundant catalysts for fuel cells. Semi-empirical molecular dynamics (SEMD) simulation will be used to study the oxidation of hydrogen by platinum and comparisons made with the same process but in the presence of a recently discovered catalyst Fe(PO₃)₂. Preliminary SEMD simulations of possible catalysts for photocatalytic water splitting will also be presented.

Keywords: Catalyst, Water Splitting, Molecular Dynamics, Semi-empirical, Fuel Cells.

CO 22

Li states on a C-H vacancy in graphane: A first-principles study

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Using a hybrid density functional theory approach, we study the interaction of a Li atom with a C-H pair vacancy defect (V_{CH}) in a *graphane* monolayer. The effects of a Li atom on the thermodynamic stability, structural, magnetic and electronic properties of a V_{CH} defective *graphane* monolayer are explored, taking into account the effect of charge doping. We find that the Li ions enhance the thermodynamic stability of a V_{CH} defective *graphane* monolayer. The partial density of states analysis suggests that the Li- V_{CH} system is spin polarized, possesses a pronounced magnetic moment and half-metallic behaviour arising from the hybridization between C 2p states and Li 2s states at the vicinity of the Fermi level. When charging the Li- V_{CH} system, it is found that the -1 (+1) charge doping is more energetically stable in the p-type (n-type) region respectively, suggesting a defect charge compensating character. The -1 (+1) charge doping increases (reduces) the induced magnetic moment in the Li- V_{CH} system, but the half-

metallic character is always maintained in both cases. These findings give an explanation for the origin of magnetism noted in a V_{CH} defective *graphane* system and suggests a feasible experimental way for controlling it.

CO 23

Determination of effective properties of granite rock: A numerical investigation

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Macroscopic strength of the rock depends on the behavior of the micro-constituents, which include, the minerals, pores and micro-cracks. It is important to determine the effect of these constituents on the overall behavior of the rock. This study seeks to estimate the effective elastic properties of granite using the finite element method. A representative volume element (RVE) of suitable size with spherical inclusions of different radii and distribution, representing the micro-constituents, is subjected to loading. The effective elastic properties are computed numerically. Results indicate increased convergence of the result with increased number of inclusions. Comparison of numerical results to those obtained from the analytical Mori-Tanaka Scheme indicate congruence. The results exhibit the finite element method as a useful tool in determination of the effective elastic properties of heterogeneous granite rock.

Keywords: RVE; elastic properties; granite; Mori-Tanaka; homogenization, finite element

CO 24

A Density Functional Theory Investigation of Hydrogen Adsorption on the LaFeO₃(010) Surface for Use in Nickel-metal Hydride Batteries

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The ABO₃ perovskite lanthanum ferrite (LaFeO₃) is a technologically important electrode material for nickel–metal hydride batteries, energy storage and catalysis. However, the electrochemical hydrogen adsorption mechanism on LaFeO₃ surfaces remains under debate. In the present study, we have employed spin-polarized density functional theory calculations, with the Hubbard U correction (DFT+U), to unravel the adsorption mechanism of H₂ on the LaFeO₃(010) surface. We show from our calculated adsorption energies that the preferred site for H₂ adsorption is the Fe–O bridge site, with an adsorption energy of -1.18 eV (including the zero point energy), which resulted in the formation of FeOH and FeH surface species. H₂ adsorption at the surface oxygen resulted in the formation of a water molecule, which leaves the surface to create an oxygen vacancy. The H₂ molecule is found to interact weakly with the Fe and La sites, where it is only physisorbed. The electronic structures of the surface–adsorption systems are discussed via projected density of state and Löwdin population analyses. The implications of the calculated adsorption strengths and structures are discussed in terms of the improved design of nickel–metal hydride (Ni–MH) battery prototypes based on LaFeO₃.

Keywords: Lanthanide ferrite; Hydrogen adsorption; Oxygen vacancy formation; Nickel-metal hydride batteries; Density functional theory

Stochastic resonance in a double well potential with non-homogeneous temperature of a semiconductor layer

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We design a semiconductor layer such that an arrangement of three split gates along the layer gives rise to an effective double well potential for the impurities to diffuse. Applying a non-homogeneous cold temperature in addition to the background uniform temperature, the system undergoes a phase transition from a double well to a three well effective potential. If we now pass a weak impurity signal along the semiconducting layer and study its dynamics for different parameters (trap potential Φ , noise level D, etc), we get rich scenarios of stochastic resonance. We carry out simulation of the impurity dynamics at low density and study its Signal-to-Noise Ratio (SNR) and spectral power amplification.

Keywords: Impurity diffusion in a semiconductor layer; Stochastic resonance

CO 26 Structural Properties and The Liquid-Liquid Phase transition of Elemental Phosphorus

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Elemental Phosphorus is a very interesting material and it tends to crystallise in many allotropes: white (molecular P4), red (amorphous), black (layered); other forms include violet Phosphorus, fibrous and nanorod-like Phosphorous. In this work, we identified the relevant crystalline phases of Phosphorus at ambient condition and performed *ab initio* calculations to study their structural properties, relative stability and band structure using advanced functionals which properly describe the van der Waals interaction present between the molecules. Semiempirical interatomic pair potentials were evaluated on the ability to reproduce the first principles results. The first order phase transition observed in Phosphorous in the liquid phase as a function of pressure and temperature between the molecular and polymeric phases is also investigated by classical Molecular Dynamics simulations using LAMMPS.

Keywords: Elemental Phosphorus, crystalline, phase transition, polymeric phases

The effect of cold spots on two symmetric locations of a quartic potential and the study of stochastic resonance in a semiconductor layer

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We design a model to investigate the dynamics of impurities along a semiconductor layer by imposing confining quartic potential assisted by thermal noise strength D and trap potential Φ . In the presence of a uniform background temperature, the impurities pile up around the center of the quartic potential. We apply two cold spots in addition to the background uniform temperature around two symmetric locations of the quartic potential. This causes the system to undergo a phase transition from a single well to a double well effective potential. The impurities diffuse away from the central region and assemble around two peripheral regions of the semiconductor layer. If we pass a weak signal on the impurities along the layer, the impurities will be thermally activated and hop. We perform simulations in order to study the dynamics of the impurities subjected to noise (random force) and weak periodic forcing at low impurity density. Using two state model approximation, we also study the integral characteristics of the stochastic resonance for the impurity dynamics in the presence of time varying signal.

Keywords: Stochastic resonance, quartic potential, bistable potential, semiconductor layer

EDO 1

Fostering Renewable Energy Research Collaboration between U.S. and African Universities through SciBridge

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SciBridge aims to promote research collaboration on renewable energy between U.S. and African universities. We provide participating students with opportunities to perform hands-on experiments on renewable energy technologies and attend webinars presented by experts from related fields. To ensure experiment resources are accessible at African universities, the SciBridge U.S. chapter fundraises, designs, builds, and ships experiment kits that contain necessary resources to universities in Africa. Since 2014, SciBridge has sent 35 experiment kits on dyesensitized solar cells, Al-air batteries, and thermoelectric generators, each with enough supplies for 40 students, to nine universities in three different African countries – Uganda, Ethiopia, and Tanzania. Examples of how these kits are utilized by our partners include extended senior design projects, outreach programs, and the completion of a Master's thesis. To date, SciBridge is developing new kits on emerging renewable energy technologies such as microbial fuel cells and is looking for new partner universities in both U.S. and Africa. Future partner universities in Africa will be able to request existing experiment kits based on their specific needs through a proposal based system. All partner universities are encouraged to establish student chapters to coordinate experiments and report how effective the kits are at promoting research. As an example, we will introduce the organization of the NC State SciBridge chapter.

Keywords: Intercontinental Scientific Collaboration, Renewable Energy, Education, Science

EDO 02

Educating the next generation of materials scientists is more than just a side note to the National Science Foundation's Division of Materials Research Birgit Schwenzer

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The National Science Foundation is well-known for supporting innovative and transformative research. Just as importantly though, significant emphasis is placed on training the next generation of STEM researchers and educators as part of the grants awarded. While every single award contains a broader impacts section to address this and other components, the most prolific examples from the Division of Materials Research (DMR) are its 'flagship', the Materials Research, Science and Engineering Centers (MRSEC), and the Partnership for Research and Education and Materials (PREM) program. In addition, many other programs exist under the umbrella of the Foundation, and DMR participates in several of them. This presentation highlights some of the successful approaches principle investigators and DMR-funded centers have developed to diversify the next generation of STEM researchers and communicate materials science with the broader public.

Keywords: National Science Foundation, STEM education, broader impacts, outreach

EDO 03 Advanced Materials for Sustainable Development Boppanna V Chowdari

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Presently used commercial lithium ion batteries (LIBs) consist of layer-type lithium cobalt oxide, spinel LiMn₂O₄ or LiFePO₄ as the cathode, graphite as the anode, and a non-aqueous Li - ion conducting solution or immobilized gelpolymer as an electrolyte¹. LIBs are extensively used in the present-day portable electronic devices and high-power applications like back-up power supplies and electric/hybrid electric vehicles. However, LIBs need to satisfy several additional criteria, namely, cost-reduction, improvement in the energy density, safety-in-operation at high current charge/discharge rates and improvement in the low-temperature-operation. Several simple and complex oxide nanomaterials are synthesized by molten salt and graphenenothermal reduction methods. These materials are characterized by Rietveld refinement X-ray diffraction, X-ray absorption fine structure, X-ray photoelectron spectroscopy, SEM, TEM, density and BET surface area methods, cyclic voltammetry, galvanostatic cycling and electrochemical impedance spectroscopy techniques. Results based on the study of binary metal oxides like MO (M= Co, Ni, Fe, Mn and Cu) and nano SnO₂ and ternary oxides Nano-MCo₂O₄ (M= Mn, Cu, Mg, Zn) will be discussed. Advantages of nano size and matrix elements on capacity values, average charge-discharge voltages, voltage hysteresis and Electrochemical performances will be highlighted.

EDO 04 Integrating Data Sciences into Materials Science and Engineering Graduate Education <u>Elizabeth C.Dickey</u>

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"Big Data," defined as high-volume, high-velocity and/or high-variety data, is becoming more prevalent in materials science, especially as high-throughput computation, large synchrotron scattering sources, and in-situ characterization tools become more widely available to the research community. As such, materials scientists need to be better educated in in statistical data sciences, while data scientists have growing opportunities to address application opportunities and data-science research challenges in the physical sciences. This talk will discuss emerging trends in interdisciplinary graduate education that intend to capitalize on emerging research methods to prepare students for a more data-intensive research and development environment. Several pilot graduate programs are being developed in the United States under the support of the US National Science Foundation (NSF) through its NSF Research Traineeship Program. One such program is the Science and Engineering of Atomic Structure Traineeship at North Carolina State University. This interdisciplinary traineeship is motivated by the unprecedented opportunities for integrating information from multiple characterization and modelling data sets for determining materials structure across different length scales. The academic program integrates of Bayesian statistics, uncertainty quantification and materials informatics into the academic curriculum and fosters collaborative interactions and fluency across several physical sciences and mathematical disciplines.

Keywords: Education, Big Data, Statistics, Graduate Traineeship

EDO 05

Promoting Interests in Energy Research: Developing a Low Cost Potentiostat for African Universities as Teaching Tool

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Many students in Africa are interested in solar energy conversion, energy storage, and other energy-related research. However, labs in Africa tend to be poorly equipped and resources are not available for students to study electrochemistry, one of the fundamental methods of characterizing materials for energy research. Our international team met at the 2016 Joint Undertaking for an African Materials Institute (JUAMI) and we have developed a versatile, low-cost, Arduino based potentiostat and undergraduate-level electrochemistry teaching experiments for African universities that lack electroanalytical instrumentation. This project will connect the undergraduate theoretical coursework with the techniques needed for cutting-edge research in energy technology, thereby fostering a community of students excited and prepared for graduate-level research. With careful experiment design, we have achieved our goal of keeping the total cost of the potentiostat and the materials for the introductory experiments under \$100 (US) per module. Our project aims to address the lack of laboratory equipment in African universities. Integration of the electrochemistry experiments in an undergraduate curriculum will bolster interest in students who want to pursue a materials science career. Potentiostats are powerful instruments that can be used in many areas of research such as photoelectrochemistry, electrocatalysis, electrocanalytical, contaminant detection, and electrodeposition, all of which are directly related to common needs in Africa. The potential impacts of the outcome will benefit many African students and potentially lead them toward a career in science, technology, engineering, or mathematics (STEM). Our team will present our recent progress in developing and deploying these electrochemistry modules, and will give a brief demonstration of the working potentiostat.

Keywords: Potentiostat, Arduino, Electrochemistry, Materials Education, Energy Research

EDO 06 R&D in Semiconductor Industry: from Materials to Microchips <u>Francesca Iacopi</u>

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Innovation in Nanotechnology and Materials is underpinning almost all of the most significant technology advances of our times. Micro and nano-electronics is no exception. Whether it is about pursuing the ultimate miniaturization by following Moore's Law of device scaling, or it is about achieving the ultimate multifunctional system integration (sensing, computing, energy, communications, etc.) according to the More than Moore trend, electronic materials and their integration processes are a major enabler. However, the R&D road going from a novel material in the research lab to a commercial product is particularly long in the semiconductor industry, not rarely over 10 years. In this talk I will explain how the research and development phase of a material and its integration in a microsystem is so critical, how a close collaboration between Academia and Industry is key for a successful R&D phase, and will introduce the fundamental concepts of yield, quality and reliability.

Keywords: R&D, materials integration, miniaturization, reliability

EDO 07

Scientific integrity in 21st century Africa: The case for responsible conduct of research training in materials science education

Francis Barchi

EDO 08 A perspective on the role of key collaborations in creating new directions in nanomaterials and interface science <u>Ganpati Ramanath</u>

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This talk will provide a perspective on the crucial role of transdisciplinary and international collaborations in charting new directions to realize thin film and bulk nanomaterials and interfaces with atomic-level control over multiple properties. I will discuss examples from my research career to illustrate multifaceted benefits such as, expanding research interests by building new expertise, devising creative strategies through complementary activities, combining theory and experiment, all of which contribute to enhancing the quality and impact of the research, and enriching the student experience. In particular, I will describe the roles of undergraduate research projects and key collaborations that led us to pioneer the use of molecular nanolayers at thin film interfaces to modify a slew of properties, e.g., chemical, adhesion, thermal and electronic transport, and create and modify organized nanostructured assemblies. The influx of new expertise and synergies from these collaborations seeded completely new activities on synthesizing and modifying nanostructures, chemically-functionalized porous thin films, and bulk thermoelectric nanomaterials unprecedented properties, and understanding relationships between electronic- and atomic-structure, processing, and properties. These also seeded new collaborations, and new avenues of interacting with industry, thereby creating a vibrant environment, and opening up networking opportunities that fostered student excellence in research, innovation, and entrepreneurship. Outcomes of activities such as exchange visits and

joint experimentation and analyses included high impact papers and inventions, students winning international awards, and founding a start-up company.

Keywords: Transdisciplinary collaborations, education, atomistic design, entrepreneurship

EDO 09

Funding for Tools for Materials Research at the National Science Foundation <u>Guebre Tessema</u>

EDO 10

Implementation of professional and academic development camp for Liberian women undergraduate engineers at the University of Liberia J. K. Wenderott¹, Caroline Mills²

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Under the auspices of the University of Michigan's Society of Women Engineers (UM-SWE), a two-weeklong camp for forty Liberian women undergraduate engineers was realized in August 2017 at the University of Liberia in Monrovia. The planning stage involved development of curriculum that included workshops focused on professional, career, and leadership development and hands-on engineering demonstrations with accompanying lessons intended for academic development. Eight UM-SWE members, four graduate and four undergraduate, travelled to Monrovia for the implementation of the camp and were hosted by local collaborator and recently-formed Liberia SWE (L-SWE). Here, we report on the objectives of the 2017 camp and curriculum, as well as the overarching goals of the partnership between UM-SWE and L-SWE. We discuss success of the camp through the results of our monitoring and evaluation (M&E) exercises and propose areas for improvement. The M&E activities, comprised of pre- and postcamp surveys and short reflections following the workshops and demonstrations, were utilized to assess camp participant personal growth and satisfaction and to support sustainability of the camp through quantitative assessment of its success. We also note progress on the broader goals of the UM-SWE and L-SWE partnership and suggest how this partnership could be achieved between other US SWE chapters and African universities to promote women in science and engineering through global connections.

Keywords: education, professional development, leadership camp

EDO 11

Building Research, Agribusiness and Innovation Capacities of HEI's in Agriculture through Regional Partnerships

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Food security and poverty remain one of the major challenges to Africa's development, affecting about 33% of its population. Among the key contributing factors to food insecurity are occurrence of frequent droughts, rampant crop and livestock diseases, poor infrastructure, policies, market access; high input costs, inadequate technical capacity, limited technologies and innovations. The above challenges can be addressed by building capacity along the agricultural value chain through strengthening of agricultural training, promotion and upscaling of tested technologies. The African Centre of Excellence in Sustainable Agriculture and Agribusiness Management (CESAAM) at Egerton University, Kenya, is modelled to address the above issues. Egerton University has a long history of agricultural training and research, and is centrally placed within the Eastern Africa region. The region has a number of countries emerging from conflict that need to re-build their human capacity to address food insecurity. The broad objective of CESAAM is to contribute to sustainable agricultural and agribusiness management through capacity development, research and technology transfer for enhanced food security. The specific objectives are to develop capacity along the agricultural Value Chain in the Eastern and Southern Africa region; undertake innovative research, for increased crop and livestock productivity, enhance the capacity of the University's agro-science park to assist partner universities establish a similar model for incubation of technological innovations, and to develop evidence based agricultural policy briefs and disseminate best practices through agricultural knowledge centers in Egerton (CESAAM) and partner universities. Expected outputs include increased capacity to offer quality training and conduct research nationally and regionally, equipped research laboratories, increased innovation products, increased dissemination of agricultural best practices and evidence-based policy briefs. The cumulative impacts of these outputs are increased productivity along the agricultural value chain and improved food security.

Keywords: research, collaborations, innovation, agriculture, agribusiness

EDO 12 Fostering an Entrepreneurial Mindset Kudakwashe Mzembe

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Energy access is fundamental to the full enjoyment of life and advancement of any society. To date, more than 600 million people in Sub Saharan Africa have no access to electricity. This has a direct impact on the rate of development on the continent. The continent accounts for 13 percent of the world's population, but only 4 percent of the energy demand. Due to the high cost of setting up sufficient energy infrastructure, it is paramount to focus on alternative means of energy generation to begin to address this challenge. It is also of vital importance to begin to equip Africa's young people with the right tools, platforms and resources to engender an entrepreneurial culture. Africa has the youngest population in the world and this presents a massive opportunity. Solar energy is emerging and the technology has been improving in leaps and bounds over the last few years meaning that the cost is decreasing and becoming less prohibitive. With the right kind of focus and policy framework, African countries can begin to raise
energy entrepreneurs and "intrapreneurs". In as much as there is an urgent need for scientists and "home grown" academics, there is an equal need for the fostering of an entrepreneurial mindset in the different African countries. Most African countries are strategically positioned to have maximum daylight hours and this makes solar very favorable energy source for Africa. Solar energy has multiple entry points and one does not need a sophisticated education to learn the basics and tap into its potential. There are multiple opportunities within the solar energy supply chain that Africans can begin to take advantage of immediately.

Keywords: Solar Energy and Entrepreneurship

EDO 13

Mother is Gold: Experiments in Teaching and Learning Materials Science and Engineering with African Proverbs Kwadwo Osseo-Asare

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Ghana's first president, Kwame Nkrumah, is quoted as saying "I am an African not because I was born in Africa, but because Africa was born in me." African proverbs represent a potent pedagogical resource, which if mined and applied judiciously can help nurture this seed of Africa and orient it in a direction that promotes critical thinking and innovation. Many observers have noted that African educational institutions tend to stress mastery of lower-order cognitive skills such as attention span and memorization. In contrast, higher-order skills, including logic, analytical reasoning, creativity, critical analysis, visualization, and synthesis, are often neglected. To encourage students to develop a conceptual understanding of materials science and engineering rooted in the African soil, a new approach has been developed in which the indirection characteristic of African proverbial discourse is appropriated to serve as a teaching and learning aid. This presentation shares highlights of this experiment in pedagogy, based on interactions with undergraduate and graduate students in Ghana and Nigeria, including initial reactions to assignments to provide proverbs with materials connections, and samples of the proverbs provided. Suggestions for extension of this methodology are also offered.

Keywords: Conceptual Understanding; African Proverbs; Teaching and Learning; Materials Science and Engineering

EDO 14 International-related activities and funding

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International activities are an important component of basic materials research. Innovation is the key to successful research results. This requires collaborations with counterparts worldwide. For Africa to tap into cutting edge innovations, Africa needs to seek funding to enable collaborations with other researchers worldwide. There are many avenues that lead to funding for these activities.

EDO 15

Generating partnerships for collaborative research: synchrotron light source data for African materials science

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Synchrotron light source facilities are foundational to modern science, including high resolution and multi-scale characterization of material structure, but there is currently no such facility located on the African continent. In this talk, I will detail ways in which researchers in Africa can gain access to synchrotron facilities for their work, even when direct travel to foreign facilities is not possible. In particular, I will discuss open communication and collaboration avenues between African and other researchers in order to obtain measurements and expertise on data analysis and interpretation. Examples in forming international collaborations will be given, including one recently formed out of the Joint-US Africa Materials Institute (JUAMI), for characterizing the atomic structure of microporous materials for energy applications.

Keywords: total scattering, nanostructure, collaboration

EDO 16

Aiding learning process and creating a collaborative network in materials science through the use of mobile and web based platform

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Smartphones have made it easier for us to check facts, take photos, Read the news, Dictionary, Watch, Translator among so many other uses, which is why the use of Mobile Smartphone as a mode of teaching is the future of education, thus the need for an app or learning platform where students can go and learn more about Materials science and form a collaborative network with students worldwide to study and follow the latest trends in Materials study. A mobile classroom is easy to use and gives the student the opportunity to learn at his/her own pace and also associate with top Materials Science Researchers around the globe. An app was developed for students to learn programming in various languages this was used alongside students who were taught through the normal method class teacher interactions. For a period of one month and on various programming languages. Also, the students

were grouped in various collaborative teams and networks to help each other and overcome challenges. The students were accessed at the end of the month and the results showed a huge disparity between the two class of students with those who learnt through the Web/Mobile platform learning more programming languages and covering more topics than expected. Overall it was concluded that with the use of mobile/web based platform for teaching and learning proved more impactful and effective than going to a class to study. Also, the Collaborations built from the various networks showed how well student with different background can learn and also help each other in finding and solving our daily problems.

EDO 17 Youth Science Laboratory Kits for Resource-Limited Settings Nam-Joon Cho[†]

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Innovation across science and technology is a key driving force in the global economy, and it is critical that nations adopt sustainable practices to develop highly capable workforces. These efforts start with science, technology, engineering, and mathematics (STEM) education at the youth level, although school curriculums typically favor conceptual understanding over experiential learning, especially in resource-limited settings. In this talk, I will present recent efforts to develop science laboratory kits for middle-school age students, including curriculum development and content creation. The objective of these kits is to enable students to acquire hands-on experiences that reinforce conceptual understanding and allow them to see the utility of STEM topics in practical applications. Indeed, the kit curriculum covers a series of fundamental topics that build upon one another in order to deliver a solid knowledge of a particular subject (*e.g.*, physics). Particular emphasis has been placed on using common materials and self-guiding instructions so that students worldwide can use the kits in informal settings. The affordable cost of these kits is aimed at encouraging buy-in from global stakeholders, with an aim towards providing students with a strong science education that will enable them to become the leaders of tomorrow.

EDO 18

Enabling Science Learning in Tanzanian Rural High Schools: A collaborative project of Tanzanian and Swiss Materials Engineers and Educators (2009-2016) <u>Nava Setter^{1,2}</u>, Kalafunja M. O-saki³

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In Europe and North-America, high-school students do not have enough interest in science, resulting in an increasing shortage of scientists and engineers. This issue is even more severe in Africa where poor infrastructure impedes access of youth to appropriate science education. Insufficient in-service training programs for science teachers further worsen the situation. In a joint project between Tanzanian and Swiss materials engineers and educators we developed infrastructure, prepared and implemented integrated science modules [ISMs], and developed and tested a program for in-service training of high-school science teachers with the aim to facilitate high-school science learning in rural areas in Tanzania. The infrastructure consisted of a 'technology package' containing solar-unit, beamer, and a laptop computer. A typical Integrated science module counts several lessons and few practical sessions. The lessons contained, in addition to frontal interactive teaching, an introductory video showing relevance of the studied subject in the context of a technology encourages inquiry-based learning. KIASTE, Kisimiri in-service training of A-level science teachers was established aiming to serve as a model in-service

training unit training teachers in the use of the science modules and providing teachers with block-courses (one week duration) in various subjects of A-level science curriculum. KIASTE has been providing a modest number of such courses in chemistry, physics and mathematics for high-school teachers of the Arusha-Moshi region since 2012. This 'prototype' could be expanded into a full-scale network of mini-centers for in-service training of high school teachers. Two PhD theses in Science Education (University of Dodoma), one PhD and four Master theses in Materials Engineering (EPFL) were accomplished during the project. The financial support of the Swiss Foreign Ministry (Department of Development and Cooperation), the EPFL, and the Talent Foundation is acknowledged.

Keywords: Science-education, Science modules, Engineers-educators collaboration, Technology & society

EDO 19

African School on Electronic Structure Methods and Applications (ASESMA) - Building African Networks for Computational Materials and Biological Sciences

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The African School on Electronic Structure Methods and Applications (ASESMA) is a series of workshops held every two years in different Sub-Saharan countries, designed to foster a collaborative network for research and higher education within Africa. Participants are drawn from across the continent through a competitive process, and the lecturers and mentors are outstanding scientists from across the world including Africa. ASESMA is sponsored for the years 2010 to 2020 by the International Union of Pure and Applied Physics (IUPAP) as a joint mission of the Commissions on Physics Development, Computational Physics, Physics Education and the Structure and Dynamics of Condensed Matter, and it is supported by the International Centre for Theoretical Physics, the National Research Foundation in South Africa, the U.S. Liaison Committee for IUPAP, the American Physical Society and as well as a number of international organizations and industries. The core guiding principle is that computation makes it possible for world-class research to be done with modest investment, and it is an essential part of education for the future. The skills acquired are useful for teaching at the university level and are transferable to other disciplines. The participants are the teachers who will educate future generations of Africans! The focus of ASESMA is computational methods and applications of electronic structure, chosen because it is an important field that is narrow enough to build up a network for joint work and collaboration, yet broad enough to span the range from fundamental physics to applications in materials science, chemistry, biology and many other fields. In each workshop participants learn the basic theory and computational methods with hands-on computing, and each participant is involved in a project in an area of current research that can be continued after the school. The main applications are to materials that are crucial for many areas of technology, including solar energy and the vast reserves of minerals and materials mined in Africa. The important need now is for funding for research, for ASESMA participants to attend meetings, and for short visits to international institutions that are all essential for scientists to participate fully in the global community. ASESMA has shown that it is possible to build a network across sub-Sharan Africa with worldclass research. It already is expanding to involve more chemistry and materials science, and the next school will be an introduction into biological systems. These are steps toward fulfilling the vision of building African Networks for Computational Materials and Biological Sciences.

EDO 20 Nanoscience, Nanotechnology, and Beyond <u>Paul Weiss</u>

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The birth and development of the fields of nanoscience and nanotechnology have (uniquely) led to our ability to work and to communicate across fields. We have learned to share both problems and approaches. These skills have led to new approaches not only for our fields but for others. It is not accidental that nonscientists have led the efforts worldwide to address problems in energy, water, security, medicine, neuroscience, the microbiome, and other areas. I will discuss how we can accelerate these efforts and leverage our skills to shape a safer, healthier world.

Keywords: nanoscience, nanotechnology, education, communication, impact

EDO 21 To achieve research excellence in Africa through networking and collaboration: Lessons learnt from the African Materials Science and Engineering Network <u>P.K. Jain</u>

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As Africa aspires to achieve development level of the western world, undoubtedly scientific research, and innovation has a major role to play. However, due to the lack of research infrastructure, lack of skilled manpower to lead research, and above all limited capacity of African countries to invest in science and technology research, Africa lags behind the developed countries by decades. These barriers to science and technology based development in Africa can be overcome to a large extent through fostering regional and international collaborations, networking and sharing of research infrastructure and skills by the neighboring countries at the least, and ideally extending these initiatives beyond the confines of Africa even. First part of the paper presents an overview of the current status of research in Africa, and makes a case for the need for networking to overcome the prevailing impediments to research in Africa. In the second part experience gained, and lessons learned from the African Materials Science and Engineering Network (AMSEN) of six Southern, East and West African universities are presented. The AMSEN has been supported with funding from the Carnegie Corporation of New York (USA) through the Regional Initiative in Science and Education (RISE) at the Institute of Science (IAS) at Princeton, USA. Significance of innovation driven entrepreneurial research is also stressed. From the achievements and benefits drawn by the AMSEN member universities, it is concluded that networking and collaborations is undeniably necessary for Africa to make rapid advances in the highly competitive and fast evolving global research and innovation land scape.

Keywords: Research excellence, Networking, Research infrastructure, Skills development, Africa

EDO 22 Scientific User Facilities Role in Education

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The ability to perform high-impact science can be accelerated through access to world leading capabilities. However, it is often cost-prohibitive for individual groups to procure all of the apparatus needed to perform cutting edge research. One solution to this dilemma has been the creation of user facilities, where a funder purchases and maintains equipment in a centralized facility for all researcher to access. In this presentation we will explore some of the high impact science being done by academic users at the Center for Integrated Nanotechnologies, a US Department of Energy National User Facility. We will also discuss way to improve the accessibility of these tools and capabilities to the global research community. Sandia National Laboratories is a multimission laboratory managed and operated by National Technology and Engineering Solutions of Sandia LLC, a wholly owned subsidiary of Honeywell International Inc. for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.

Keywords: Nanoscience, education, User facilities, CINT

EDO 23 Training the Next Generation of Leaders: Graduate Education in Sustainability <u>A. Stanley Meiburg</u>¹

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Sustainable materials management requires leaders who think in fundamentally different ways. Traditional engineering skills are important but insufficient by themselves: vision, courage, innovation, and the ability to exercise influence beyond authority are indispensable attributes for a new generation of leaders. At the Wake Forest University Graduate Program in Sustainability, we are developing such leaders with a novel curriculum whose core attributes are scientific literacy, systems thinking, and exposure to practical approaches that are useful across the broad field of sustainability. The author will describe how Wake Forest applies this curriculum in our one year Masters of Arts in Sustainability program, and illustrate its value using examples from his 39 year career with the U.S. Environmental Protection Agency, including 2 years as EPA's Acting Deputy Administrator.

Keywords: Education, Sustainability, Leadership, Masters, EPA

EDO 24

Lack of Entrepreneurship Skills as a Barrier to Nanotechnology Commercialisation in Africa

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Nanotechnology is amongst the most profound alternative solutions and game changers in the early 21st Century, with its widespread potential to make an impact in fields such as health, water, energy, agriculture, mining and construction. In the last two decades, many African governments have invested a substantial amount of funds into nanotechnology research and development (R&D). At present, there is a significant number of R&D outputs and patents filed by African researchers in the field of nanotechnology. However, despite immense potential that nanotechnology holds for African countries, only a few of those patents and/or R&D products are at the commercialisation stage. Therefore, there is a need to find smart commercialisation strategies, in order to capitalise on existing and future nanotechnology patents and/or R&D products. Nanotechnology commercialisation in African countries is facing several critical barriers such as lack of infrastructure, sustainable investment and entrepreneur skills. In this presentation we will be focusing on the lack of entrepreneurship skills as the major barrier towards commercialisation of nanotechnology R&D outputs in African countries. We will also highlight the following: entrepreneurship tools that are required to convert those research results into commercial products; the strategies that could boost the launching of new ventures such as creation of the clusters of nanotech entrepreneurs; and commercialisation through public-private partnerships. In addition, we will look at other constraints and the politics surrounding nanotechnology commercialisation in African countries. Finally, we will provide recommendations to policy-makers on the continent on nanotechnology commercialisation employing an entrepreneurial approach.

EDO 25

Towards Industrialization Through Value Addition

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Africa faces serious economic growth challenges since it depends strongly on exporting unprocessed commodities and serves as a market for finished products. With its abundant raw materials, Africa has a potential to become a dominant force on the global market through value addition. Essentially, every technology depends on materials development and innovation, hence, by harnessing its natural resources to get the maximum possible value, Africa can realize a positive economic transformation. Indeed, value addition provides an opportunity to industrialize for economic growth, economic transformation and poverty alleviation through employment creation, thus reducing the dependence on producing and exporting unprocessed commodities. However, to promote economic transformation through value addition, sound and sustainable economic development policies towards industrial development need to be designed and implemented. We present on policies which Africa might need to adopt and implement to promote economic transformation, job creation and industrialization.

Keywords: value addition, industrialization, economic development

EDO 26 Materials Science Research in Uganda

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Materials Science is one of the fields which is researched on at the Department of Physics, Makerere University. As a Department, we have developed Human Resource both in Uganda and the East African Region. We are part of the Materials Science & Solar Energy for Eastern and Southern Africa (MSSEESA) network that was founded in 2002 whose main aims are building research in materials science and solar energy in the region. The network has been very important in the region since it has encouraged exchange of students and staff as well as sharing of equipment that are in the different universities across the East African region. Expanding this network to other regions in Africa and the rest of the world is now our focus for research in the field of Science. This we have partly been able to achieve through Joint US-Africa Materials Institute (JUAMI) workshops and networks have been born out of these workshops already between the alumni.